Supporting Information for

Atropisomerism in Amidinoquinoxaline N-Oxides: Effect of the Ring Size and Substituents on the Enantiomerization Barriers

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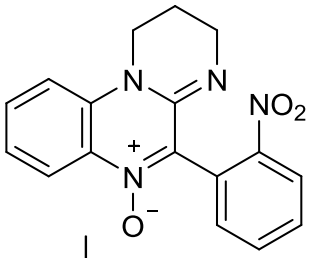
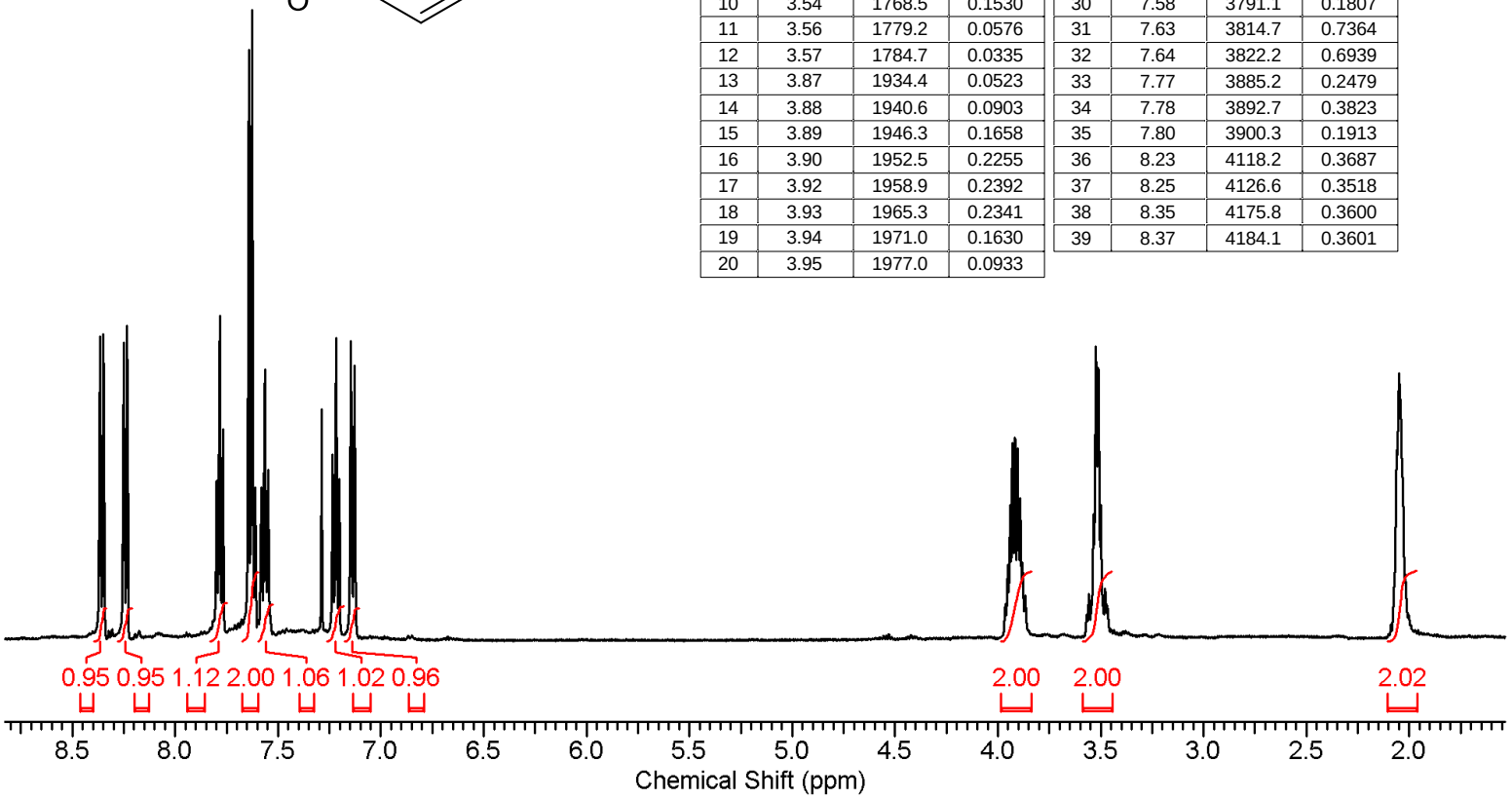
^{1}H NMR (500 MHz, $CDCl_3$) for compound **1b**

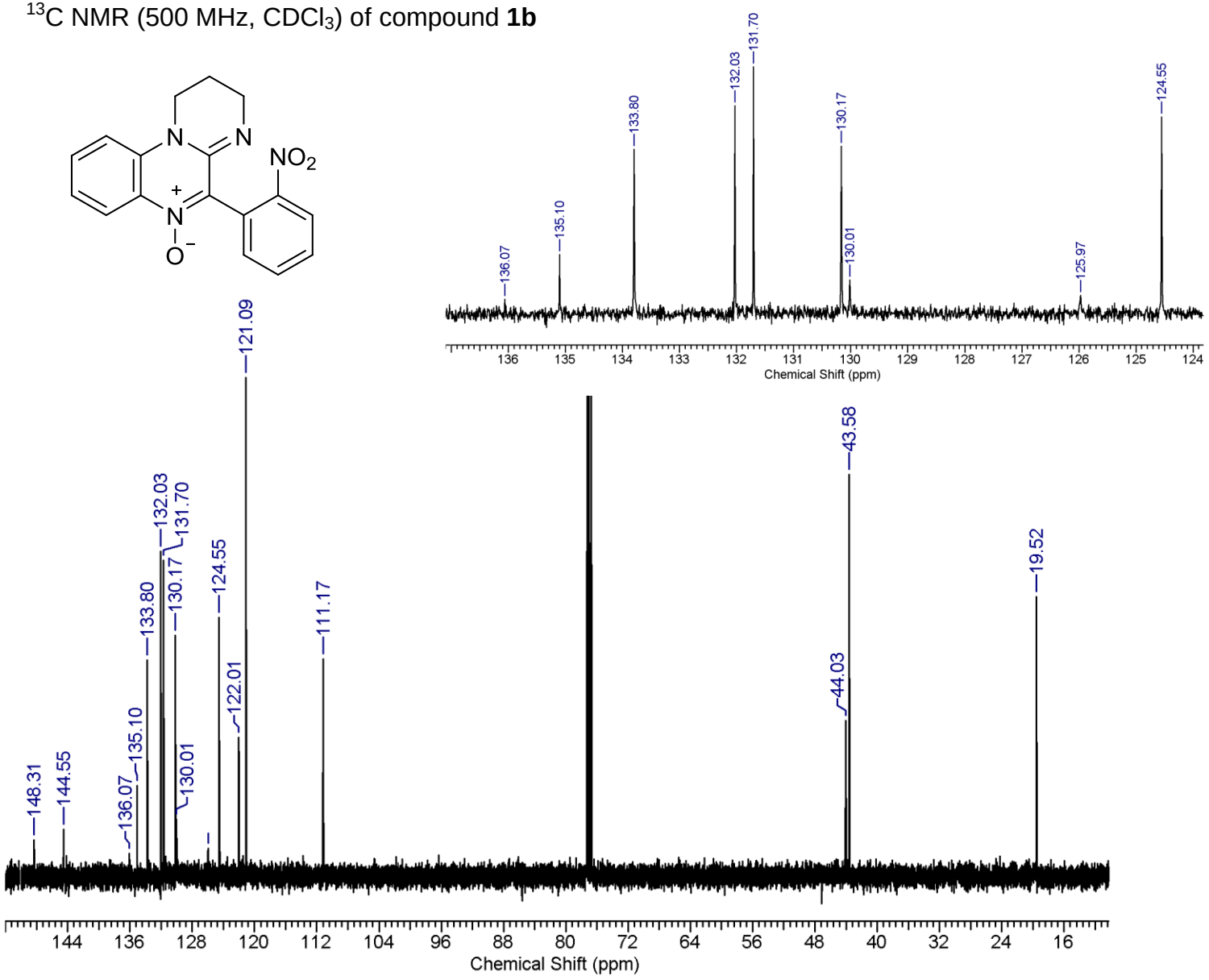


No.	(ppm)	(Hz)	Height
1	2.02	1010.2	0.0753
2	2.03	1016.8	0.1922
3	2.05	1025.1	0.3153
4	2.06	1030.6	0.2281
5	3.47	1734.6	0.0399
6	3.48	1739.6	0.0598
7	3.50	1750.2	0.1564
8	3.51	1756.6	0.3189
9	3.52	1762.5	0.3471
10	3.54	1768.5	0.1530
11	3.56	1779.2	0.0576
12	3.57	1784.7	0.0335
13	3.87	1934.4	0.0523
14	3.88	1940.6	0.0903
15	3.89	1946.3	0.1658
16	3.90	1952.5	0.2255
17	3.92	1958.9	0.2392
18	3.93	1965.3	0.2341
19	3.94	1971.0	0.1630
20	3.95	1977.0	0.0933

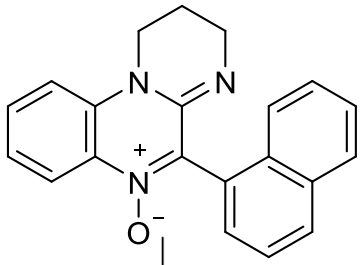
No.	(ppm)	(Hz)	Height
21	3.96	1982.7	0.0473
22	7.13	3565.4	0.3198
23	7.15	3573.9	0.3521
24	7.20	3602.7	0.1887
25	7.22	3610.3	0.3538
26	7.23	3618.3	0.2204
27	7.29	3644.4	0.2703
28	7.55	3775.3	0.1983
29	7.56	3782.9	0.3166
30	7.58	3791.1	0.1807
31	7.63	3814.7	0.7364
32	7.64	3822.2	0.6939
33	7.77	3885.2	0.2479
34	7.78	3892.7	0.3823
35	7.80	3900.3	0.1913
36	8.23	4118.2	0.3687
37	8.25	4126.6	0.3518
38	8.35	4175.8	0.3600
39	8.37	4184.1	0.3601



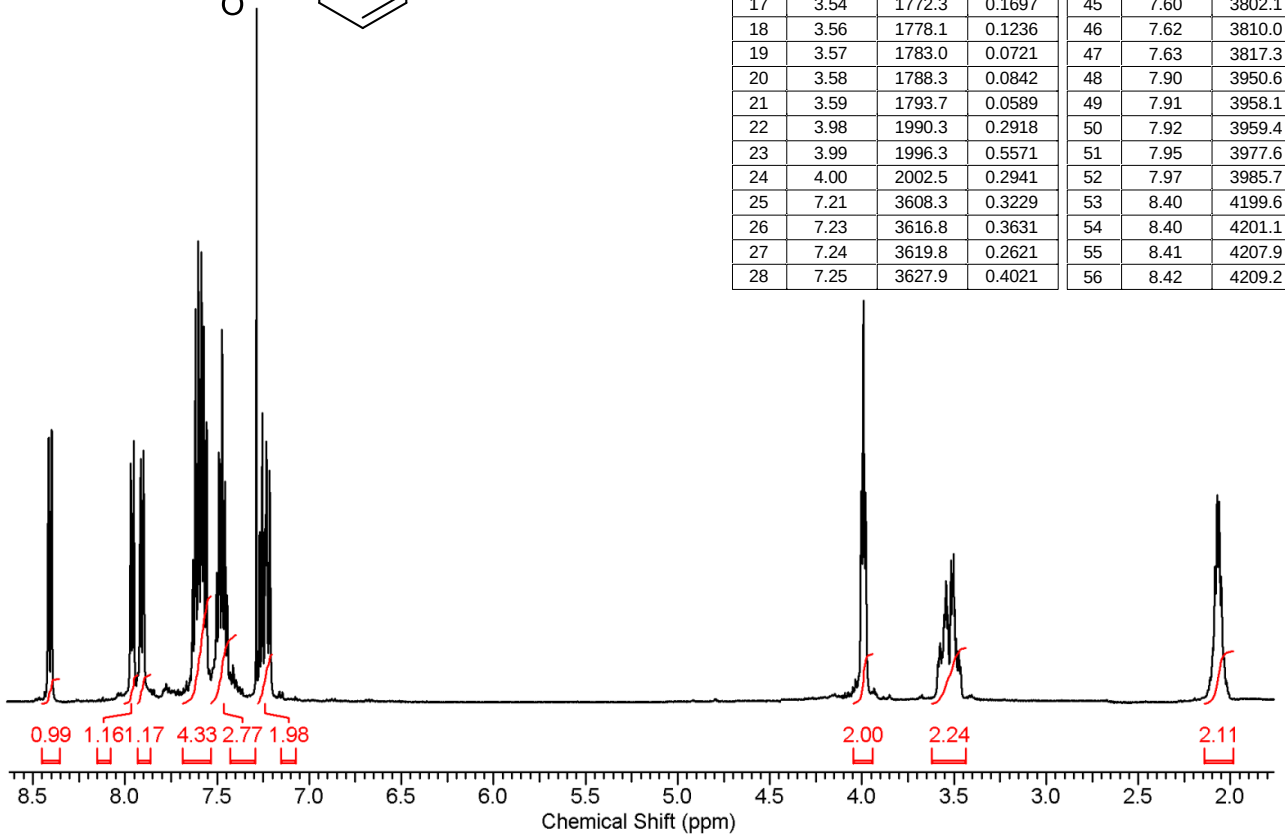
^{13}C NMR (500 MHz, $CDCl_3$) of compound **1b**



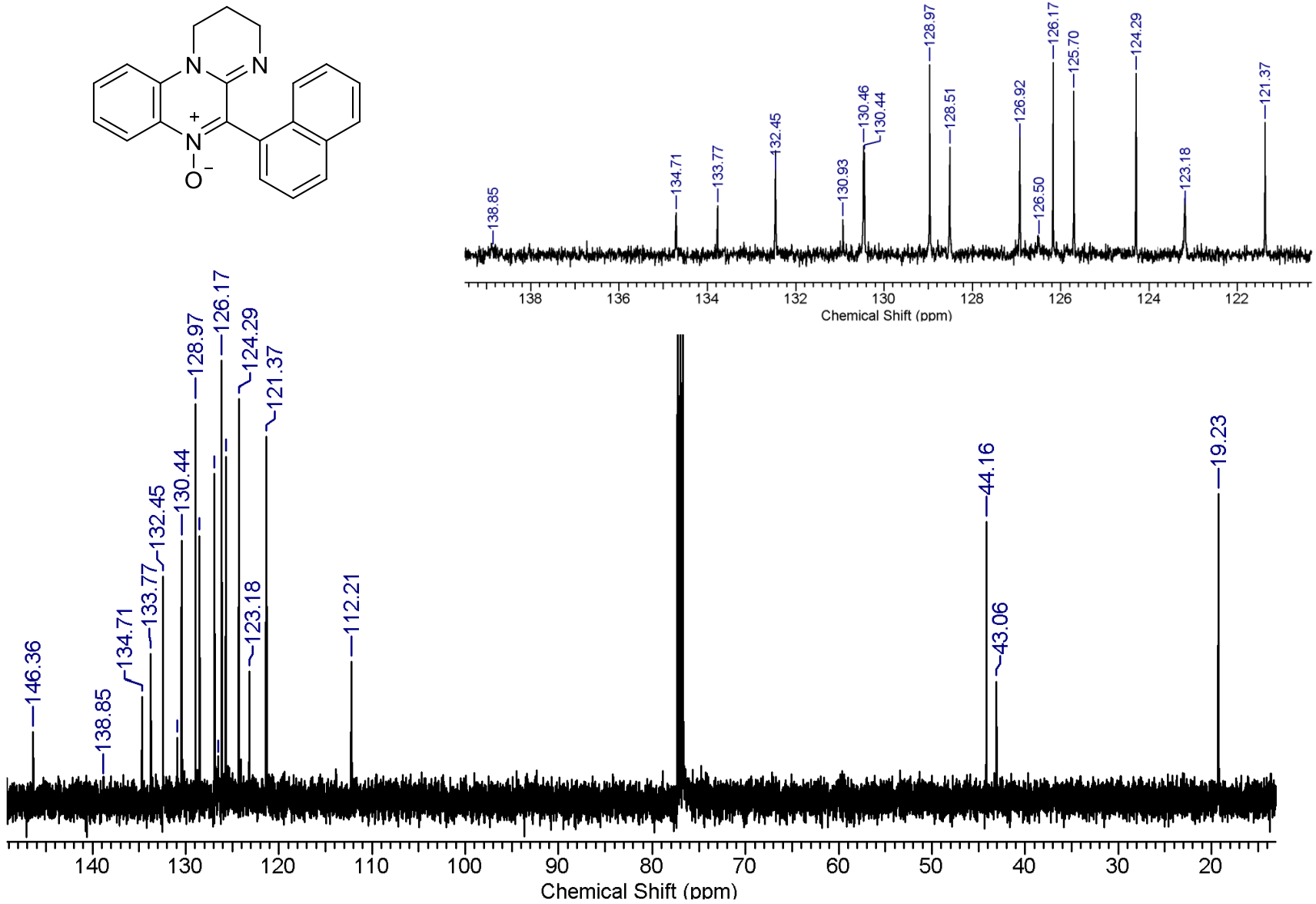
^{1}H NMR (500 MHz, $CDCl_3$) for compound **1c**



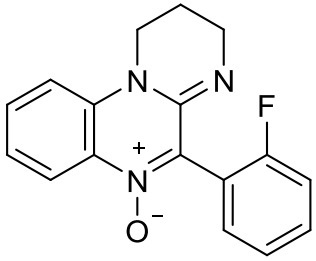
1	2.02	1011.3	0.0324	29	7.27	3635.4	0.2378
2	2.04	1018.5	0.0690	30	7.29	3644.6	0.9609
3	2.05	1025.0	0.1759	31	7.44	3722.0	0.1276
4	2.06	1031.2	0.2799	32	7.44	3723.2	0.1506
5	2.07	1035.9	0.2881	33	7.46	3728.8	0.2891
6	2.08	1042.1	0.1900	34	7.46	3729.9	0.3077
7	2.10	1048.2	0.0776	35	7.47	3737.1	0.4903
8	2.11	1055.5	0.0365	36	7.47	3738.2	0.5172
9	3.47	1733.0	0.0509	37	7.49	3745.2	0.3309
10	3.48	1738.7	0.0727	38	7.49	3746.5	0.3478
11	3.49	1744.5	0.0906	39	7.50	3752.1	0.1818
12	3.50	1748.8	0.1302	40	7.50	3753.4	0.1555
13	3.50	1751.6	0.2072	41	7.56	3779.9	0.3896
14	3.51	1754.8	0.1794	42	7.57	3787.6	0.5212
15	3.52	1758.6	0.1987	43	7.58	3793.3	0.6233
16	3.53	1767.4	0.1233	44	7.59	3794.4	0.6244
17	3.54	1772.3	0.1697	45	7.60	3802.1	0.6397
18	3.56	1778.1	0.1236	46	7.62	3810.0	0.5454
19	3.57	1783.0	0.0721	47	7.63	3817.3	0.1992
20	3.58	1788.3	0.0842	48	7.90	3950.6	0.3505
21	3.59	1793.7	0.0589	49	7.91	3958.1	0.3389
22	3.98	1990.3	0.2918	50	7.92	3959.4	0.3204
23	3.99	1996.3	0.5571	51	7.95	3977.6	0.3637
24	4.00	2002.5	0.2941	52	7.97	3985.7	0.3325
25	7.21	3608.3	0.3229	53	8.40	4199.6	0.3748
26	7.23	3616.8	0.3631	54	8.40	4201.1	0.3785
27	7.24	3619.8	0.2621	55	8.41	4207.9	0.3684
28	7.25	3627.9	0.4021	56	8.42	4209.2	0.3655



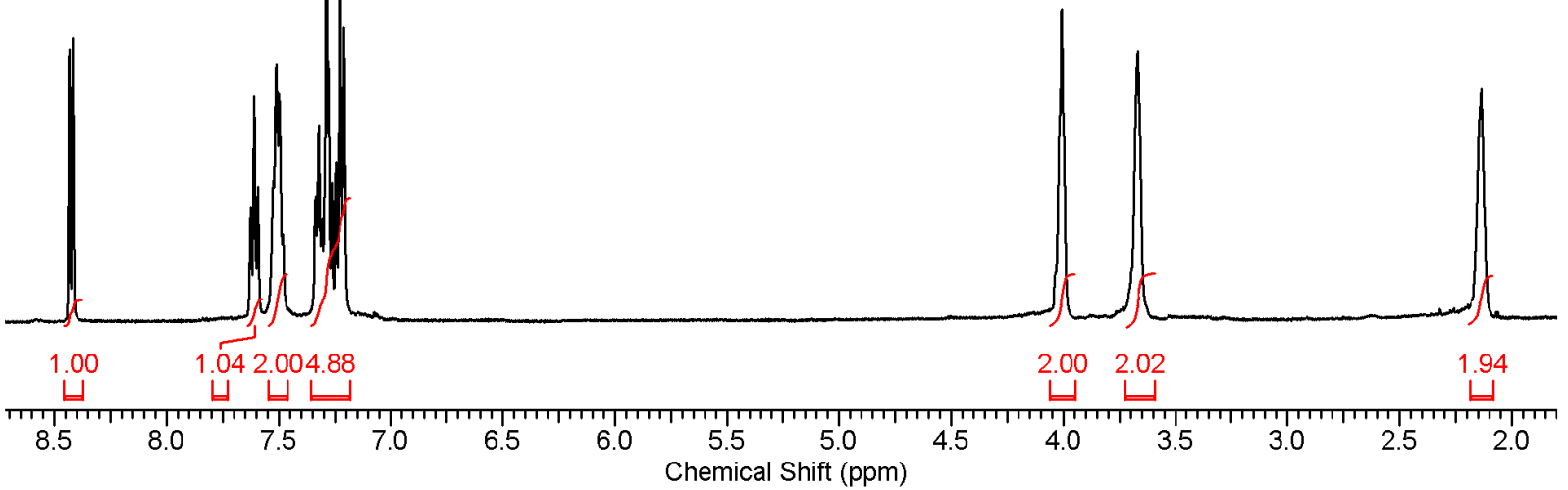
^{13}C NMR (500 MHz, $CDCl_3$) of compound **1c**



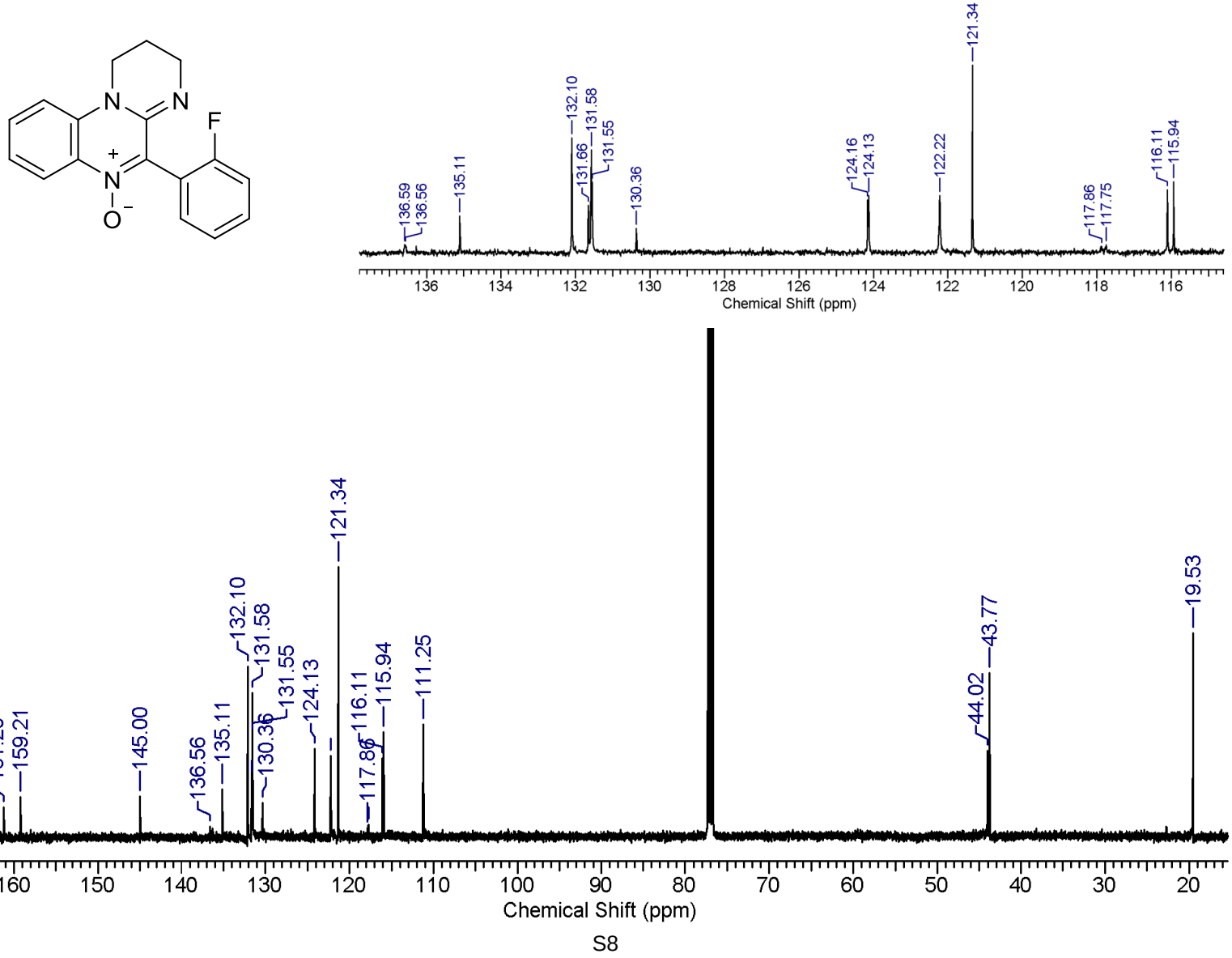
^{1}H NMR (500 MHz, $CDCl_3$) for compound **1g**



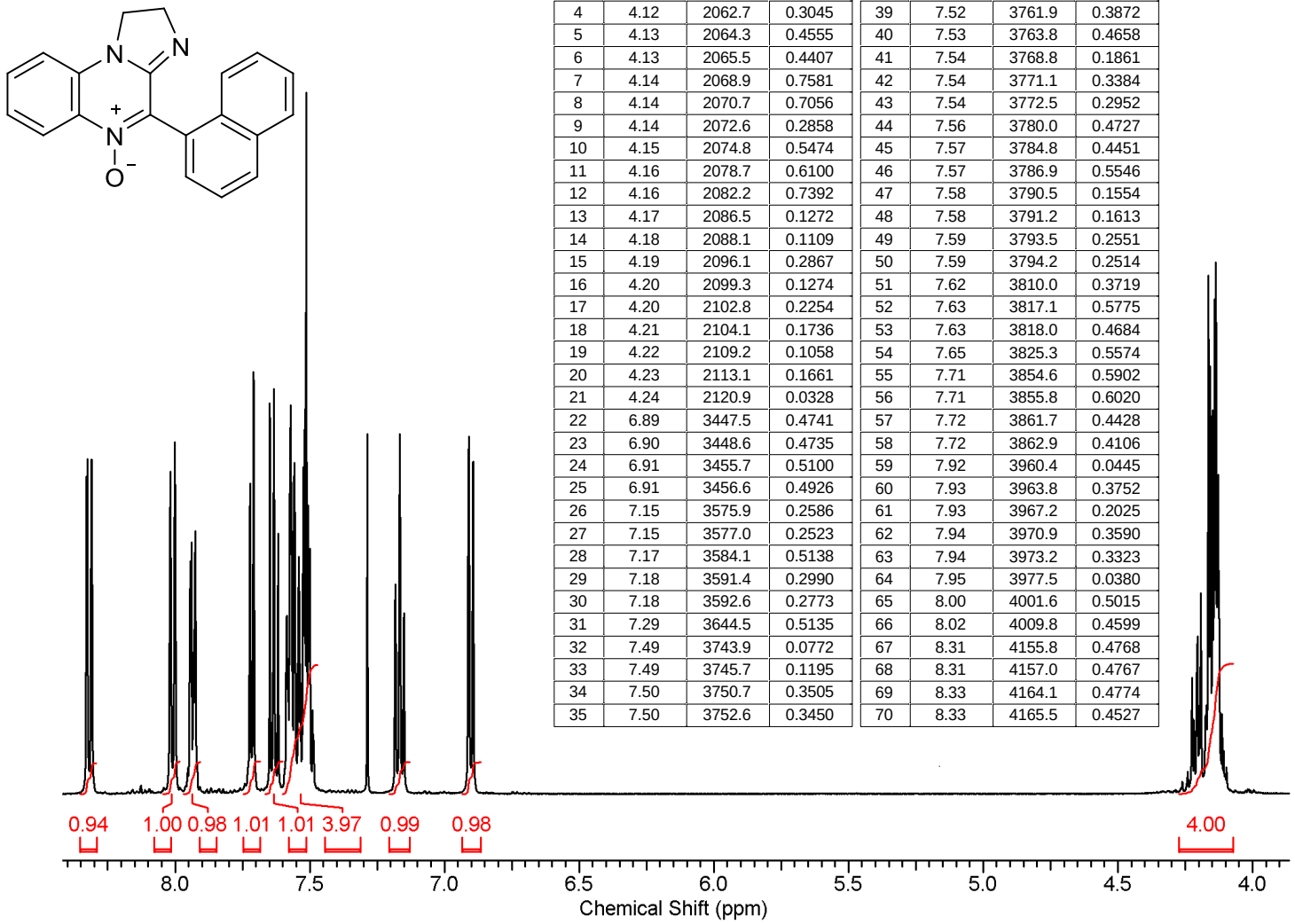
No.	(ppm)	(Hz)	Height
1	2.14	1068.5	0.2623
2	3.67	1834.2	0.3040
3	4.01	2004.2	0.3511
4	7.21	3605.2	0.3314
5	7.23	3613.9	0.4316
6	7.25	3623.6	0.1810
7	7.26	3632.5	0.1590
8	7.28	3640.5	0.2939
9	7.29	3644.6	0.8402
10	7.31	3654.0	0.1186
11	7.32	3661.5	0.2222
12	7.34	3668.6	0.1429
13	7.48	3741.9	0.1018
14	7.50	3749.7	0.2569
15	7.51	3756.5	0.2902
16	7.52	3762.7	0.1620
17	7.59	3797.5	0.1544
18	7.61	3805.3	0.2546
19	7.62	3813.3	0.1316
20	8.42	4210.0	0.3190
21	8.43	4218.2	0.3059



^{13}C NMR (500 MHz, $CDCl_3$) of compound **1g**

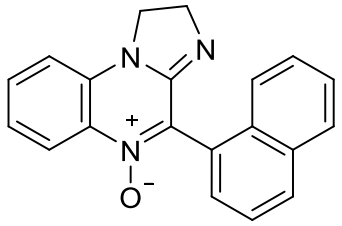


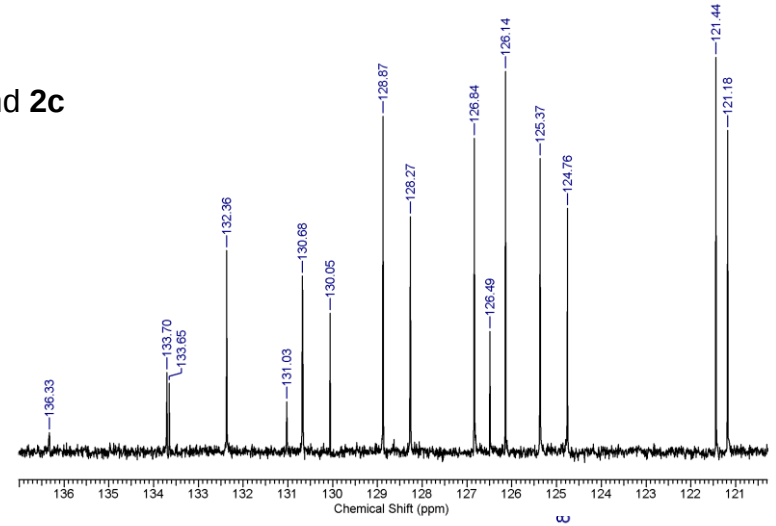
1H NMR (500 MHz, $CDCl_3$) for compound **2c**

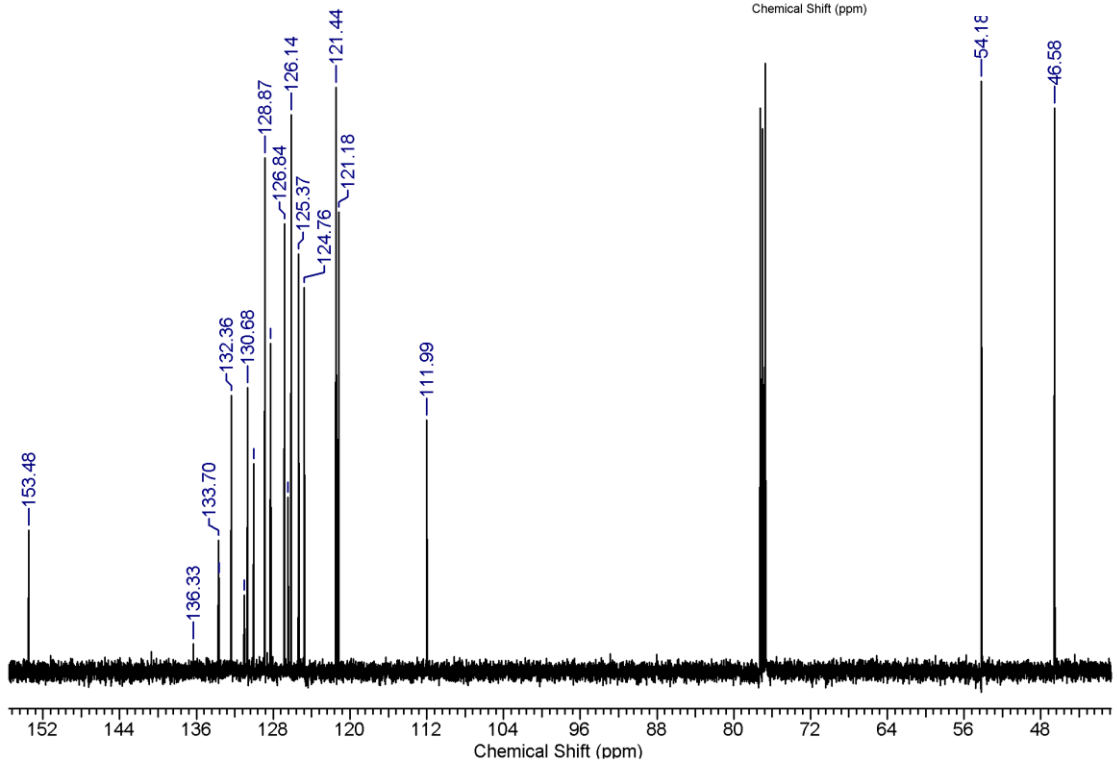


No.	(ppm)	(Hz)	Height
1	4.10	2049.0	0.0389
2	4.11	2054.2	0.0618
3	4.11	2057.0	0.1146
4	4.12	2062.7	0.3045
5	4.13	2064.3	0.4555
6	4.13	2065.5	0.4407
7	4.14	2068.9	0.7581
8	4.14	2070.7	0.7056
9	4.14	2072.6	0.2858
10	4.15	2074.8	0.5474
11	4.16	2078.7	0.6100
12	4.16	2082.2	0.7392
13	4.17	2086.5	0.1272
14	4.18	2088.1	0.1109
15	4.19	2096.1	0.2867
16	4.20	2099.3	0.1274
17	4.20	2102.8	0.2254
18	4.21	2104.1	0.1736
19	4.22	2109.2	0.1058
20	4.23	2113.1	0.1661
21	4.24	2120.9	0.0328
22	6.89	3447.5	0.4741
23	6.90	3448.6	0.4735
24	6.91	3455.7	0.5100
25	6.91	3456.6	0.4926
26	7.15	3575.9	0.2586
27	7.15	3577.0	0.2523
28	7.17	3584.1	0.5138
29	7.18	3591.4	0.2990
30	7.18	3592.6	0.2773
31	7.29	3644.5	0.5135
32	7.49	3743.9	0.0772
33	7.49	3745.7	0.1195
34	7.50	3750.7	0.3505
35	7.50	3752.6	0.3450
36	7.51	3754.2	0.4114
37	7.51	3757.4	1.0000
38	7.52	3760.3	0.5497
39	7.52	3761.9	0.3872
40	7.53	3763.8	0.4658
41	7.54	3768.8	0.1861
42	7.54	3771.1	0.3384
43	7.54	3772.5	0.2952
44	7.56	3780.0	0.4727
45	7.57	3784.8	0.4451
46	7.57	3786.9	0.5546
47	7.58	3790.5	0.1554
48	7.58	3791.2	0.1613
49	7.59	3793.5	0.2551
50	7.59	3794.2	0.2514
51	7.62	3810.0	0.3719
52	7.63	3817.1	0.5775
53	7.63	3818.0	0.4684
54	7.65	3825.3	0.5574
55	7.71	3854.6	0.5902
56	7.71	3855.8	0.6020
57	7.72	3861.7	0.4428
58	7.72	3862.9	0.4106
59	7.92	3960.4	0.0445
60	7.93	3963.8	0.3752
61	7.93	3967.2	0.2025
62	7.94	3970.9	0.3590
63	7.94	3973.2	0.3323
64	7.95	3977.5	0.0380
65	8.00	4001.6	0.5015
66	8.02	4009.8	0.4599
67	8.31	4155.8	0.4768
68	8.31	4157.0	0.4767
69	8.33	4164.1	0.4774
70	8.33	4165.5	0.4527

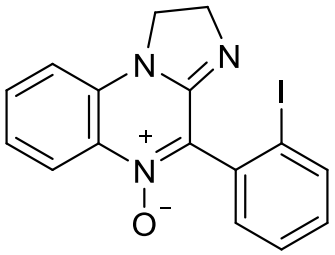
^{13}C NMR (500 MHz, $CDCl_3$) of compound **2c**



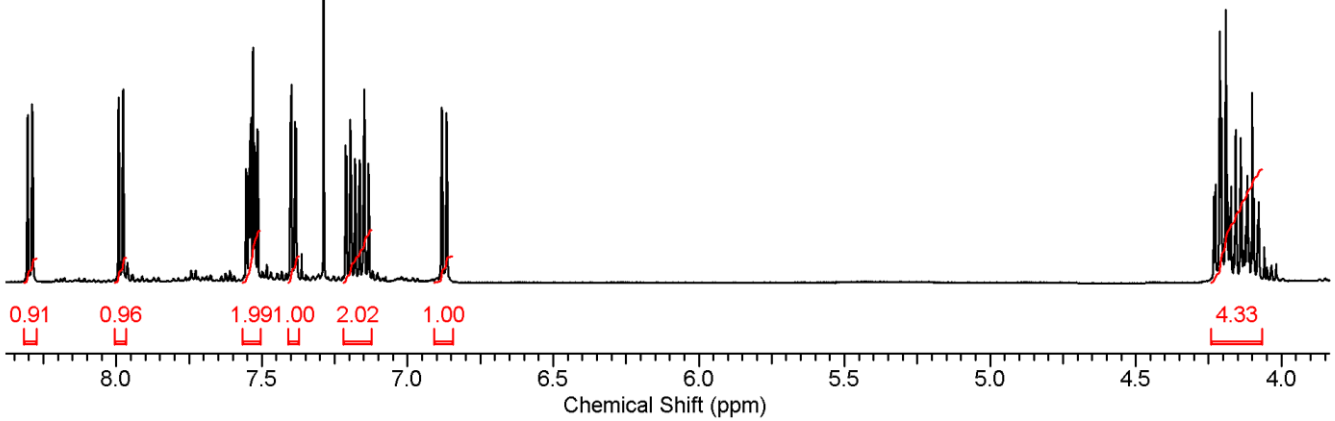




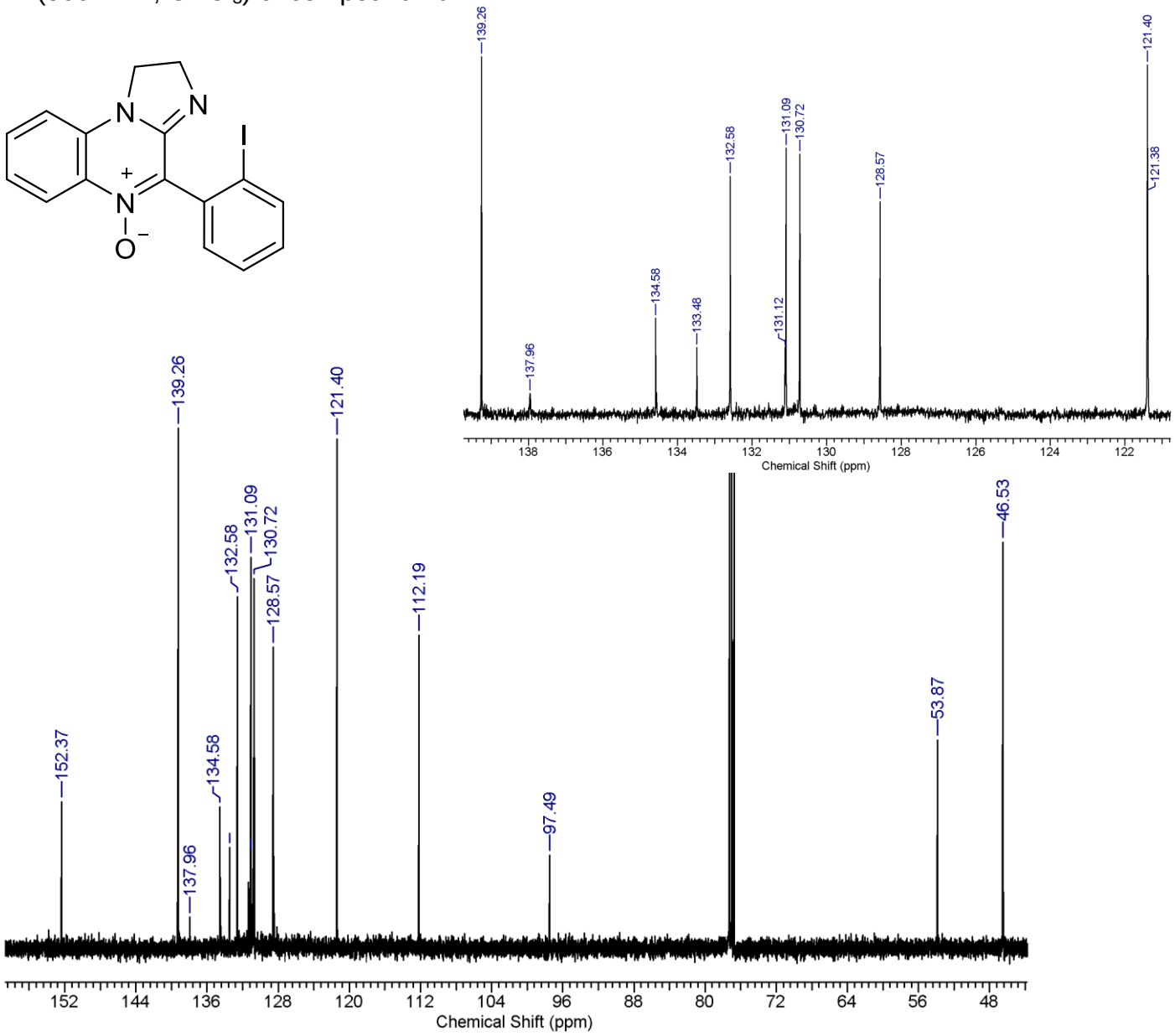
1H NMR (500 MHz, $CDCl_3$) for compound **2d**



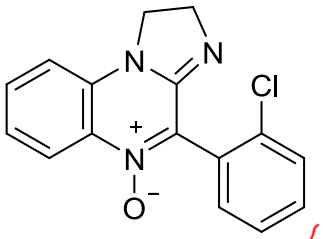
No.	(ppm)	(Hz)	Height
1	4.06	2030.1	0.0474
2	4.08	2039.0	0.1068
3	4.08	2040.4	0.0833
4	4.08	2041.5	0.0762
5	4.09	2047.7	0.1113
6	4.10	2050.9	0.2516
7	4.11	2055.7	0.0400
8	4.11	2056.9	0.0308
9	4.12	2058.7	0.1412
10	4.12	2060.5	0.1214
11	4.12	2062.6	0.0634
12	4.13	2063.5	0.0341
13	4.13	2066.2	0.0426
14	4.14	2069.2	0.1530
15	4.14	2070.8	0.1917
16	4.15	2076.8	0.0606
17	4.15	2077.7	0.0949
18	4.16	2079.3	0.2025
19	4.16	2082.3	0.0379
20	4.17	2087.1	0.1274
21	4.18	2089.4	0.0882
22	4.18	2091.0	0.0366
23	4.19	2093.5	0.1438
24	4.19	2096.2	0.3614
25	4.20	2100.1	0.0332
26	4.20	2101.5	0.0380
27	4.21	2103.6	0.2178
28	4.21	2105.2	0.2590
29	4.21	2106.3	0.3327
30	4.23	2113.9	0.1296
31	4.23	2116.8	0.1138
32	6.86	3433.4	0.2129
33	6.87	3434.3	0.2244
34	6.88	3441.4	0.2281
35	6.88	3442.5	0.2316
36	7.13	3566.8	0.1438
37	7.13	3567.9	0.1575
38	7.15	3574.1	0.1761
39	7.15	3575.3	0.2556
40	7.15	3576.2	0.1699
41	7.16	3582.4	0.1574
42	7.17	3583.7	0.1619
43	7.18	3589.9	0.1567
44	7.18	3591.5	0.1641
45	7.19	3597.5	0.2007
46	7.19	3597.9	0.2018
47	7.20	3599.1	0.2158
48	7.20	3599.5	0.2065
49	7.21	3605.5	0.1671
50	7.21	3607.1	0.1814
51	7.29	3644.6	1.0000
52	7.38	3692.2	0.2045
53	7.39	3693.8	0.2128
54	7.40	3700.2	0.2625
55	7.40	3701.6	0.2480
56	7.51	3757.7	0.2002
57	7.52	3758.8	0.2030
58	7.52	3761.8	0.1733
59	7.52	3763.2	0.1812
60	7.53	3765.2	0.3114
61	7.53	3766.4	0.3059
62	7.54	3769.1	0.1909
63	7.54	3769.8	0.2182
64	7.54	3770.5	0.2027
65	7.54	3771.2	0.1878
66	7.54	3772.8	0.1517
67	7.55	3773.9	0.1419
68	7.55	3777.4	0.1462
69	7.56	3778.7	0.1502
70	7.98	3988.6	0.2559
71	7.98	3989.5	0.2540
72	7.99	3996.6	0.2450
73	7.99	3997.6	0.2290
74	8.29	4144.3	0.2260
75	8.29	4145.4	0.2362
76	8.30	4152.5	0.2216
77	8.31	4153.7	0.2187



^{13}C NMR (500 MHz, $CDCl_3$) of compound **2d**

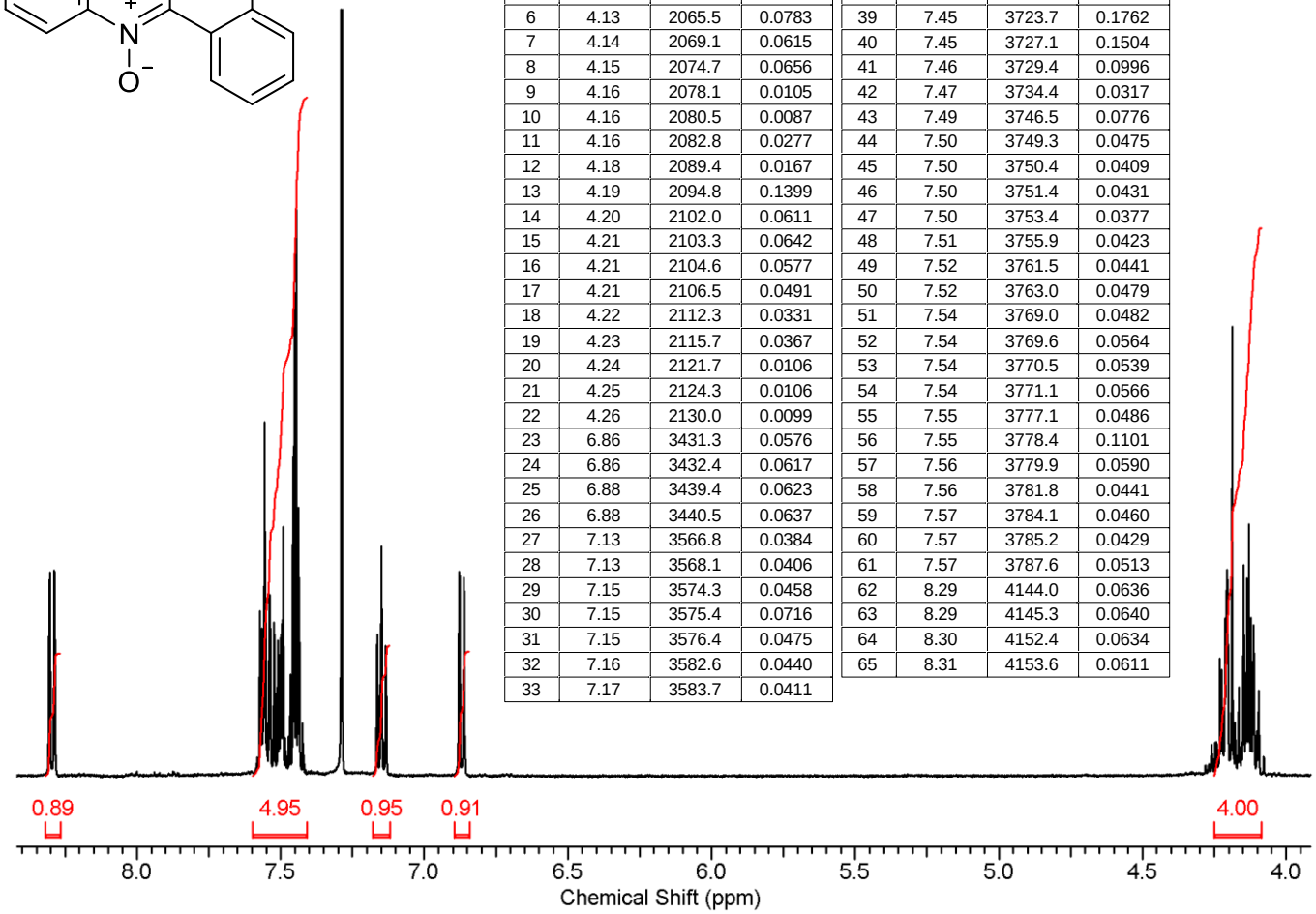


^{1}H NMR (500 MHz, $CDCl_3$) for compound **2f**

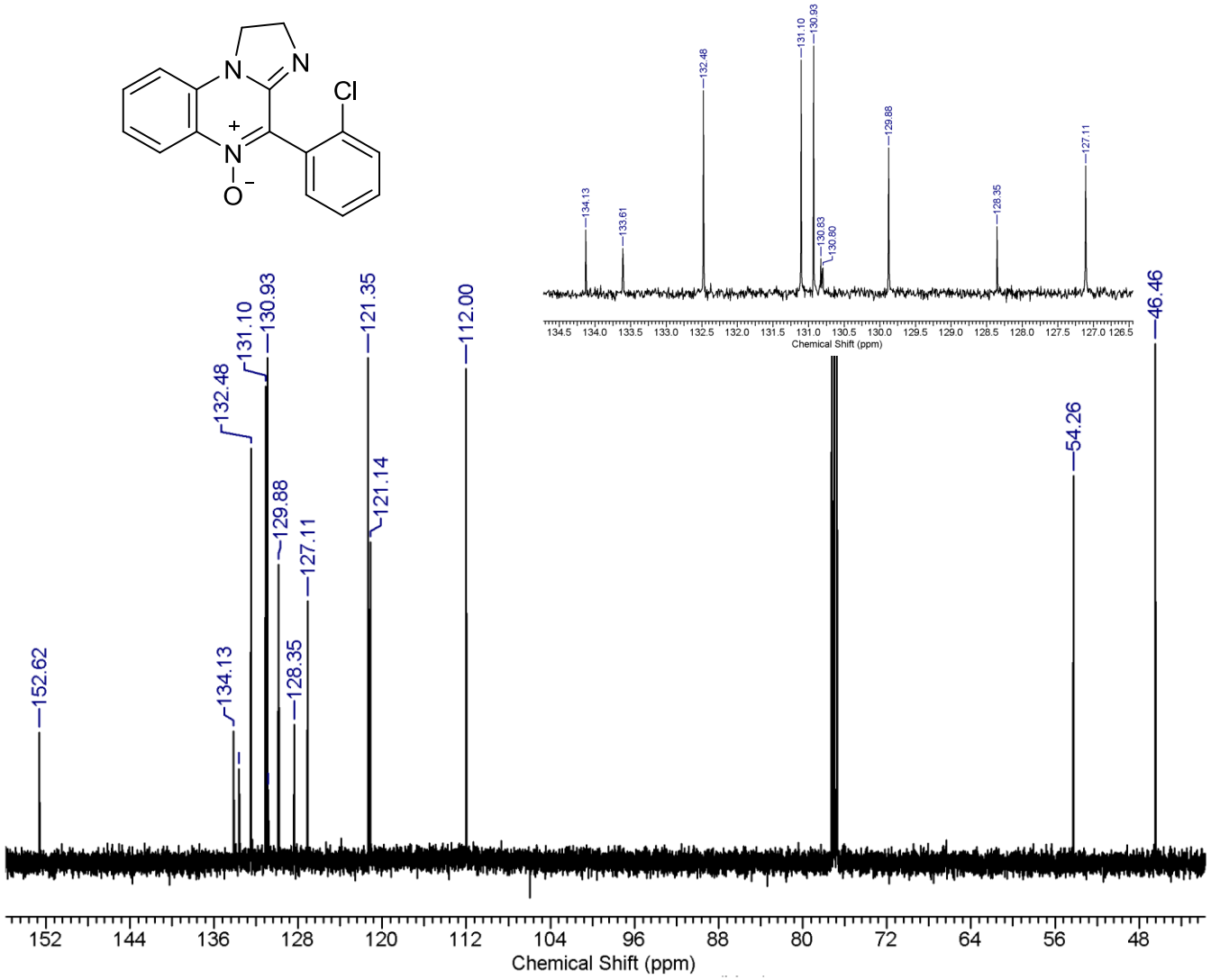


No.	(ppm)	(Hz)	Height
1	4.08	2039.4	0.0062
2	4.10	2048.4	0.0267
3	4.10	2051.6	0.0141
4	4.11	2056.7	0.0471
5	4.12	2061.4	0.0492
6	4.13	2065.5	0.0783
7	4.14	2069.1	0.0615
8	4.15	2074.7	0.0656
9	4.16	2078.1	0.0105
10	4.16	2080.5	0.0087
11	4.16	2082.8	0.0277
12	4.18	2089.4	0.0167
13	4.19	2094.8	0.1399
14	4.20	2102.0	0.0611
15	4.21	2103.3	0.0642
16	4.21	2104.6	0.0577
17	4.21	2106.5	0.0491
18	4.22	2112.3	0.0331
19	4.23	2115.7	0.0367
20	4.24	2121.7	0.0106
21	4.25	2124.3	0.0106
22	4.26	2130.0	0.0099
23	6.86	3431.3	0.0576
24	6.86	3432.4	0.0617
25	6.88	3439.4	0.0623
26	6.88	3440.5	0.0637
27	7.13	3566.8	0.0384
28	7.13	3568.1	0.0406
29	7.15	3574.3	0.0458
30	7.15	3575.4	0.0716
31	7.15	3576.4	0.0475
32	7.16	3582.6	0.0440
33	7.17	3583.7	0.0411

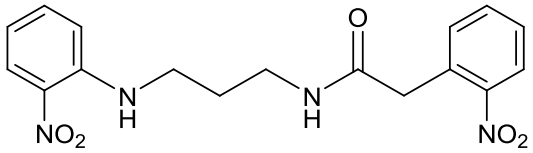
No.	(ppm)	(Hz)	Height
34	7.29	3644.6	1.0000
35	7.42	3712.8	0.0165
36	7.43	3718.3	0.0618
37	7.44	3719.6	0.0835
38	7.44	3720.2	0.0702
39	7.45	3723.7	0.1762
40	7.45	3727.1	0.1504
41	7.46	3729.4	0.0996
42	7.47	3734.4	0.0317
43	7.49	3746.5	0.0776
44	7.50	3749.3	0.0475
45	7.50	3750.4	0.0409
46	7.50	3751.4	0.0431
47	7.50	3753.4	0.0377
48	7.51	3755.9	0.0423
49	7.52	3761.5	0.0441
50	7.52	3763.0	0.0479
51	7.54	3769.0	0.0482
52	7.54	3769.6	0.0564
53	7.54	3770.5	0.0539
54	7.54	3771.1	0.0566
55	7.55	3777.1	0.0486
56	7.55	3778.4	0.1101
57	7.56	3779.9	0.0590
58	7.56	3781.8	0.0441
59	7.57	3784.1	0.0460
60	7.57	3785.2	0.0429
61	7.57	3787.6	0.0513
62	8.29	4144.0	0.0636
63	8.29	4145.3	0.0640
64	8.30	4152.4	0.0634
65	8.31	4153.6	0.0611



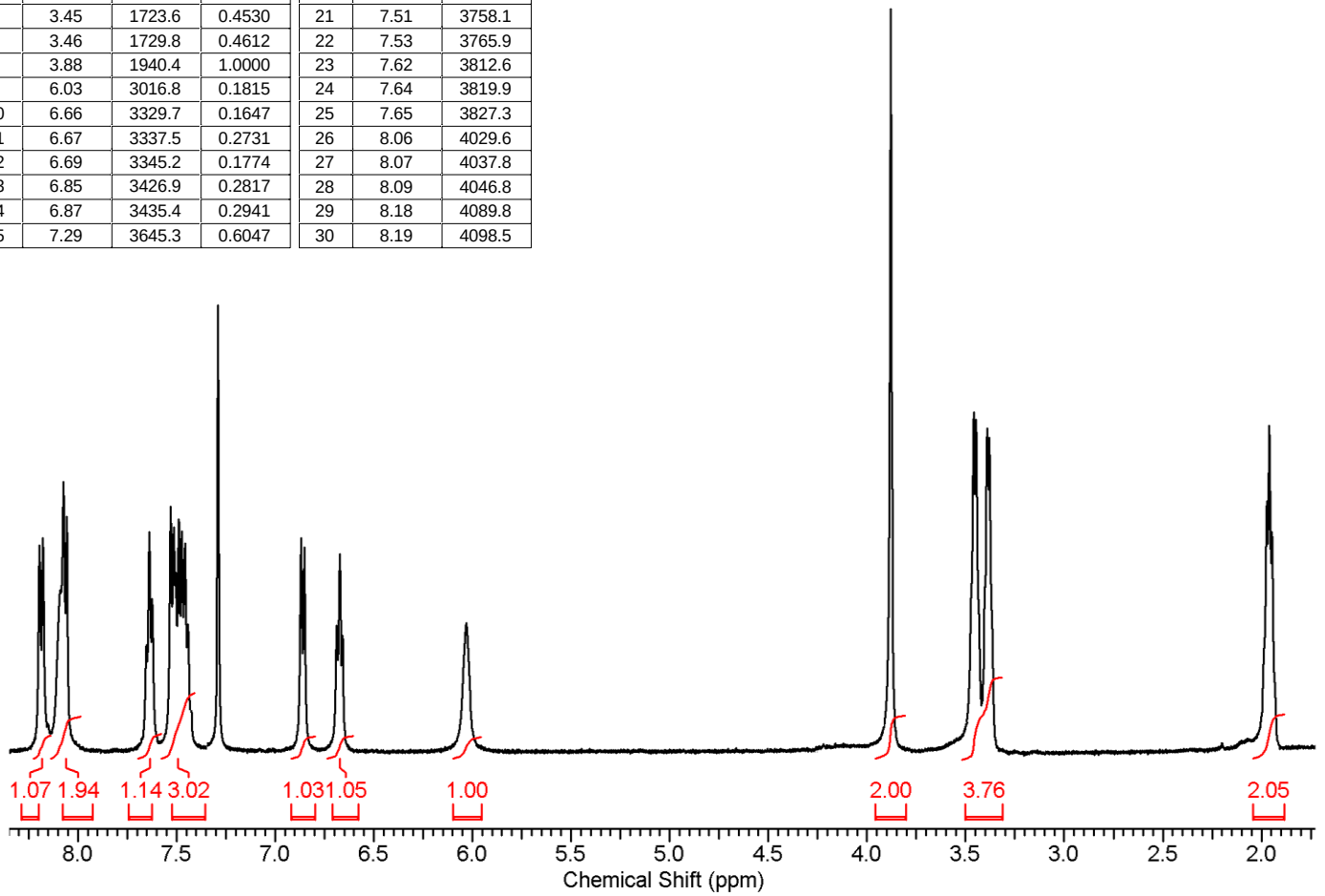
^{13}C NMR (500 MHz, $CDCl_3$) of compound **2f**



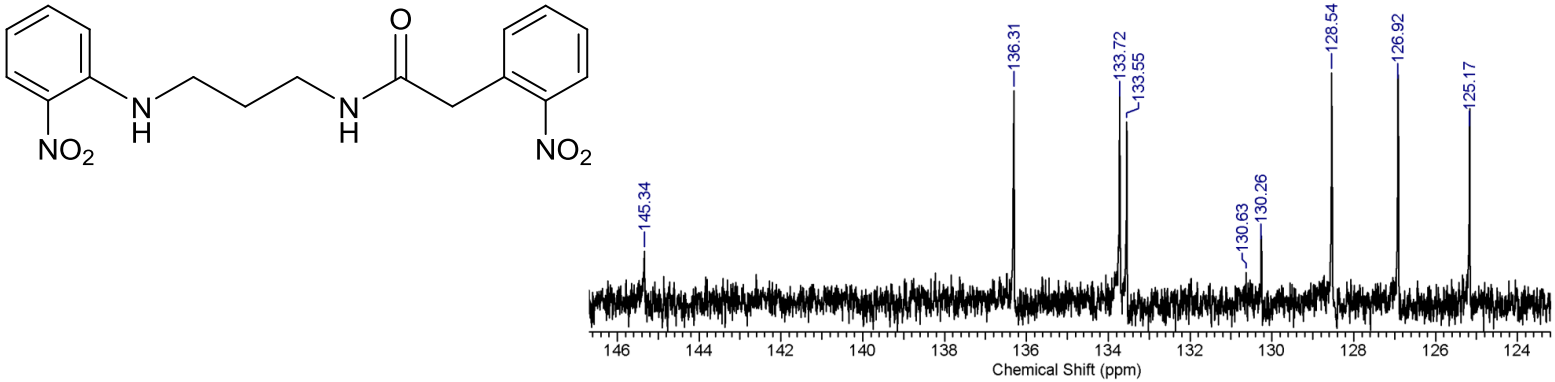
^{1}H NMR (500 MHz, $CDCl_3$) for compound **3b**

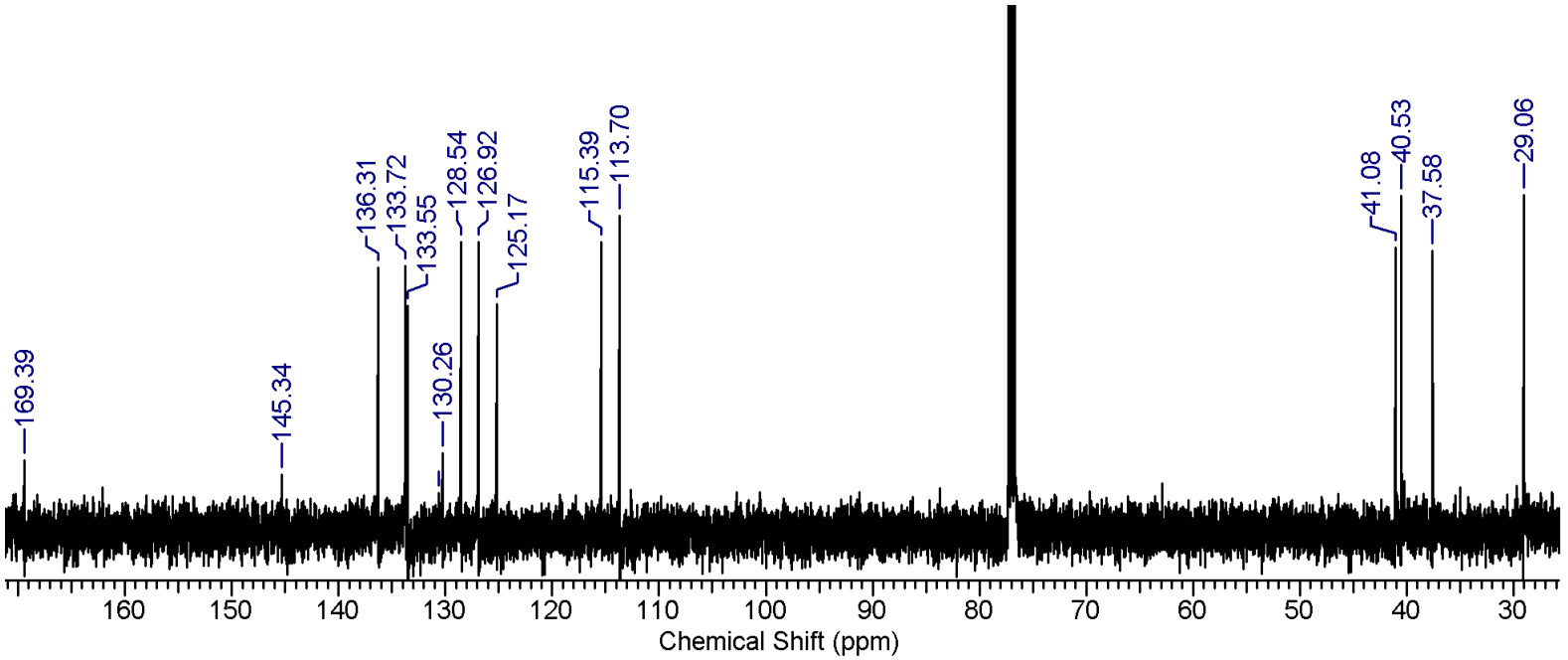


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)
1	1.95	974.0	0.3039	16	7.44	3721.7
2	1.96	980.4	0.4445	17	7.46	3729.3
3	1.97	986.8	0.3417	18	7.47	3737.1
4	3.38	1689.7	0.4299	19	7.49	3745.1
5	3.39	1695.5	0.4413	20	7.50	3753.1
6	3.45	1723.6	0.4530	21	7.51	3758.1
7	3.46	1729.8	0.4612	22	7.53	3765.9
8	3.88	1940.4	1.0000	23	7.62	3812.6
9	6.03	3016.8	0.1815	24	7.64	3819.9
10	6.66	3329.7	0.1647	25	7.65	3827.3
11	6.67	3337.5	0.2731	26	8.06	4029.6
12	6.69	3345.2	0.1774	27	8.07	4037.8
13	6.85	3426.9	0.2817	28	8.09	4046.8
14	6.87	3435.4	0.2941	29	8.18	4089.8
15	7.29	3645.3	0.6047	30	8.19	4098.5



^{13}C NMR (500 MHz, $CDCl_3$) of compound **3b**



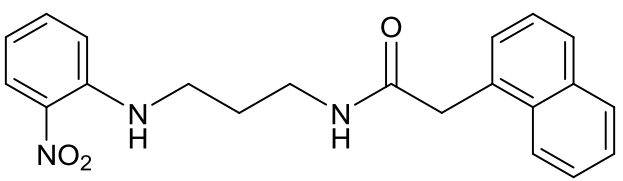


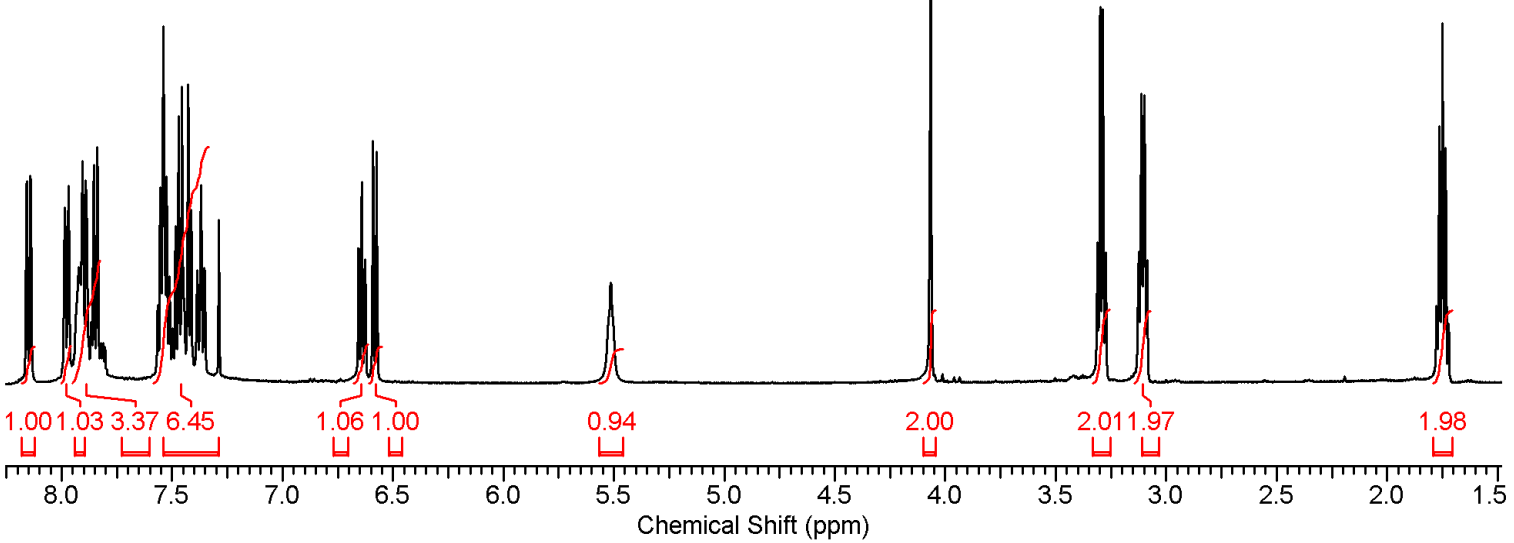
^{1}H NMR (500 MHz, $CDCl_3$) for compound **3c**

No.	(ppm)	(Hz)	Height
1	1.72	861.2	0.0576
2	1.74	867.8	0.2266
3	1.75	874.7	0.3466
4	1.76	881.6	0.2474
5	1.78	888.4	0.0749
6	3.09	1543.7	0.1187
7	3.10	1550.3	0.2773
8	3.11	1556.3	0.2787
9	3.13	1562.9	0.1270
10	3.27	1637.1	0.1259
11	3.29	1643.5	0.3596
12	3.30	1649.9	0.3624
13	3.31	1656.5	0.1357
14	4.07	2033.7	1.0000
15	5.51	2757.9	0.0975
16	6.57	3287.6	0.2229
17	6.59	3296.3	0.2334

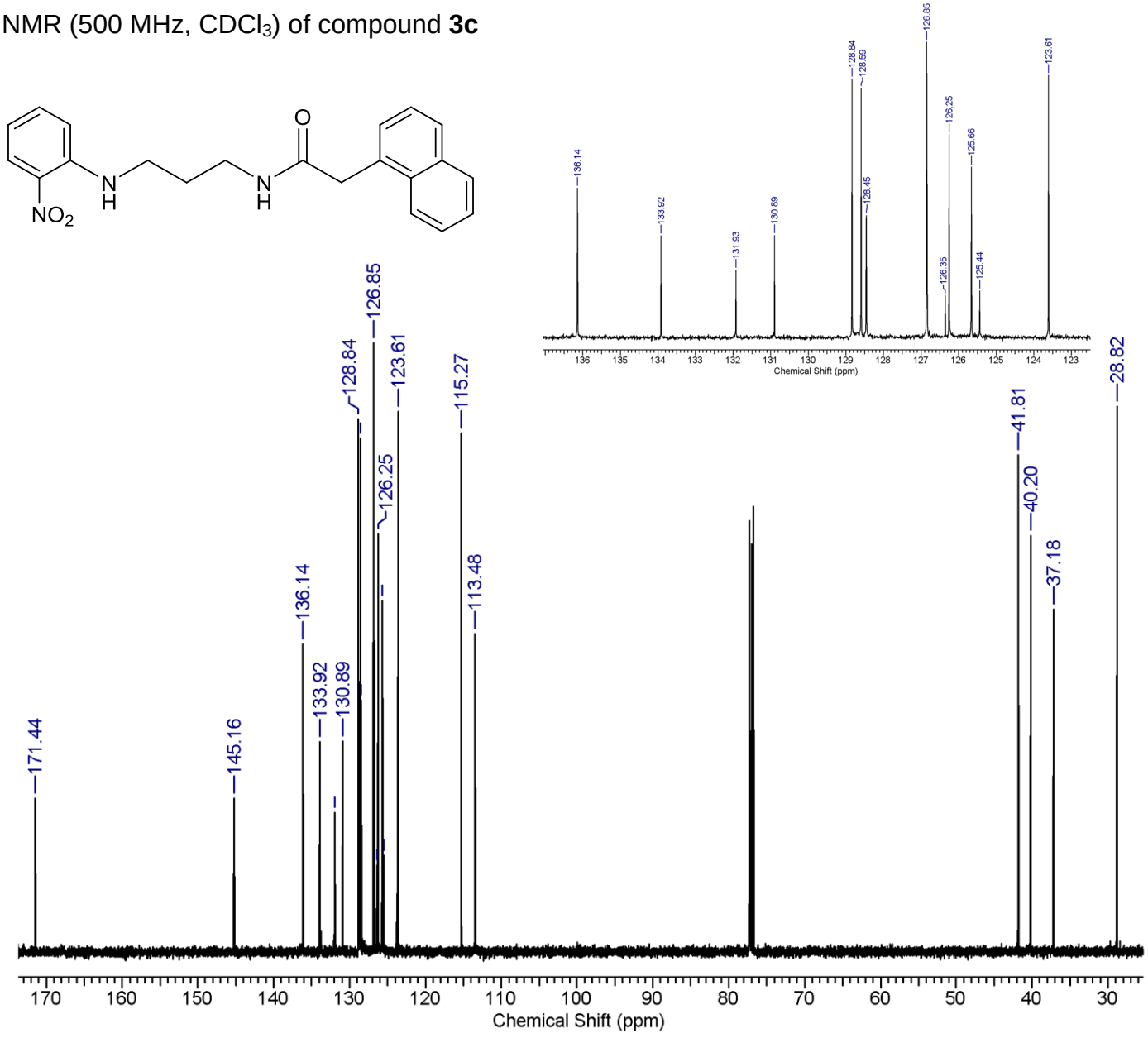
No.	(ppm)	(Hz)	Height
18	6.63	3313.4	0.1196
19	6.64	3321.4	0.1936
20	6.66	3329.0	0.1300
21	7.29	3645.1	0.1574
22	7.36	3678.5	0.1115
23	7.37	3685.8	0.1908
24	7.39	3694.1	0.1091
25	7.41	3708.0	0.1673
26	7.43	3714.9	0.2874
27	7.44	3723.3	0.0823
28	7.45	3725.2	0.0856
29	7.45	3728.2	0.2857
30	7.47	3735.9	0.2571
31	7.48	3743.0	0.1513
32	7.50	3749.9	0.0532
33	7.51	3757.5	0.1030
34	7.52	3763.2	0.1994

No.	(ppm)	(Hz)
35	7.54	3770.3
36	7.55	3777.8
37	7.56	3783.1
38	7.84	3920.0
39	7.85	3928.0
40	7.87	3934.1
41	7.89	3945.1
42	7.89	3947.0
43	7.91	3954.3
44	7.92	3961.8
45	7.97	3985.6
46	7.98	3993.4
47	8.14	4071.7
48	8.16	4079.0
49	8.16	4080.2

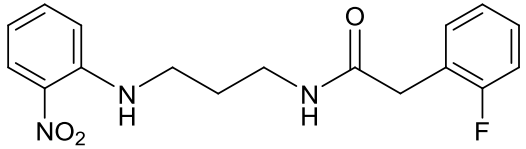




^{13}C NMR (500 MHz, $CDCl_3$) of compound **3c**



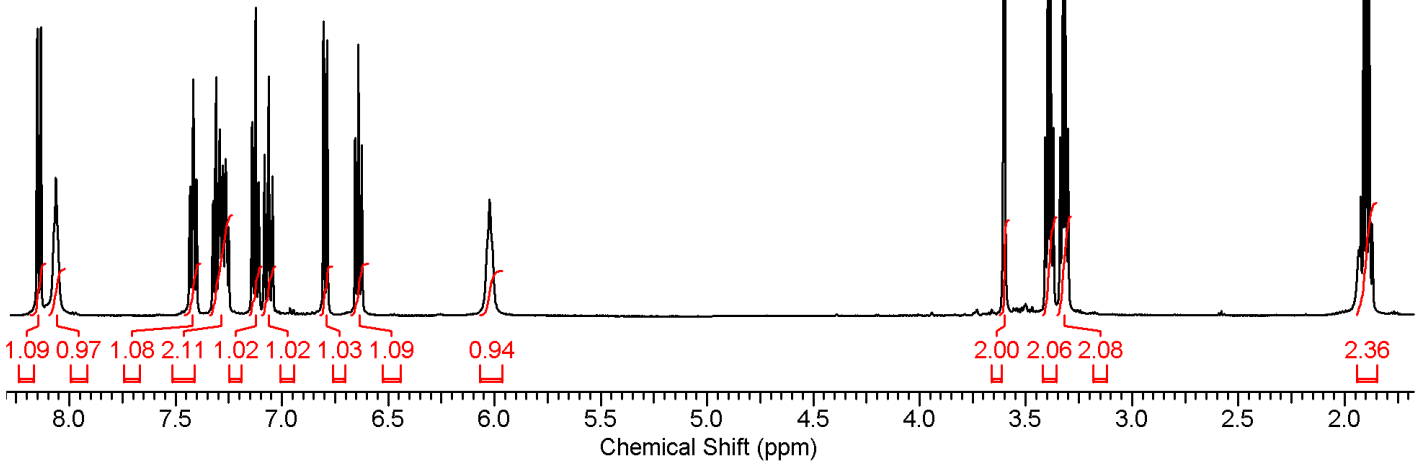
^{1}H NMR (500 MHz, $CDCl_3$) for compound **3g**



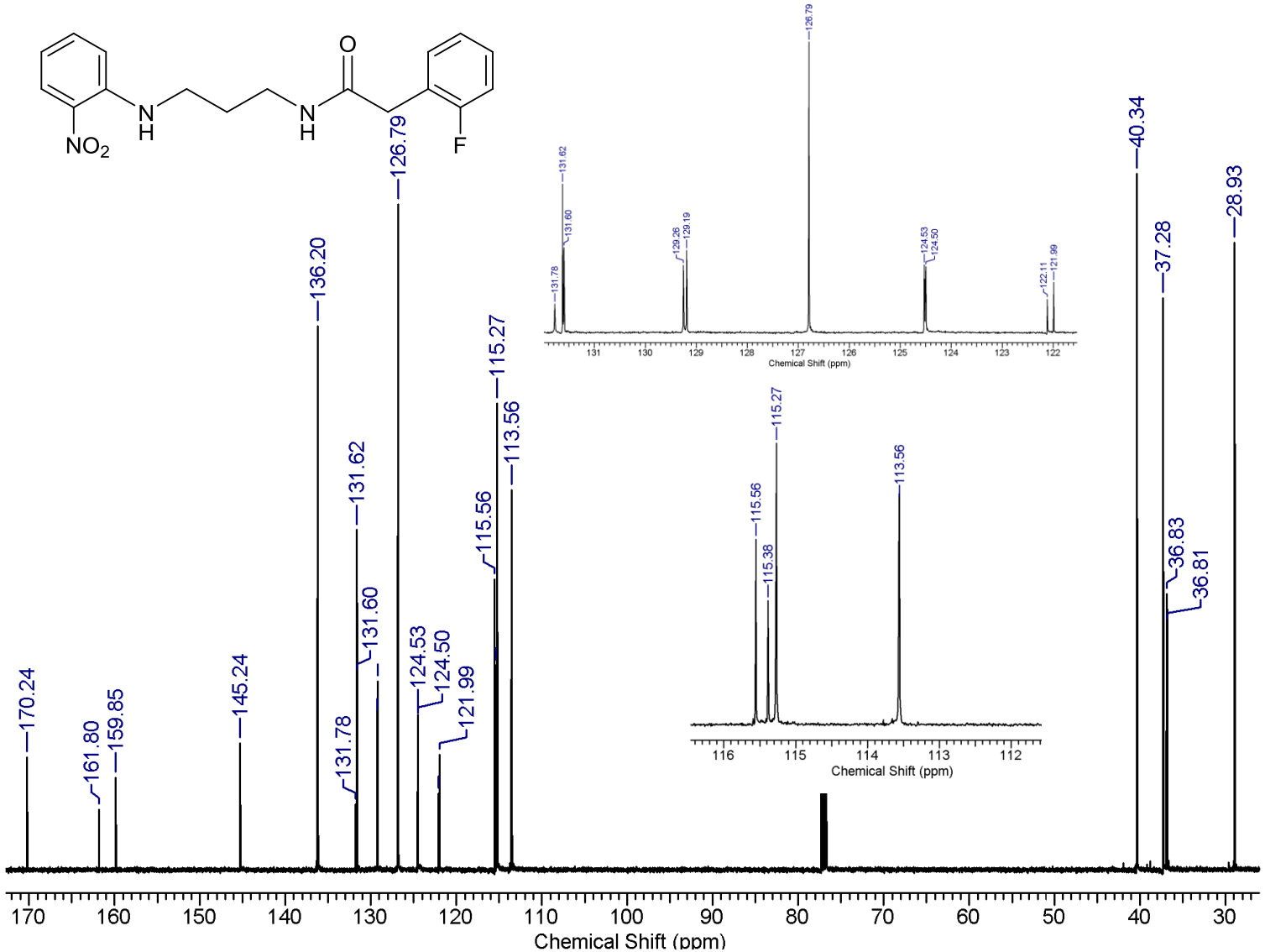
No.	(ppm)	(Hz)	Height
1	1.87	935.1	0.0944
2	1.88	941.7	0.3387
3	1.90	948.6	0.4991
4	1.91	955.7	0.3507
5	1.92	962.3	0.1226
6	3.30	1651.1	0.1924
7	3.31	1657.9	0.4024
8	3.33	1663.4	0.4027
9	3.34	1670.3	0.1832
10	3.37	1685.6	0.1929
11	3.38	1692.3	0.5035
12	3.40	1698.4	0.4969
13	3.41	1705.1	0.1836
14	3.60	1801.0	1.0000
15	6.02	3012.2	0.1196
16	6.62	3312.3	0.1666
17	6.63	3313.6	0.1751
18	6.64	3319.4	0.2014
19	6.64	3320.7	0.2785
20	6.64	3322.1	0.2028
21	6.65	3327.8	0.1824

No.	(ppm)	(Hz)	Height
22	6.66	3329.0	0.1780
23	6.79	3394.7	0.2830
24	6.80	3402.7	0.3025
25	7.04	3523.1	0.1366
26	7.05	3524.0	0.1428
27	7.06	3532.5	0.2458
28	7.08	3541.2	0.1561
29	7.08	3542.1	0.1657
30	7.11	3555.6	0.1370
31	7.11	3556.5	0.1351
32	7.12	3562.9	0.3165
33	7.13	3564.0	0.3079
34	7.14	3570.5	0.1991
35	7.14	3571.6	0.1886
36	7.25	3625.4	0.0771
37	7.25	3627.2	0.0909
38	7.26	3630.7	0.0888
39	7.26	3632.7	0.1611
40	7.27	3634.8	0.1303
41	7.28	3638.9	0.1220
42	7.28	3640.7	0.1544

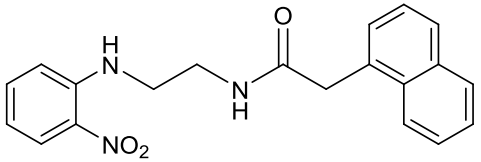
No.	(ppm)	(Hz)	Height
43	7.28	3642.8	0.0832
44	7.29	3644.8	0.1432
45	7.29	3647.8	0.1913
46	7.31	3655.4	0.2447
47	7.31	3656.7	0.2179
48	7.32	3662.9	0.1177
49	7.33	3664.3	0.1047
50	7.40	3701.4	0.1388
51	7.40	3702.5	0.1403
52	7.41	3708.5	0.1651
53	7.42	3709.8	0.2430
54	7.42	3711.0	0.1665
55	7.43	3716.9	0.1326
56	7.43	3718.1	0.1298
57	8.06	4033.0	0.1413
58	8.13	4067.6	0.2961
59	8.14	4069.0	0.2923
60	8.15	4076.3	0.2948
61	8.15	4077.7	0.2846



^{13}C NMR (500 MHz, $CDCl_3$) of compound **3g**



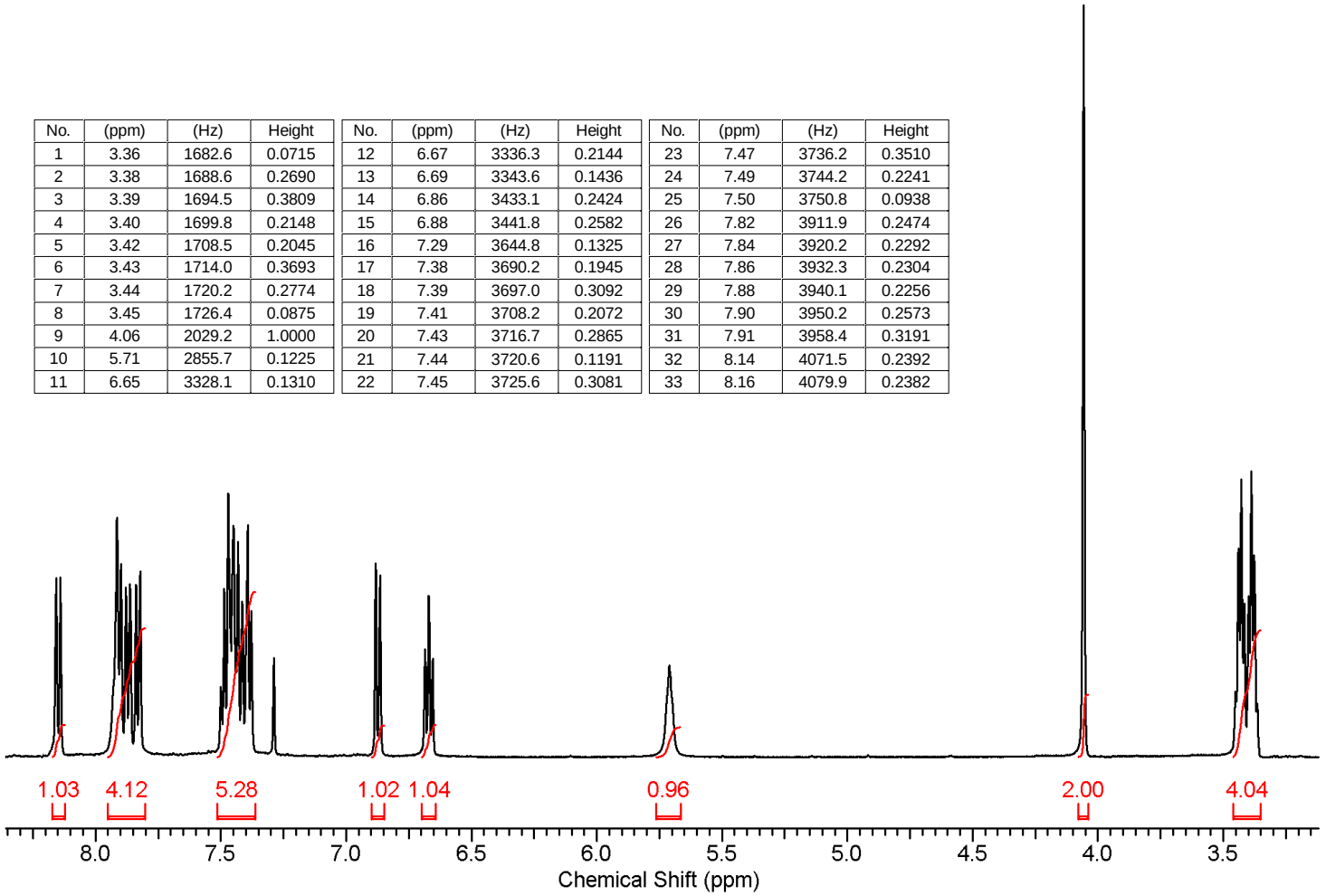
^{1}H NMR (500 MHz, $CDCl_3$) for compound **4c**



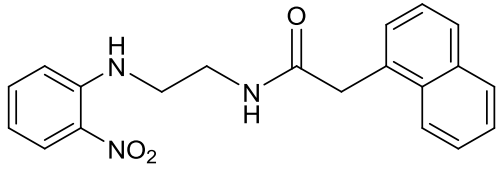
No.	(ppm)	(Hz)	Height
1	3.36	1682.6	0.0715
2	3.38	1688.6	0.2690
3	3.39	1694.5	0.3809
4	3.40	1699.8	0.2148
5	3.42	1708.5	0.2045
6	3.43	1714.0	0.3693
7	3.44	1720.2	0.2774
8	3.45	1726.4	0.0875
9	4.06	2029.2	1.0000
10	5.71	2855.7	0.1225
11	6.65	3328.1	0.1310

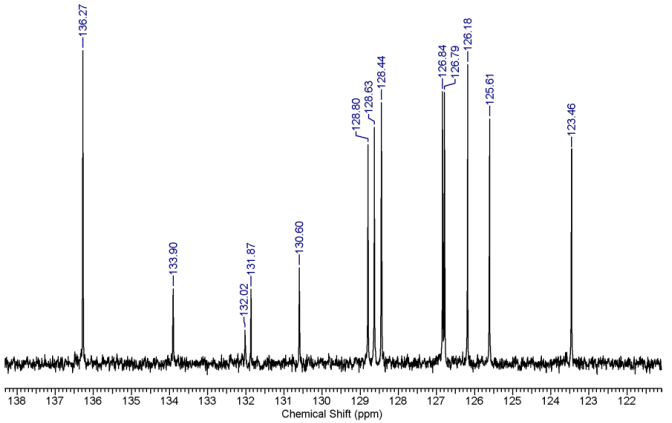
No.	(ppm)	(Hz)	Height
12	6.67	3336.3	0.2144
13	6.69	3343.6	0.1436
14	6.86	3433.1	0.2424
15	6.88	3441.8	0.2582
16	7.29	3644.8	0.1325
17	7.38	3690.2	0.1945
18	7.39	3697.0	0.3092
19	7.41	3708.2	0.2072
20	7.43	3716.7	0.2865
21	7.44	3720.6	0.1191
22	7.45	3725.6	0.3081

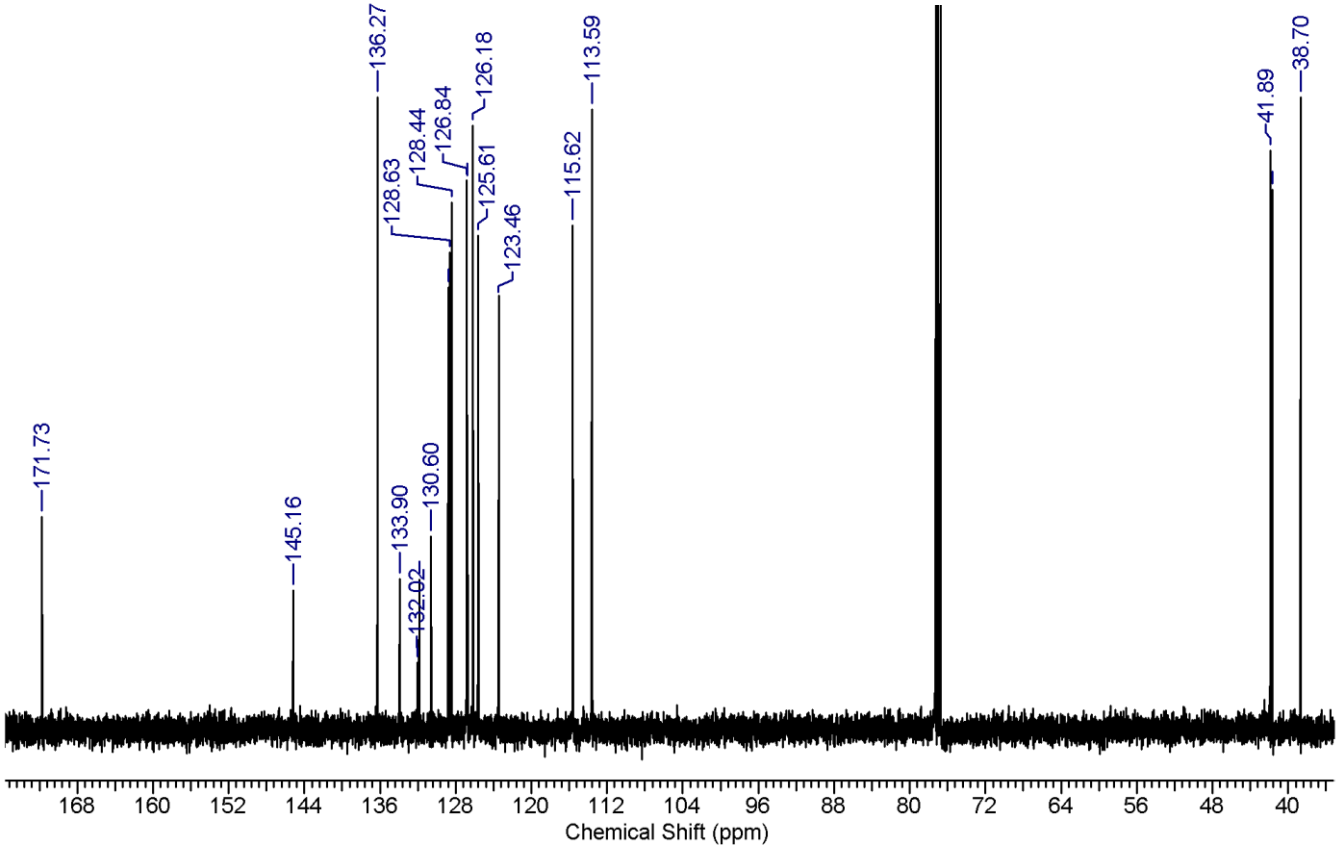
No.	(ppm)	(Hz)	Height
23	7.47	3736.2	0.3510
24	7.49	3744.2	0.2241
25	7.50	3750.8	0.0938
26	7.82	3911.9	0.2474
27	7.84	3920.2	0.2292
28	7.86	3932.3	0.2304
29	7.88	3940.1	0.2256
30	7.90	3950.2	0.2573
31	7.91	3958.4	0.3191
32	8.14	4071.5	0.2392
33	8.16	4079.9	0.2382



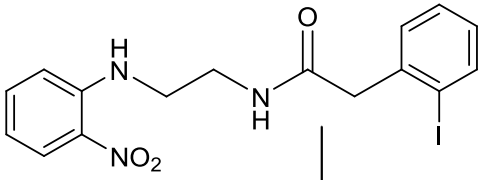
^{13}C NMR (500 MHz, $CDCl_3$) of compound **4c**







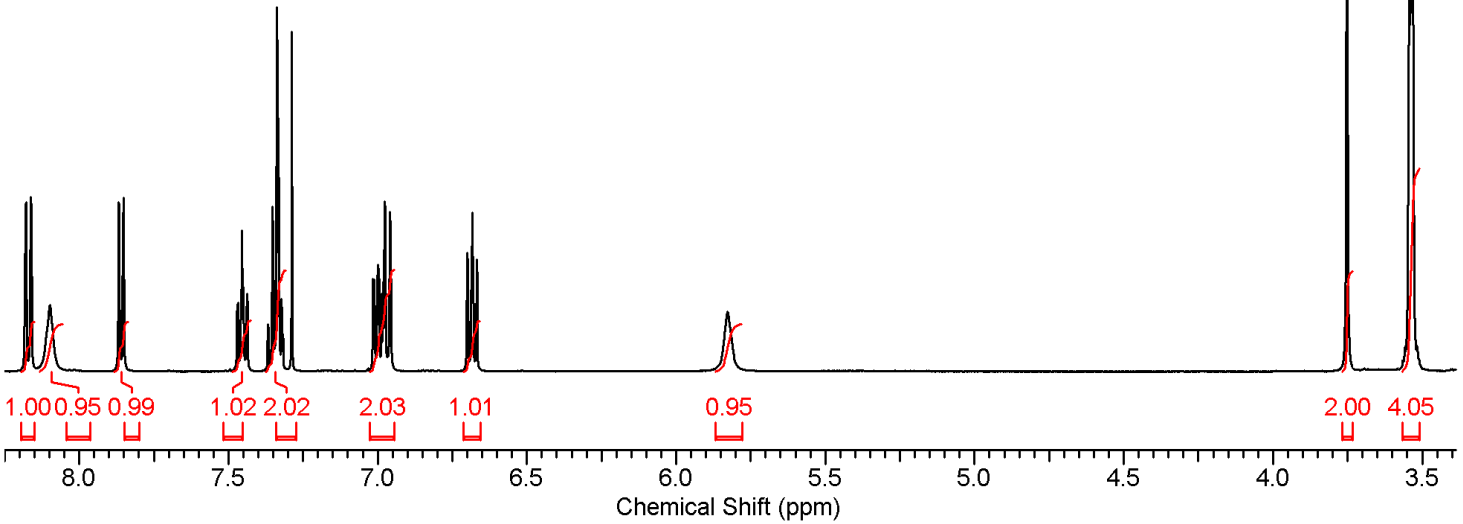
^{1}H NMR (500 MHz, $CDCl_3$) for compound **4d**



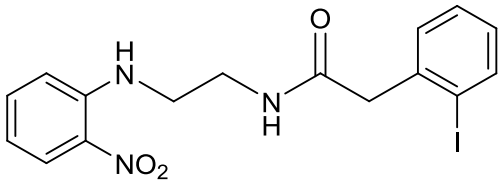
No.	(ppm)	(Hz)	Height
1	3.53	1766.2	0.4553
2	3.54	1768.8	0.4793
3	3.54	1771.9	0.4459
4	3.75	1876.4	1.0000
5	5.83	2914.2	0.0600
6	6.67	3334.1	0.0994
7	6.67	3335.3	0.1120
8	6.68	3341.0	0.1149
9	6.68	3342.4	0.1589
10	6.69	3343.8	0.1258
11	6.70	3349.6	0.1129
12	6.70	3350.8	0.1190
13	6.96	3479.5	0.1481
14	6.96	3480.5	0.1596
15	6.97	3488.1	0.1660
16	6.98	3489.0	0.1700
17	6.98	3491.4	0.0902
18	6.99	3494.0	0.0776
19	6.99	3498.1	0.0926

No.	(ppm)	(Hz)	Height
20	7.00	3499.5	0.1032
21	7.00	3500.7	0.1072
22	7.00	3501.7	0.0962
23	7.01	3506.2	0.0924
24	7.02	3508.6	0.0926
25	7.29	3644.7	0.3397
26	7.32	3659.7	0.0378
27	7.32	3662.1	0.0725
28	7.33	3667.4	0.2537
29	7.34	3669.3	0.3643
30	7.34	3670.2	0.3276
31	7.35	3676.0	0.1511
32	7.35	3677.1	0.1650
33	7.37	3683.6	0.0442
34	7.37	3684.8	0.0475
35	7.44	3719.3	0.0768
36	7.44	3720.3	0.0779
37	7.44	3721.0	0.0760
38	7.45	3726.3	0.0843

No.	(ppm)	(Hz)	Height
39	7.45	3727.5	0.1300
40	7.45	3727.9	0.1408
41	7.46	3728.9	0.0841
42	7.46	3729.6	0.0799
43	7.47	3734.4	0.0625
44	7.47	3734.8	0.0693
45	7.47	3736.0	0.0677
46	7.47	3736.5	0.0676
47	7.85	3926.3	0.1735
48	7.85	3927.0	0.1701
49	7.87	3934.2	0.1665
50	7.87	3935.1	0.1693
51	8.10	4050.5	0.0670
52	8.16	4081.3	0.1681
53	8.16	4082.7	0.1745
54	8.18	4089.8	0.1692
55	8.18	4091.3	0.1679



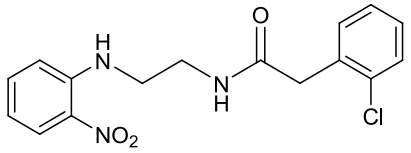
^{13}C NMR (500 MHz, $CDCl_3$) of compound **4d**

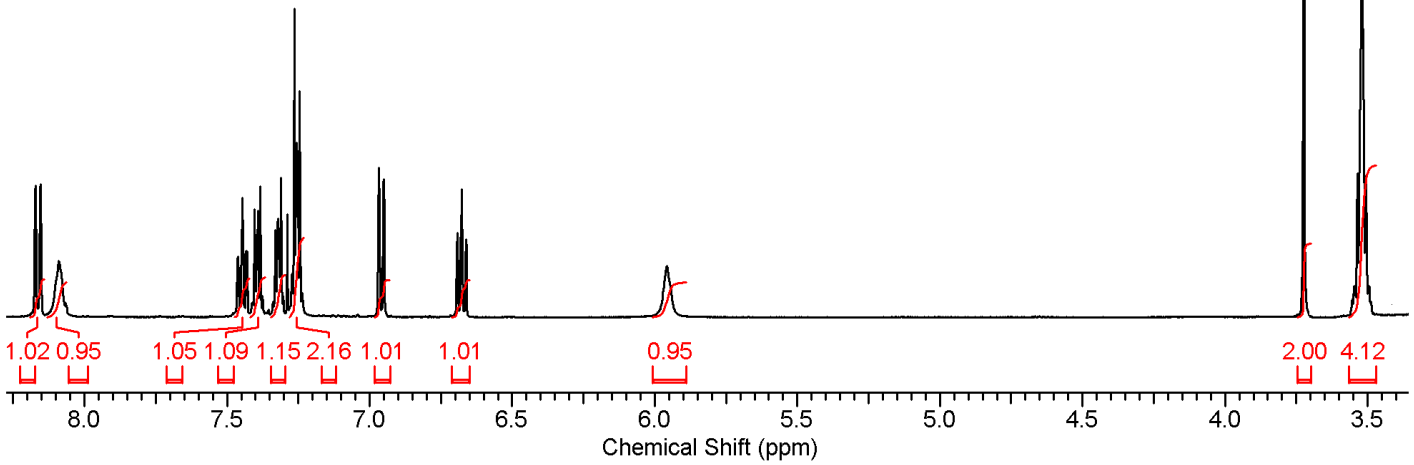


^{1}H NMR (500 MHz, $CDCl_3$) for compound **4f**

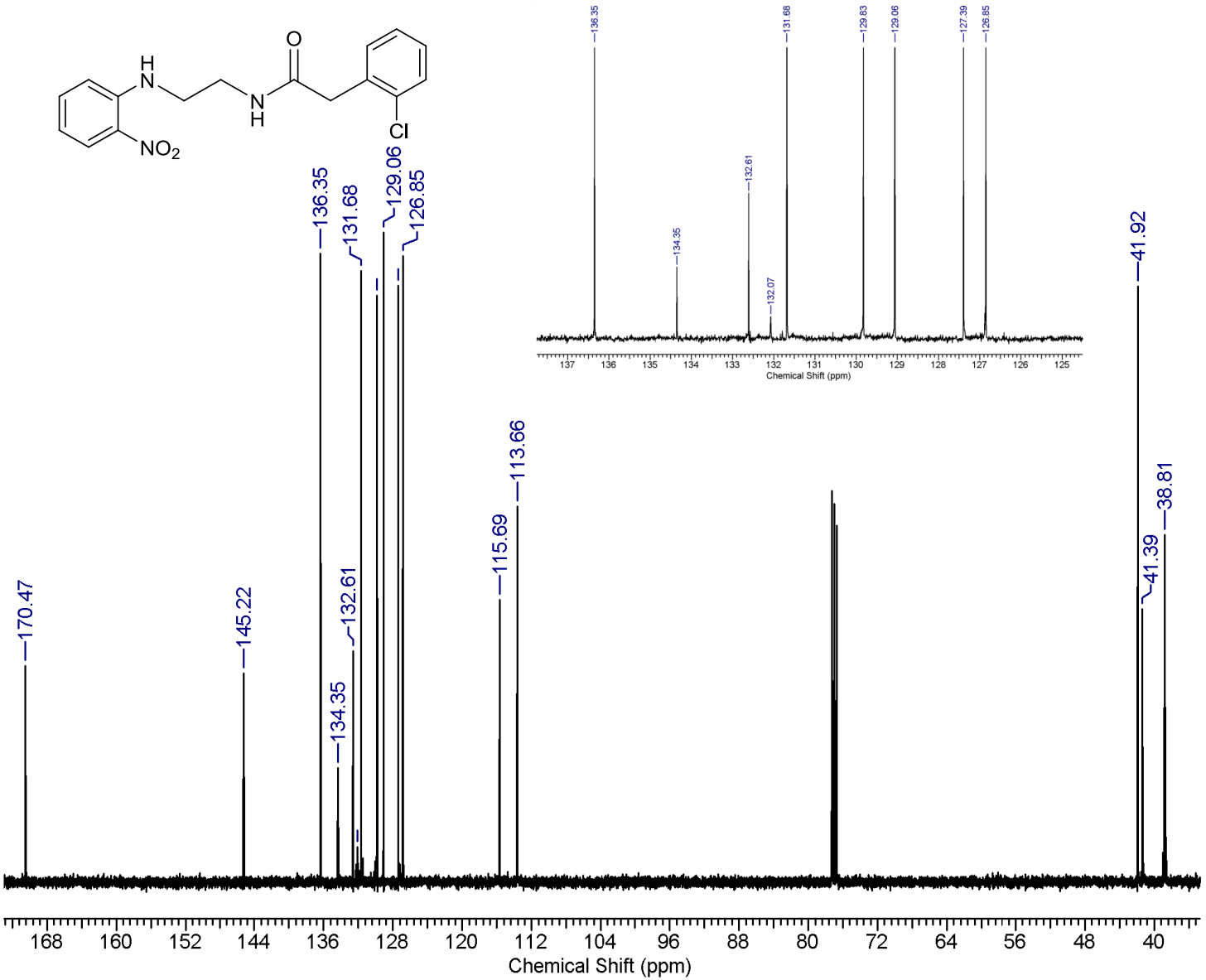
No.	(ppm)	(Hz)	Height
1	3.49	1747.9	0.0389
2	3.51	1753.4	0.1767
3	3.52	1760.7	0.4485
4	3.54	1768.2	0.1792
5	3.55	1773.7	0.0388
6	3.72	1862.8	1.0000
7	5.96	2979.0	0.0640
8	6.66	3331.3	0.0968
9	6.66	3332.4	0.0941
10	6.67	3338.4	0.1092
11	6.68	3339.5	0.1594
12	6.68	3340.9	0.1011
13	6.69	3346.8	0.1049
14	6.69	3348.0	0.0981
15	6.95	3475.9	0.1718
16	6.97	3484.6	0.1864
17	7.24	3619.2	0.0306
18	7.25	3623.6	0.2814
19	7.25	3626.8	0.2065
20	7.25	3627.4	0.1962
21	7.26	3629.0	0.2179
22	7.26	3629.7	0.2026
23	7.26	3632.9	0.3840

No.	(ppm)	(Hz)
24	7.27	3636.6
25	7.27	3637.3
26	7.29	3645.3
27	7.31	3656.7
28	7.32	3659.5
29	7.32	3661.3
30	7.32	3662.2
31	7.33	3665.9
32	7.38	3693.1
33	7.39	3696.6
34	7.39	3698.2
35	7.40	3702.3
36	7.43	3715.8
37	7.43	3717.2
38	7.45	3724.3
39	7.46	3731.4
40	7.46	3732.7
41	8.09	4045.8
42	8.15	4077.7
43	8.16	4079.0
44	8.17	4086.4
45	8.17	4087.7





^{13}C NMR (500 MHz, $CDCl_3$) of compound **4f**



Chiral HPLC Screening for compound **1a**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2 (min)	k_2	α	R
Chiralcel OJ-H	9,13	2,04 (-)	18,37	5,12 (+)	2,51	8,33
Chiralcel OD-H	5,51	0,84 (+)	8,42	1,81 (-)	2,16	4,81
Chiralpak AS-H	5,18	0,73 (-)	5,99	1,00 (+)	1,37	1,69
Sepapak-2-HR	11,14	2,71 (+)	13,96	3,65 (-)	1,35	2,38
Chiralpak AD-H	8,61	1,87 (-)	9,27	2,09 (+)	1,12	1,10
Chiralcel OB-H	4,33	0,44			1	0

Chiral HPLC Screening for compound **1b**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2 (min)	k_2	α	R	
Chiralpak AS-H	7,38	1,46			1	0	
Chiralpak IC	4,44	4,44			1	0	
Chiralcel OB-H	9,24	2,08			1	0	

Chiral HPLC Screening for compound **1c**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2(min)	k_2	α	R
Chiralpak AS-H	7.91	1.64 (-)	15.13	4.04 (+)	2.47	6.07
Chiralcel OJ-H	12.73	3.24 (+)	26.79	7.93 (-)	2.45	5.51
Chiralpak AD-H	10.27	2.42 (-)	14.80	3.93 (+)	1.62	5.46
Chiralcel OD-H	7.73	1.58 (+)	10.66	2.55 (-)	1.62	3.13
Chiralpak IC	22.89	6.63 (-)	28.91	8.64 (+)	1.30	2.90
Sepapak-2-HR	16.09	4.36 (+)	18.04	5.01 (-)	1.15	1.44

Chiral HPLC Screening for compound **2a**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2 (min)	k_2	α	R
Chiralcel OC	24,26	7,09 (+)	32,14	9,71 (-)	1,37	2,12
Chiralcel OB-H	6,81	1,27 (-)	8,20	1,73 (+)	1,36	0,60
Chiralpak AS-H	4,96	0,65 (-)	5,63	0,88 (+)	1,35	2,06
Chiralpak AD-H	8,31	1,77 (-)	9,59	2,20 (+)	1,24	2,60
Sepapak-2-HR	11,39	2,80 (-)	12,94	3,31 (+)	1,19	2,53
Chiralcel OJ-H	14,31	3,77 (-)	16,33	4,44 (+)	1,18	2,05
Ulmo	13,59	3,53 (-)	14,41	3,80 (+)	1,08	0
Chiralcel OD-H	6,56	1,19			1	0

Chiral HPLC Screening for compound **2c**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2 (min)	k_2	α	R
Chiralcel OJ-H	14,60	3,87 (+)	25,64	7,55 (-)	1,95	5,64
Chiralpak AD-H	10,06	2,35 (-)	16,54	4,51 (+)	1,92	8,81
Chiralpak AS-H	6,91	1,30 (-)	10,44	2,48 (+)	1,90	5,52
Sepapak-2-HR	16,80	4,60 (-)	21,30	6,10 (+)	1,33	4,18
Chiralcel OD-H	7,66	1,55 (+)	8,82	1,94 (-)	1,25	1,47
Chiralcel OD-H*	11,09	2,70 (+)	13,07	3,36 (-)	1,25	1,66
Chiralcel OB-H	11,75	2,92 (+)	13,88	3,63 (-)	1,24	0
Chiralpak IC	18,64	5,51 (-)	22,15	6,38 (+)	1,22	2,06

* Mobile phase: hexane/ethanol (70/30)

Chiral HPLC Screening for compound **2f**

Mobile phase: hexane/ethanol (50/50);

Flow: 1 mL/min;

Temperature: 25 °C;

UV detection at 254 nm

Sign determined by on-line circular dichroism at 254 nm

Column	Rt_1 (min)	k_1	Rt_2 (min)	k_2	α	R
Chiralpak AD-H	9,89	2,30 (-)	13,84	3,61 (+)	1,57	6,04
Chiralcel OD-H	6,49	1,16 (+)	7,79	1,60 (-)	1,37	2,38
Chiralcel OB-H	10,21	2,40 (-)	12,57	3,19 (+)	1,33	0,44
Chiralpak AS-H	5,26	0,75 (+)	5,94	0,98 (-)	1,30	1,83
Chiralpak IC	12,47	3,16 (+)	15,08	4,03 (-)	1,28	2,98
Sepapak-2-HR	13,05	3,35 (+)	14,64	3,88 (-)	1,16	2,28
Whelk	29,32	8,77 (+)	33,33	10,11 (-)	1,15	1,02
Chiralcel OJ-H	21,99	6,33			1	0
Ulmo	13,96	3,65			1	0

Enantiomerization kinetics of compound **1a**

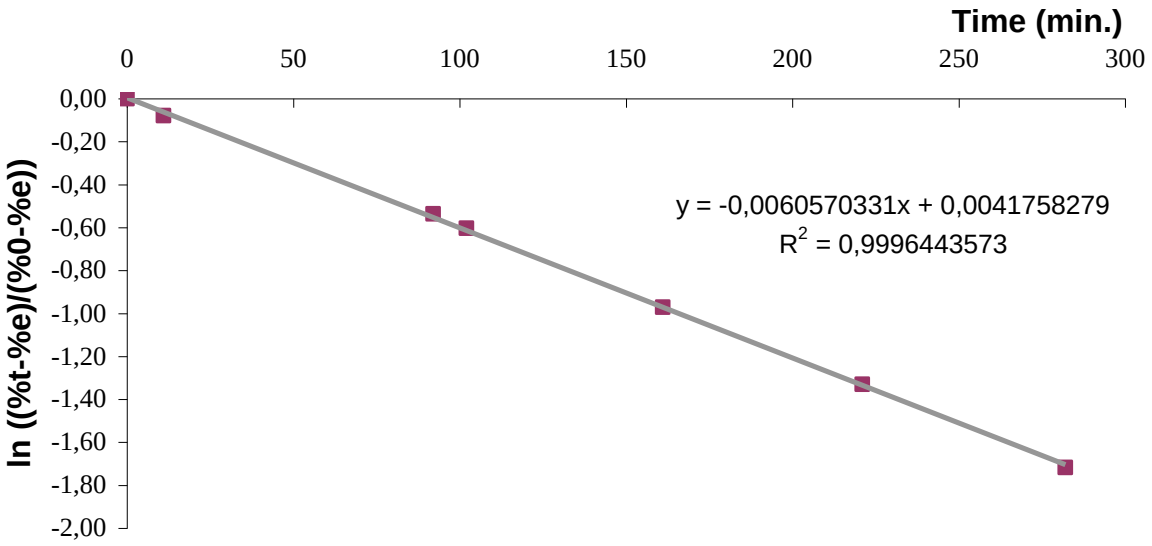
About 2 mg of an enriched sample of one of the enantiomers of **1a** is heated in about 10 mL of ethanol at 30 °C. 20 µL are taken and then injected at different time intervals on 3-Cellucoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **1a**	ln ((%t-%e)/(%0-%e))
0	72,736	0,0000
11	71,023	-0,0783
92	63,299	-0,5363
102	62,447	-0,6025
161	58,610	-0,9710
221	56,014	-1,3299
282	54,086	-1,7164

k_{rot}= 5.0475 x 10-5 s^{-1} (30°C)

$\Delta G^{\neq}_{rot}$ = 99.23 KJ/mol (30°C)

$t_{1/2}$= 1.91 hs (30°C)



Enantiomerization kinetics of compound **1c**

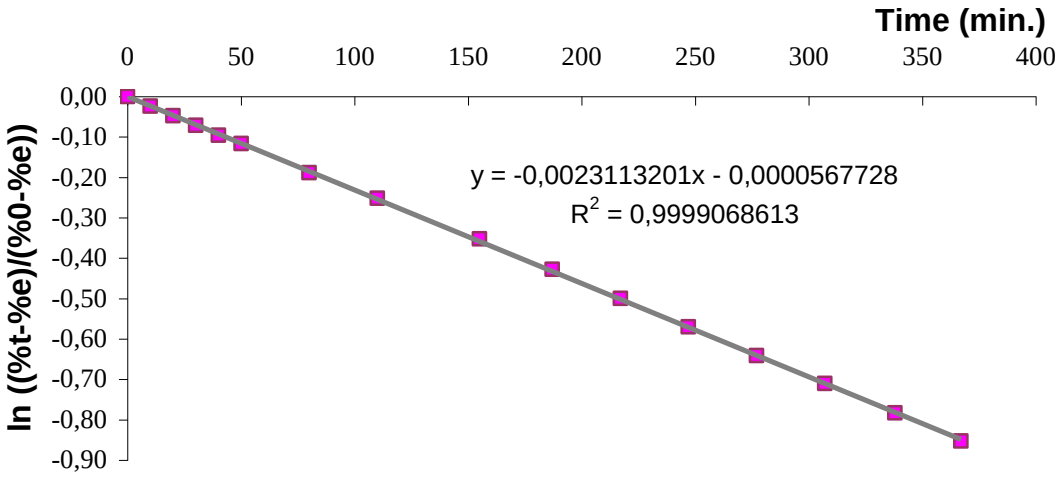
About 2 mg of an enriched sample of one of the enantiomers of **1b** is heated in about 10 mL of ethanol at 40 °C. 20 µL are taken and then injected at different time intervals on 3-Amycoat (ethanol, 0.7 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **1c**	ln ((%t-%e)/(%0-%e))
0	88,688	0,0000
10	87,770	-0,0240
20	86,904	-0,0472
30	86,042	-0,0708
40	85,168	-0,0954
50	84,441	-0,1163
80	82,047	-0,1883
110	80,085	-0,2515
155	77,199	-0,3523
187	75,227	-0,4276
217	73,481	-0,4993
247	71,889	-0,5695
277	70,379	-0,6410
307	69,022	-0,7099
338	67,687	-0,7827
367	66,488	-0,8529

k_{rot}= 1.9261 x 10-5 s^{-1} (40°C)

$\Delta G^{\neq}_{rot}$ = 105.10 KJ/mol (40°C)

$t_{1/2}$= 5.00 hs (40°C)



Enantiomerization kinetics of compound **1d**

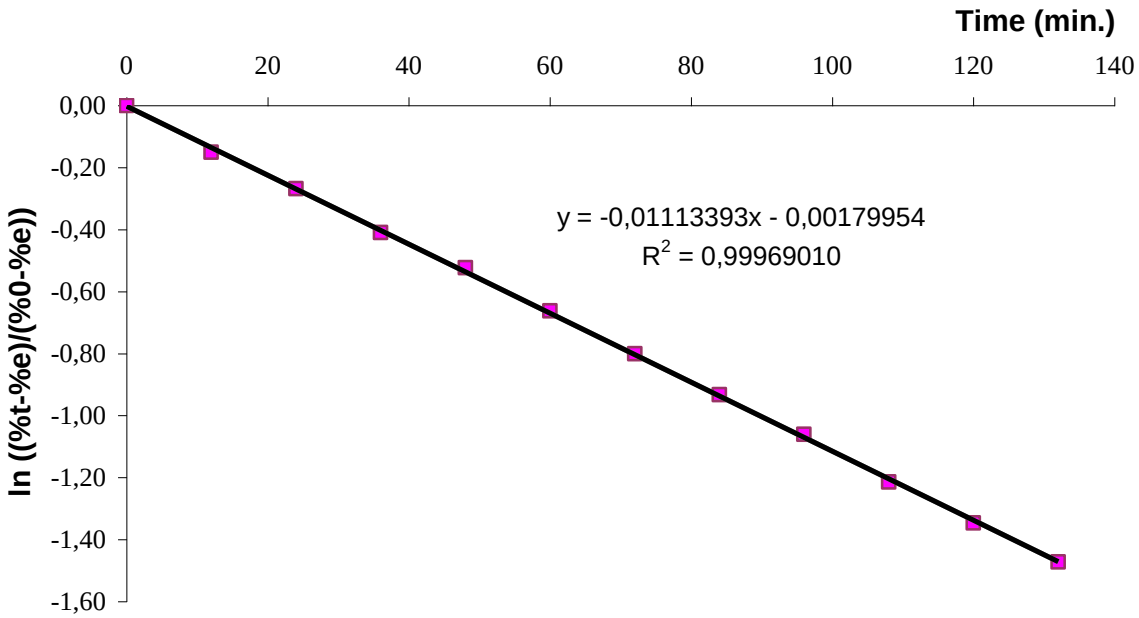
About 2 mg of an enriched sample of one of the enantiomers of **1c** is heated in about 10 mL of ethanol at 78 °C. 20 µL are taken and then injected at different time intervals on 3-Amycoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **1d**	ln ((%t-%e)/(%0-%e))
0	98,423	0,0000
12	91,674	-0,1501
24	87,049	-0,2677
36	82,155	-0,4094
48	78,702	-0,5230
60	74,959	-0,6627
72	71,751	-0,8003
84	69,053	-0,9328
96	66,766	-1,0606
108	64,381	-1,2141
120	62,598	-1,3464
132	61,106	-1,4725

k_{rot}= 9.2783 x 10-5 s^{-1} (78°C)

$\Delta G^{\neq}_{rot}$ = 113.59 KJ/mol (78°C)

$t_{1/2}$= 1.04 hs (78°C)



Enantiomerization kinetics of compound **1e**

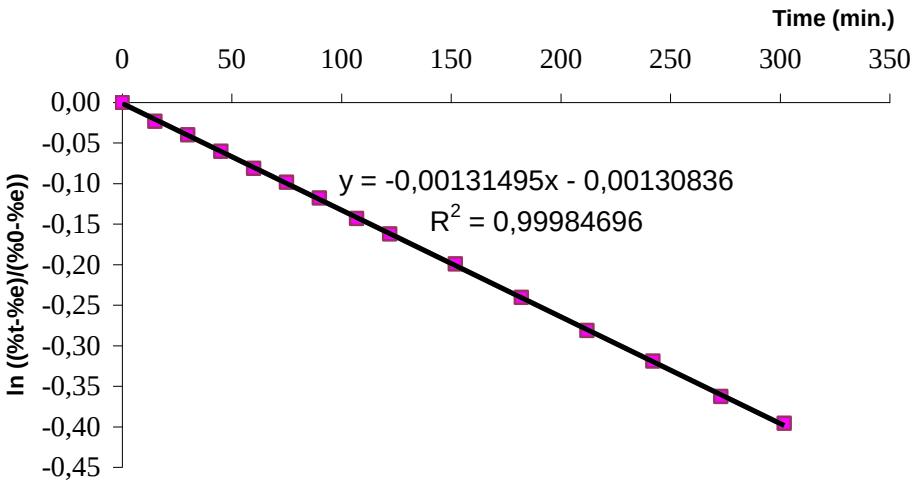
About 2 mg of an enriched sample of one of the enantiomers of **1d** is heated in about 10 mL of ethanol at 50 °C. 20 µL are taken and then injected at different time intervals on 3-Amycoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **1e**	ln ((%t-%e)/(%0-%e))
0	96,280	0,0000
15	95,209	-0,0234
30	94,462	-0,0401
45	93,575	-0,0602
60	92,657	-0,0815
75	91,932	-0,0987
90	91,127	-0,1180
107	90,103	-0,1433
122	89,345	-0,1623
152	87,916	-0,1993
182	86,381	-0,2407
212	84,926	-0,2815
242	83,628	-0,3194
273	82,194	-0,3629
302	81,149	-0,3959
334	79,810	-0,4399
362	78,685	-0,4783
392	77,590	-0,5173

k_{rot}= 1.0958 x 10-5 s^{-1} (50°C)

$\Delta G^{\neq}_{rot}$ = 110.05 KJ/mol (50°C)

$t_{1/2}$= 8.79 hs (50°C)


Time (min.)
0
50
100
150
200
250
300
350
0,00
-0,05
-0,10
-0,15
-0,20
-0,25
-0,30
-0,35
-0,40
-0,45
ln ((%t-%e)/(%0-%e))
y = -0,00131495x - 0,00130836
R2 = 0,99984696

Enantiomerization kinetics of compound **1f**

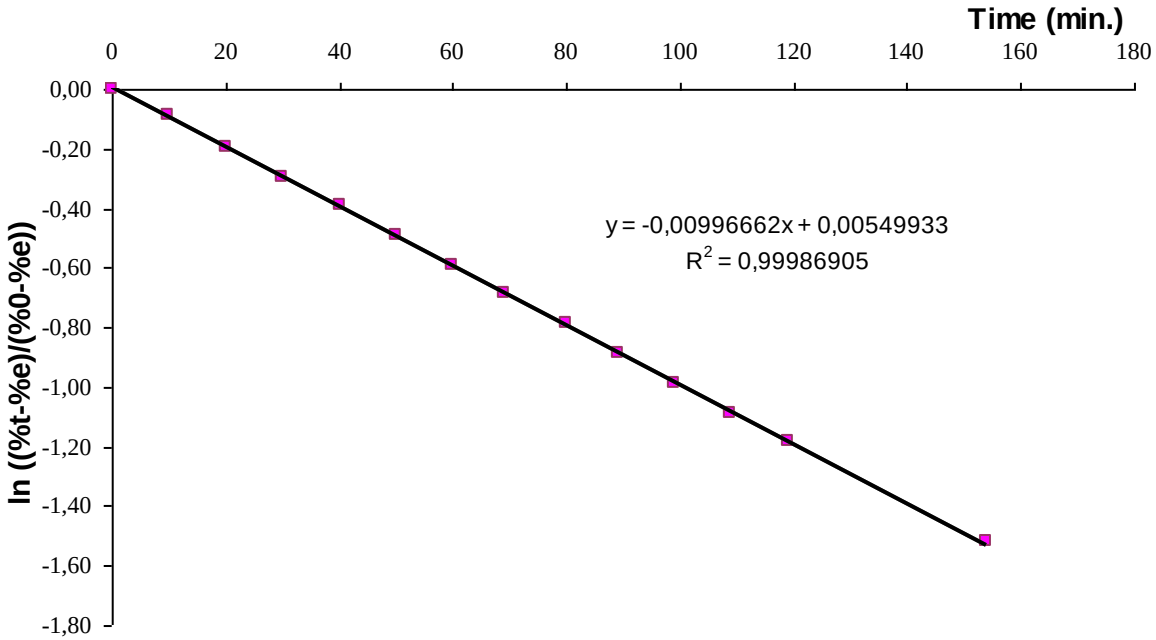
About 2 mg an enriched sample of one of the enantiomers of **1e** is heated in about 10 mL of ethanol at 50 °C. 20 µL are taken and then injected at different time intervals on 3-Amycoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **1f**	ln ((%t-%e)/(%0-%e))
0	89,809	0,0000
10	86,448	-0,0882
20	82,820	-0,1931
30	79,670	-0,2940
40	76,933	-0,3907
50	74,419	-0,4887
60	72,097	-0,5887
69	70,019	-0,6874
80	68,111	-0,7876
89	66,408	-0,8863
99	64,849	-0,9862
109	63,418	-1,0875
119	62,187	-1,1837
154	58,707	-1,5200

k_{rot}= 8.3055 x 10-5 s^{-1} (50°C)

$\Delta G^{\neq}_{rot}$ = 104.61 KJ/mol (50°C)

$t_{1/2}$= 1.16 hs (50°C)



Enantiomerization kinetics of compound **2c**

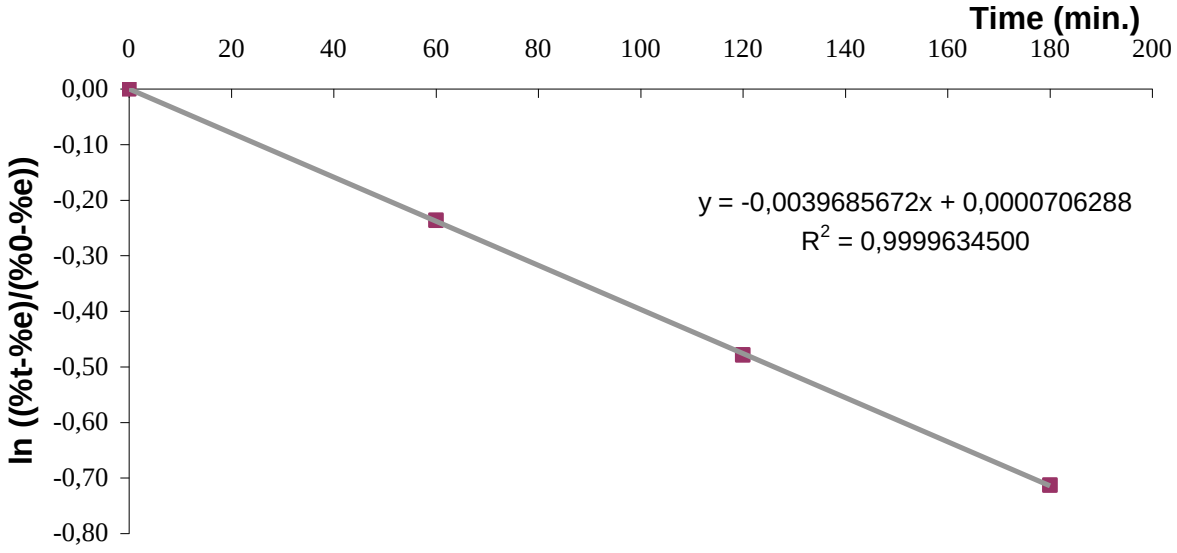
About 2 mg an enriched sample of one of the enantiomers of **2b** is heated in about 10 mL of ethanol at 30 °C. 20 µL are taken and then injected at different time intervals on 3-Amycoat (ethanol, 0.7 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **2c**	ln ((%t-%e)/(%0-%e))
0	60,782	0,0000
60	58,510	-0,2366
120	56,680	-0,4788
180	55,285	-0,7130

k_{rot}= 3.3071 x 10-5 s^{-1} (30°C)

$\Delta G^{\neq}_{rot}$ = 100.30 KJ/mol (30°C)

$t_{1/2}$= 2.91 hs (30°C)



Enantiomerization kinetics of compound **2d**

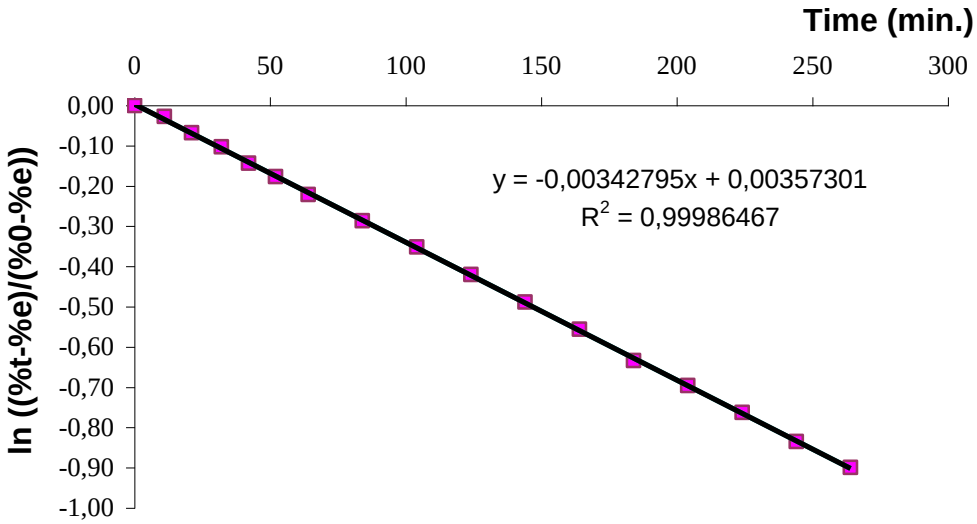
About 2 mg of an enriched sample of one of the enantiomers of **2c** is heated in about 10 mL of ethanol at 50 °C. 20 µL are taken and then injected at different time intervals on Cellucoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **2d**	ln ((%t-%e)/(%0-%e))
0	81,402	0,0000
11	80,563	-0,0271
21	79,347	-0,0677
32	78,338	-0,1027
42	77,207	-0,1434
52	76,315	-0,1767
64	75,171	-0,2212
84	73,596	-0,2858
104	72,106	-0,3510
124	70,636	-0,4198
144	69,280	-0,4878
164	68,009	-0,5560
184	66,667	-0,6334
204	65,661	-0,6957
224	64,653	-0,7622
244	63,624	-0,8350
264	62,776	-0,8993

k_{rot}= 2.8566 x 10-5 s^{-1} (50°C)

$\Delta G^{\neq}_{rot}$ = 107.48 KJ/mol (50°C)

$t_{1/2}$= 3.37 hs (50°C)



Enantiomerization kinetics of compound **2e**

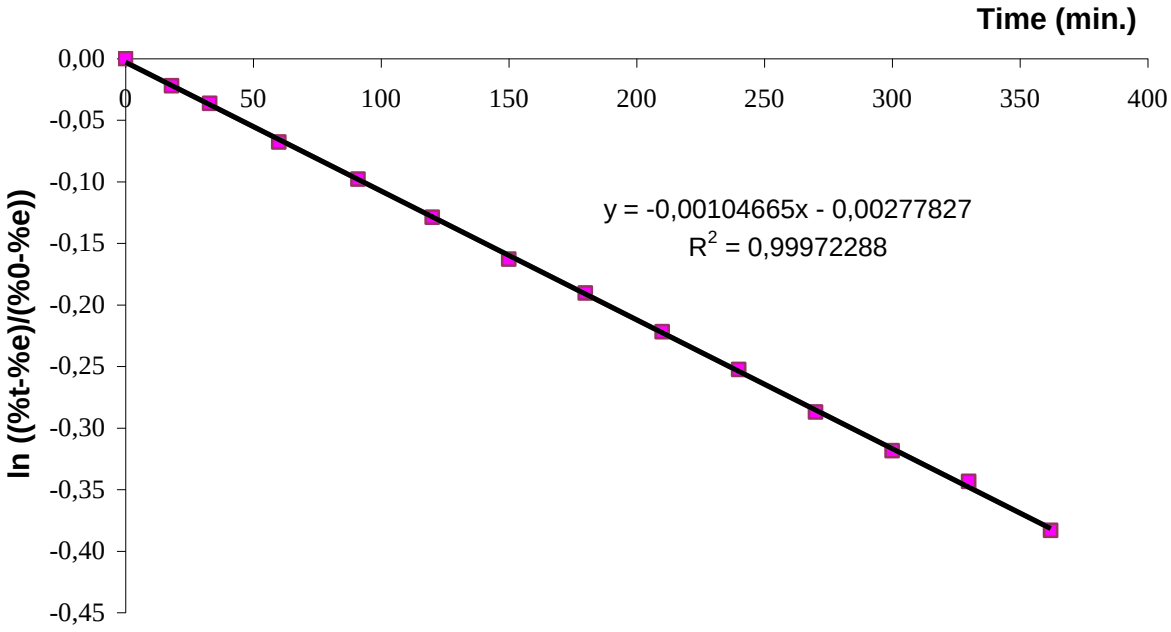
About 2 mg an enriched sample of one of the enantiomers of **2d** is heated in about 10 mL of ethanol at 40 °C. 20 µL are taken and then injected at different time intervals on Cellucoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **2e**	ln ((%t-%e)/(%0-%e))
0	81,271	0,0000
18	80,586	-0,0221
33	80,152	-0,0364
60	79,219	-0,0679
91	78,356	-0,0979
120	77,490	-0,1289
150	76,573	-0,1628
180	75,847	-0,1905
210	75,051	-0,2218
240	74,290	-0,2526
270	73,467	-0,2871
300	72,741	-0,3185
330	72,181	-0,3435
362	71,316	-0,3832

k_{rot}= 8.7221 x 10-5 s^{-1} (40°C)

$\Delta G^{\neq}_{rot}$ = 106.81 KJ/mol (40°C)

$t_{1/2}$= 11.04 hs (40°C)



Enantiomerization kinetics of compound **2f**

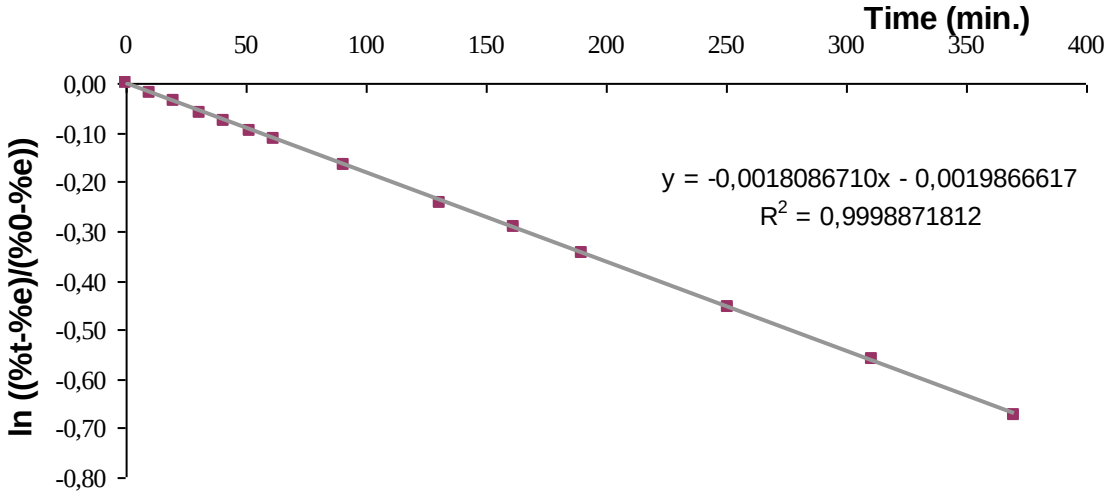
About 2 mg of an enriched sample of one of the enantiomers of **2e** is heated in about 10 mL of ethanol at 30 °C. 20 µL are taken and then injected at different time intervals on 3-Cellucoat (hexane:ethanol 50:50, 1 mL/min, UV 254 nm). The decreasing of the percentage of the enantiomer is monitored.

Time (min.)	% enantiomer **2f**	ln ((%t-%e)/(%0-%e))
0	97,763	0,0000
10	96,853	-0,0192
20	96,013	-0,0373
31	95,024	-0,0591
41	94,197	-0,0776
52	93,328	-0,0975
62	92,616	-0,1140
91	90,433	-0,1666
131	87,425	-0,2439
162	85,637	-0,2929
190	83,840	-0,3446
251	80,356	-0,4533
311	77,234	-0,5618
370	74,328	-0,6746

k_{rot}= 1.5072 x 10-5 s^{-1} (30°C)

$\Delta G^{\neq}_{rot}$ = 102.28 KJ/mol (30°C)

$t_{1/2}$= 6.39 hs (30°C)



Crystallographic data for compound 1a

Molecular formula: C18 H17 N3 O. Monoclinic, space group P 2_1/c, a = 12.5837(18), b = 7.4112(9), c = 15.4940(14), beta = 97.412(10), V = 1432.9(3) Å^3, T = 293(2) °K, Z = 4, dens$_c$ = 1.351g cm^{-3}, F(000) = 616, graphite-monochromated MoKα radiation (λ = 0.71073 Å), μ(MoKα) = 0.086mm$_{-1}$, colorless plate (0.5 × 0.4 × 0.4 mm^3), multi-scan empirical absorption correction with CrysAlisPro (transmission factors: 0.81789– 1.0), 233 frames, exposure time 10 s, 3.79 ≤ θ ≤ 28.92, –16≤ h ≤ 14, –9 ≤ k ≤ 5, –20 ≤ l ≤ 12, 10212 reflections collected, 10212 independent (R_{int} = 0.0), solution by direct methods (SHELXS97) and subsequent Fourier syntheses, full-matrix least squares on F_0^2 (SHELX97), hydrogen atoms refined with a riding model, data / restraints / parameters = 10212/ 0 / 201, $S(F^2)$ = 0.923, $R(F)$ = 0.2127 and $wR(F^2)$ = 0.2629 on all data, $R(F)$ = 0.0770 and $wR(F^2)$ = 0.2008 for 3480 reflections with $F_0 >$ 4σ(F_0), weighting scheme w = 1/[σ^2(F_0^2) + (0.1236P)^2 + 0.0000P] where P = (F_0^2 + 2F_c^2)/3, largest difference peak and hole 0.598 and -0.301e Å^{-3}. The crystal structure contains one independent molecule in the asymmetric unit. Data reduction was performed considering a twin model from two different individuals in a ratio 0.78/0.22, 4667/4603 isolated reflection from first and second individual respectively and 1497 overlapped reflections.

CCDC-978882 CIF file contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Calculations were carried out using the GAUSSIAN 03 suite of programs.[1]

Compound 1a: Ground State Conformation

Method: b3lyp/6-31+g(d,p)

SCF Done: E(RB+HF-LYP) = -935.633090698 A.U. after 15 cycles

Imaginary frequencies = 0 (35.6)

Zero-point correction= 0.317274 (Hartree/Particle)

Thermal correction to Energy= 0.334815

Thermal correction to Enthalpy= 0.335759

Thermal correction to Gibbs Free Energy= 0.271717

Sum of electronic and zero-point Energies= -935.315788

Sum of electronic and thermal Energies= -935.298247

Sum of electronic and thermal Enthalpies= -935.297303

Sum of electronic and thermal Free Energies= -935.361345

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007554	0.008927	-0.008898
2	7	0	-0.012433	0.036661	1.280663
3	6	0	2.474604	0.007166	-0.189177
4	6	0	2.385600	-0.565873	1.221290
5	6	0	1.256611	0.127425	1.982081
6	7	0	1.145165	0.062372	-0.818693
7	6	0	1.046804	0.265454	-2.189193
8	6	0	-0.216938	0.238872	-2.811063
9	6	0	-1.303146	-0.099570	-0.693553
10	7	0	-1.392219	-0.000469	-2.020439
11	6	0	2.170935	0.505378	-3.004888
12	6	0	2.021664	0.696710	-4.376845
13	6	0	0.758508	0.656639	-4.975851
14	6	0	-0.363331	0.427010	-4.185080
15	6	0	-2.542096	-0.337720	0.089331
16	6	0	-2.680113	-1.559625	0.762636
17	6	0	-3.828058	-1.846825	1.498517
18	6	0	-4.846227	-0.894921	1.579686
19	6	0	-4.704456	0.329583	0.925258
20	6	0	-3.562603	0.633181	0.171777
21	6	0	-3.443170	1.966184	-0.523472
22	8	0	-2.502585	-0.098439	-2.649701
23	1	0	3.119451	-0.621959	-0.810209
24	1	0	2.910283	1.015841	-0.168696
25	1	0	3.350883	-0.435352	1.722194
26	1	0	2.183179	-1.642509	1.172265
27	1	0	1.507377	1.188386	2.144299
28	1	0	1.128649	-0.312608	2.976940
29	1	0	3.160990	0.556091	-2.571269
30	1	0	2.905255	0.882807	-4.980195
31	1	0	0.649113	0.804881	-6.044892

32	1	0	-1.364743	0.382613	-4.593952
33	1	0	-1.877664	-2.288395	0.705500
34	1	0	-3.923445	-2.802155	2.006066
35	1	0	-5.745298	-1.101350	2.153698
36	1	0	-5.495444	1.071800	0.997728
37	1	0	-4.254983	2.636079	-0.226803
38	1	0	-2.495566	2.461626	-0.282364
39	1	0	-3.482990	1.831573	-1.610741

Compound 1a: TS1 Conformation

Method: b3lyp/6-31+g(d,p)

SCF Done: E(RB+HF-LYP) = -935.599458362 A.U. after 11 cycles

Imaginary frequencies = 1 (-60.6)

Zero-point correction= 0.317708 (Hartree/Particle)

Thermal correction to Energy= 0.334024

Thermal correction to Enthalpy= 0.334968

Thermal correction to Gibbs Free Energy= 0.274542

Sum of electronic and zero-point Energies= -935.281750

Sum of electronic and thermal Energies= -935.265434

Sum of electronic and thermal Enthalpies= -935.264490

Sum of electronic and thermal Free Energies= -935.324917

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.196782	1.003031	0.349182
2	7	0	-0.254860	1.981273	1.032375
3	6	0	1.981832	2.342024	-0.763253
4	6	0	1.005012	3.475193	-0.471468
5	6	0	0.416932	3.270775	0.926807
6	7	0	1.393482	1.040831	-0.403858
7	6	0	2.216584	-0.074991	-0.326094
8	6	0	1.718764	-1.237835	0.294880
9	6	0	-0.516799	-0.311622	0.355864
10	7	0	0.315751	-1.347160	0.608399
11	6	0	3.545288	-0.080383	-0.789201
12	6	0	4.352938	-1.198798	-0.592404
13	6	0	3.859159	-2.330595	0.064844
14	6	0	2.536694	-2.350986	0.498902
15	6	0	-1.969430	-0.529196	0.085977
16	6	0	-2.340272	-1.862789	-0.249478
17	6	0	-3.616138	-2.229038	-0.653485
18	6	0	-4.620308	-1.267841	-0.715004
19	6	0	-4.292300	0.045496	-0.399477
20	6	0	-3.003977	0.465607	-0.017934
21	8	0	-0.056618	-2.504333	1.020535
22	1	0	2.901424	2.489881	-0.181047
23	1	0	2.258512	2.322021	-1.824033
24	1	0	0.192325	3.480695	-1.207651

25	1	0	1.529673	4.432785	-0.555465
26	1	0	1.209679	3.332202	1.688030
27	1	0	-0.310320	4.054214	1.167993
28	1	0	3.949986	0.787819	-1.293999
29	1	0	5.377702	-1.179520	-0.951350
30	1	0	4.493843	-3.196030	0.223700
31	1	0	2.099527	-3.217228	0.977852
32	1	0	-1.597357	-2.639879	-0.170479
33	1	0	-3.817378	-3.267599	-0.899079
34	1	0	-5.635987	-1.527001	-1.000020
35	1	0	-5.069472	0.801856	-0.457119
36	6	0	-2.903402	1.960026	0.216438
37	1	0	-2.526868	2.199154	1.210245
38	1	0	-2.234525	2.447058	-0.498974
39	1	0	-3.894053	2.405452	0.090811

Compound 1a: TS2 Conformation

Method: b3lyp/6-31+g(d,p)

SCF Done: E(RB+HF-LYP) = -935.597871879 A.U. after 11 cycles

Imaginary frequencies = 1 (-87.7)

Zero-point correction= 0.317823 (Hartree/Particle)

Thermal correction to Energy= 0.334203

Thermal correction to Enthalpy= 0.335147

Thermal correction to Gibbs Free Energy= 0.274311

Sum of electronic and zero-point Energies= -935.280049

Sum of electronic and thermal Energies= -935.263669

Sum of electronic and thermal Enthalpies= -935.262725

Sum of electronic and thermal Free Energies= -935.323561

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.263236	1.091079	0.369468
2	7	0	0.218945	2.090269	1.013270
3	6	0	-2.240327	2.362751	-0.481674
4	6	0	-1.326303	3.553167	-0.220464
5	6	0	-0.573817	3.310066	1.088899
6	7	0	-1.539862	1.091008	-0.232927
7	6	0	-2.261649	-0.090955	-0.269782
8	6	0	-1.633865	-1.272052	0.164819
9	6	0	0.529309	-0.180886	0.247469
10	7	0	-0.218848	-1.283627	0.435752
11	6	0	-3.609375	-0.157998	-0.670164
12	6	0	-4.302928	-1.364586	-0.598006
13	6	0	-3.676314	-2.523290	-0.127856
14	6	0	-2.337137	-2.475009	0.249762
15	6	0	2.012411	-0.168348	0.015324

16	6	0	2.528081	1.114296	-0.322594
17	6	0	3.856278	1.374503	-0.627341
18	6	0	4.775382	0.332976	-0.598969
19	6	0	4.304776	-0.943544	-0.313571
20	6	0	2.960198	-1.258457	-0.032180
21	8	0	0.257035	-2.416368	0.778285
22	1	0	-2.600373	2.364727	-1.517365
23	1	0	-3.117681	2.415666	0.176739
24	1	0	-1.928772	4.466919	-0.182522
25	1	0	-0.602768	3.669674	-1.036095
26	1	0	0.099118	4.141450	1.322021
27	1	0	-1.286903	3.236878	1.925401
28	1	0	-4.118942	0.727989	-1.026715
29	1	0	-5.343909	-1.393601	-0.906010
30	1	0	-4.222583	-3.458558	-0.065708
31	1	0	-1.802242	-3.349569	0.595826
32	1	0	1.858530	1.956065	-0.318555
33	1	0	4.158620	2.388732	-0.871030
34	1	0	5.828734	0.497262	-0.807144
35	1	0	5.015174	-1.764338	-0.324302
36	6	0	2.740289	-2.755903	0.129633
37	1	0	2.392611	-3.023017	1.126749
38	1	0	2.008519	-3.148204	-0.576049
39	1	0	3.689948	-3.265960	-0.055230

Reference

1 Gaussian 03, Revision B.01, M. J. Frisch *et al.*, 2003.