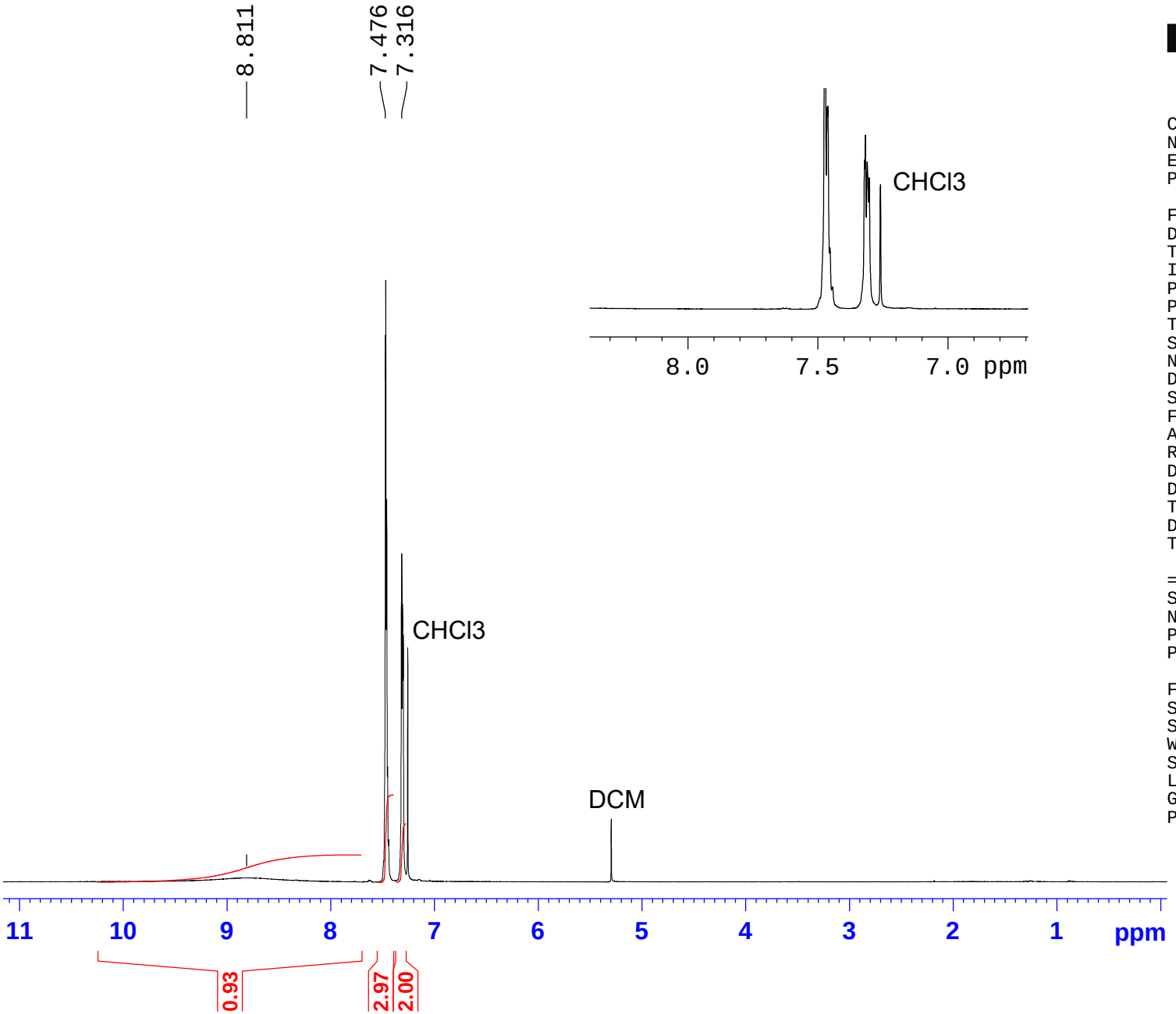
1H NMR of 3-Bromo-4-phenylisothiazole-5-carboxylic acid (12)

AK1074

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Current Data Parameters
NAME      Andreas Kalogirou
EXPNO                   554
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140107
Time                  19.03
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              10330.578 Hz
FIDRES            0.157632 Hz
AQ               3.1719425 sec
RG                      161
DW                 48.400 usec
DE                  6.50 usec
TE                  298.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          500.0361158 MHz
NUC1                     1H
P1                  11.75 usec
PLW1          15.41699982 W

F2 - Processing parameters
SI                    65536
SF            500.0330402 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
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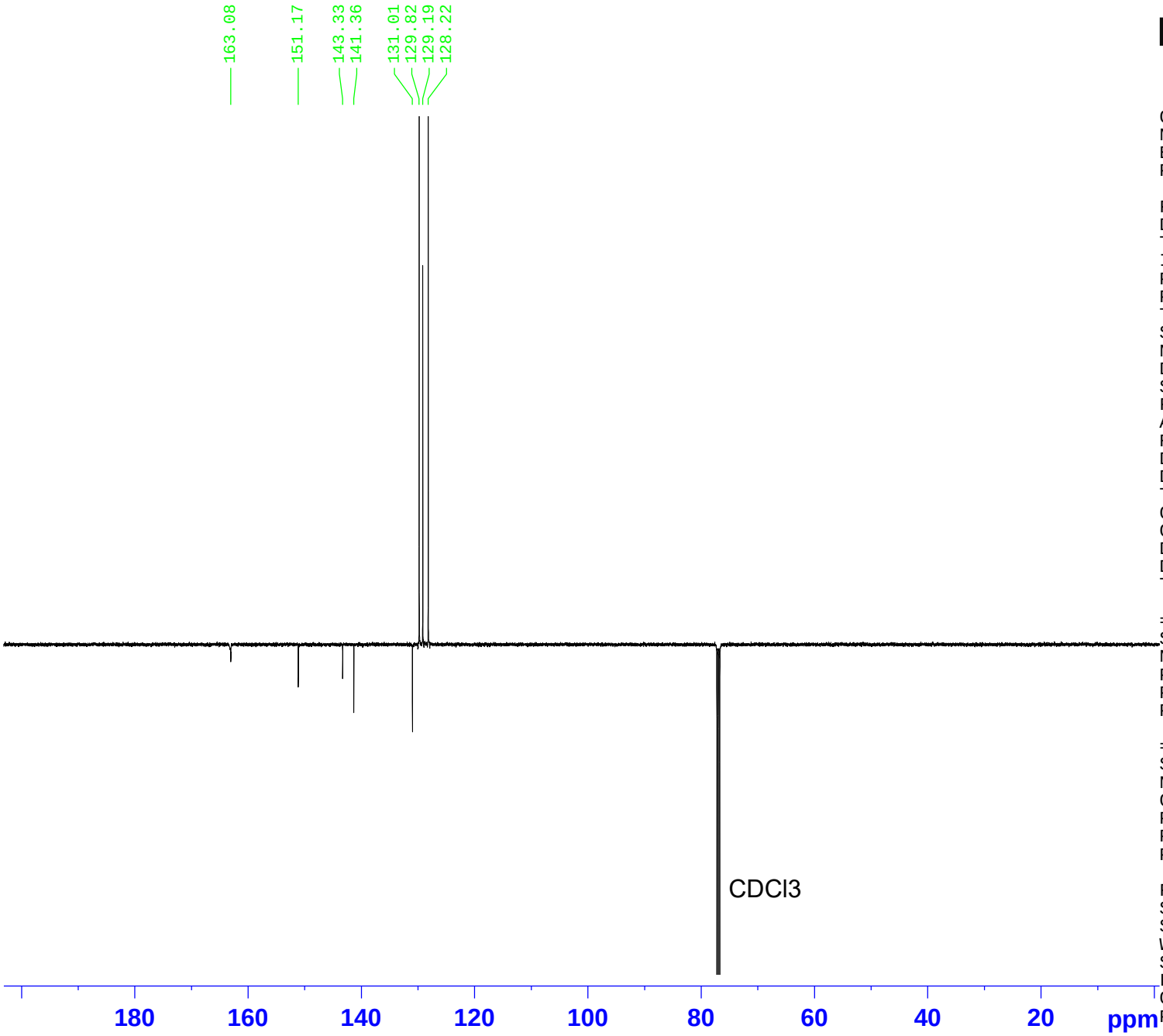
AK1074

13C NMR of 3-Bromo-4-phenylisothiazole-5-carboxylic acid (12)

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Current Data Parameters
NAME      Andreas Kalogirou
EXPNO                   555
PROCNO                    1

F2 - Acquisition Parameters
Date_           20140108
Time                9.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                 16000
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                  2050
DW                16.800 usec
DE                 6.50 usec
TE                 297.1 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7459782 MHz
NUC1                 13C
P1                  8.70 usec
P2                 17.40 usec
PLW1        138.00000000 W

======== CHANNEL f2 ========
SFO2         500.0350280 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          15.41699982 W
PLW12          0.33258000 W

F2 - Processing parameters
SI                  32768
SF           125.7334070 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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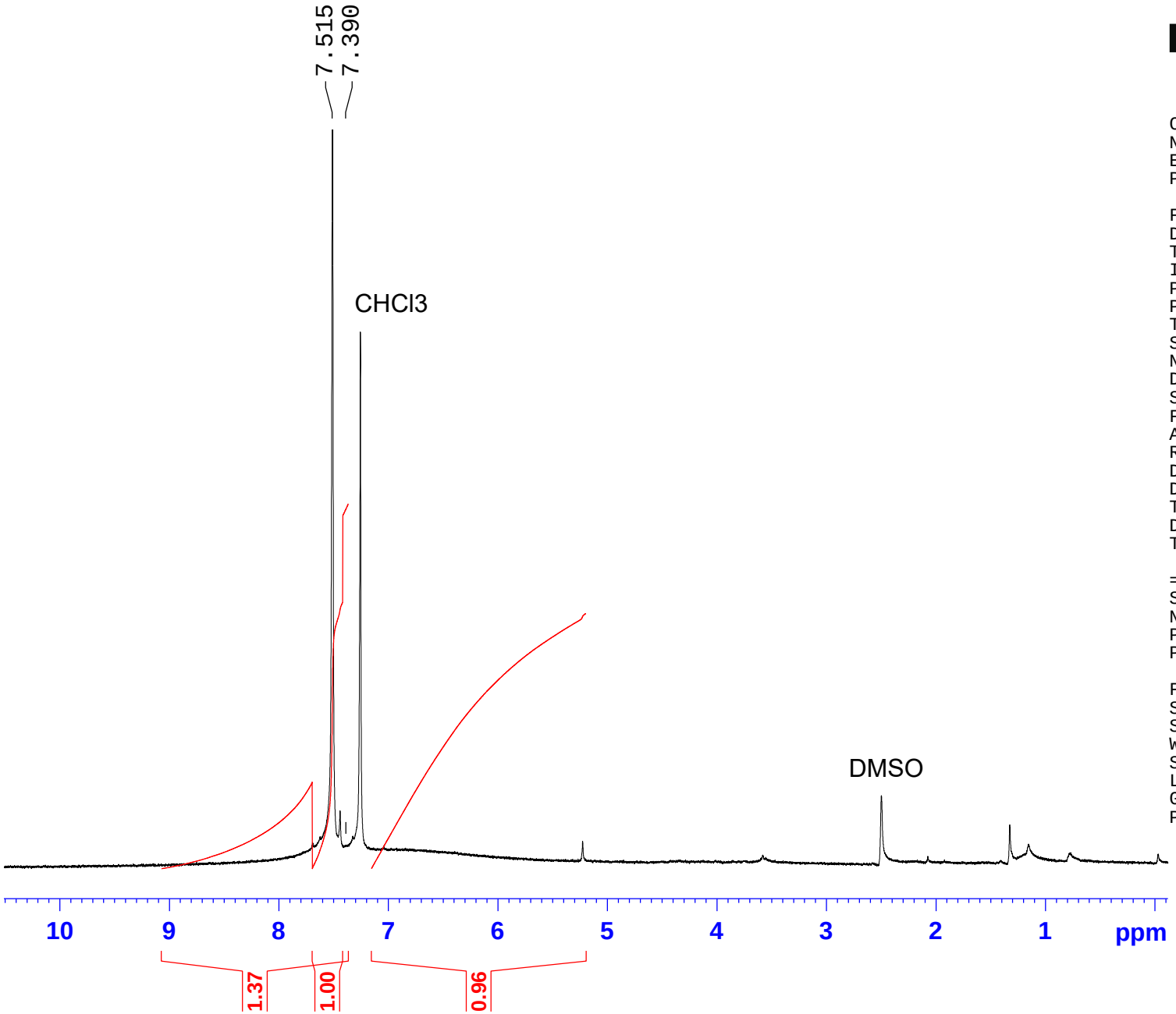
AK110

1H NMR of 3-Bromoisothiazole-5-carboxylic acid (13)

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Current Data Parameters
NAME      Andreas Kalogirou
EXPNO                   591
PROCNO                    1

F2 - Acquisition Parameters
Date_           20140204
Time               15.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                   181
DW                48.400 usec
DE                 6.50 usec
TE                297.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.0361158 MHz
NUC1                   1H
P1                 11.75 usec
PLW1         15.41699982 W

F2 - Processing parameters
SI                 65536
SF           500.0330401 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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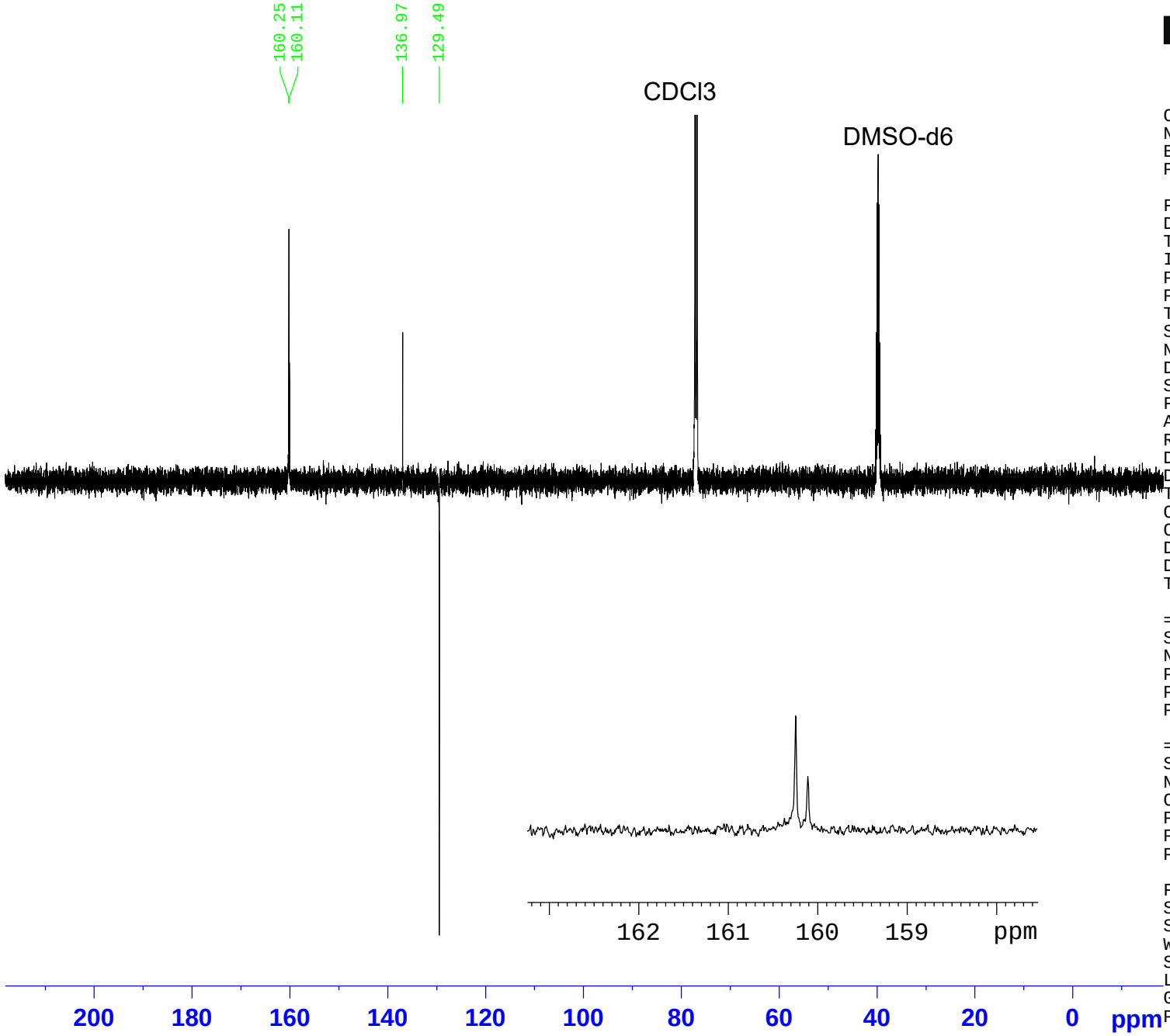
AK110

13C NMR of 3-Bromoisothiazole-5-carboxylic acid (13)

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Current Data Parameters
NAME      Andreas Kalogirou
EXPNO                   592
PROCNO                    1

F2 - Acquisition Parameters
Date_           20140204
Time               18.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             jmod
TD                 65536
SOLVENT            CDCl3
NS                  3877
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                  2050
DW                16.800 usec
DE                 6.50 usec
TE                 299.5 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7459782 MHz
NUC1                13C
P1                 8.70 usec
P2                17.40 usec
PLW1       138.00000000 W

======== CHANNEL f2 ========
SFO2         500.0350280 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.41699982 W
PLW12         0.33258000 W

F2 - Processing parameters
SI                 32768
SF           125.7334278 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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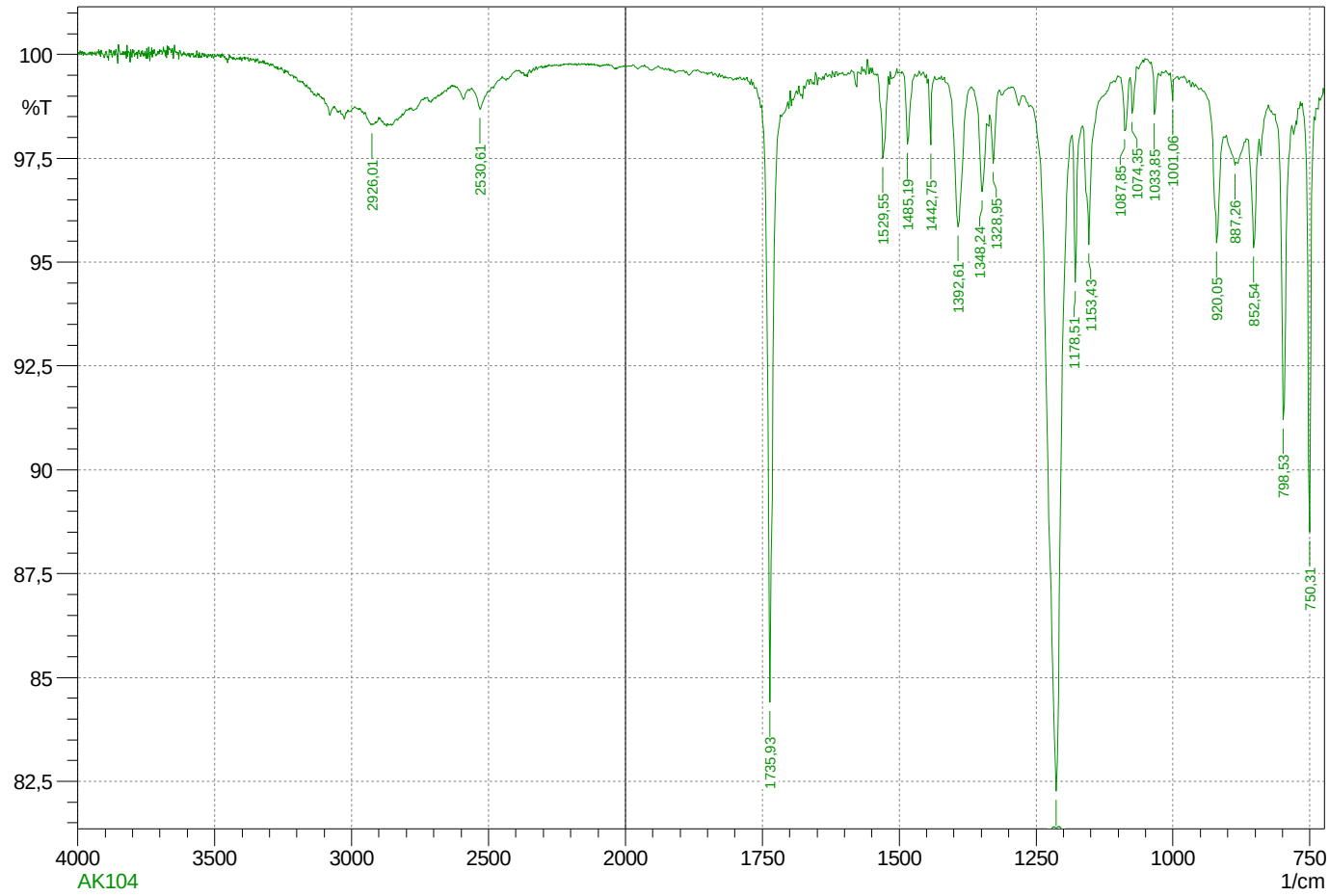
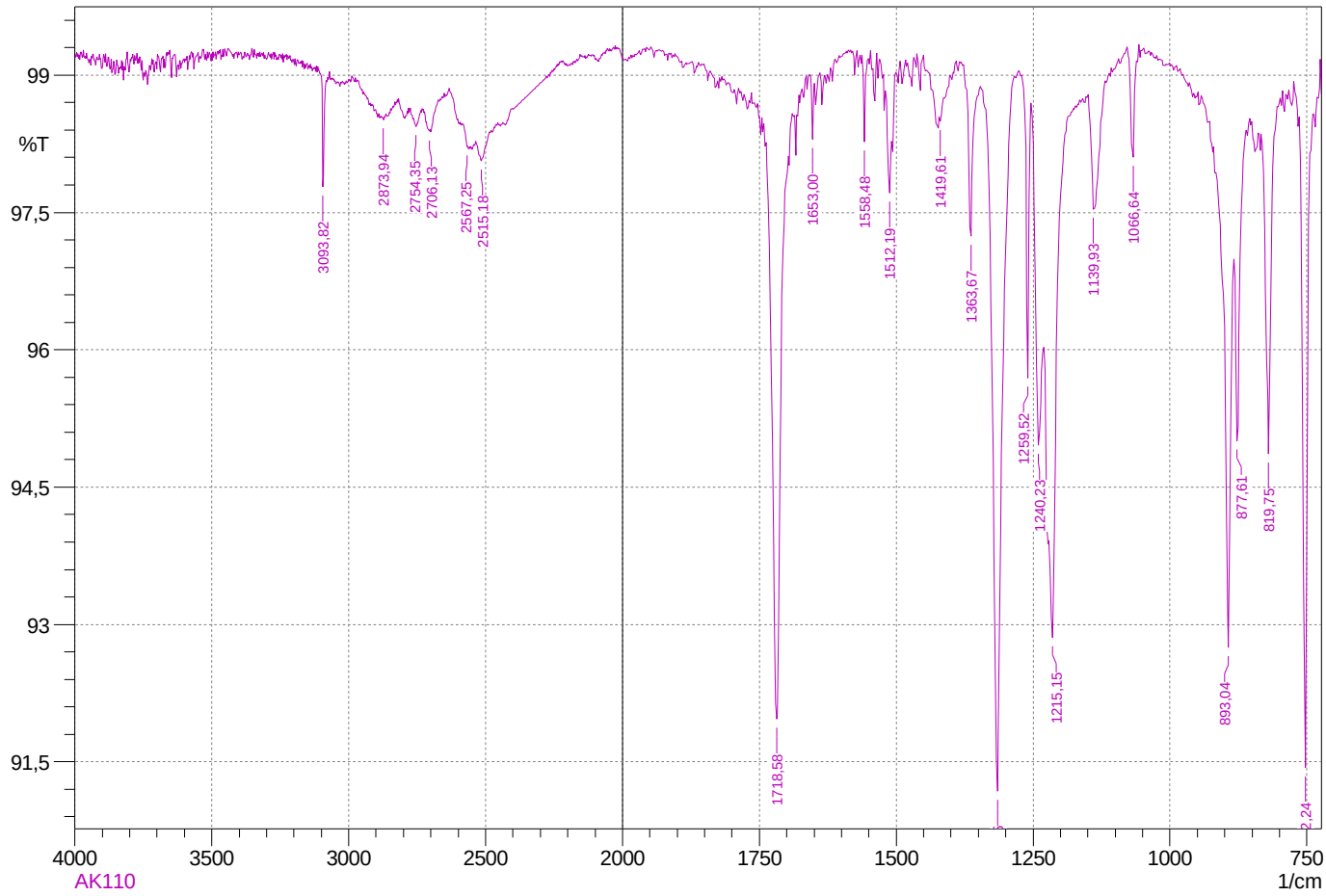
IR of 3-Bromo-4-phenylisothiazole-5-carboxylic acid (12)



	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	750,31	88,497	10,267	763,81	738,74	0,444	0,308
2	798,53	91,194	7,232	813,96	783,1	0,527	0,314
3	852,54	95,342	2,442	862,18	844,82	0,257	0,088
4	887,26	97,331	0,69	902,69	866,04	0,379	0,06
5	920,05	95,458	2,891	948,98	908,47	0,382	0,135
6	1001,06	98,889	0,646	1004,91	991,41	0,039	0,01
7	1033,85	98,557	1,149	1039,63	1026,13	0,043	0,025
8	1074,35	98,573	0,969	1078,21	1066,64	0,044	0,023
9	1087,85	98,164	1,307	1101,35	1078,21	0,098	0,045
10	1153,43	95,423	3,1	1165	1114,86	0,399	0,141
11	1178,51	94,512	3,601	1184,29	1166,93	0,228	0,087
12	1213,23	82,257	16,025	1257,59	1186,22	2,451	1,94
13	1328,95	97,378	1,367	1334,74	1317,38	0,128	0,04
14	1348,24	96,692	1,887	1367,53	1340,53	0,227	0,079
15	1392,61	95,854	3,418	1411,89	1369,46	0,381	0,245
16	1442,75	97,816	1,61	1446,61	1435,04	0,055	0,026
17	1485,19	97,841	1,721	1494,83	1471,69	0,105	0,061
18	1529,55	97,496	2	1539,2	1519,91	0,122	0,08
19	1735,93	84,406	14,422	1761,01	1716,65	0,936	0,714
20	2530,61	98,687	0,474	2555,68	2490,1	0,297	0,06
21	2926,01	98,306	0,156	2951,09	2912,51	0,272	0,017

IR of 3-Bromoisothiazole-5-carboxylic acid (13)



	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	752,24	91,4354	7,1251	763,81	738,74	0,4436	0,2858
2	819,75	94,8601	3,6383	833,25	804,32	0,3565	0,1676
3	877,61	95,0039	2,338	883,4	860,25	0,3083	0,0736
4	893,04	92,7471	4,5651	920,05	883,4	0,613	0,2266
5	1066,64	98,1024	1,1022	1078,21	1060,85	0,0938	0,0356
6	1139,93	97,5342	1,3017	1149,57	1118,71	0,2439	0,0906
7	1215,15	92,8591	1,6731	1220,94	1176,58	0,6412	-0,0955
8	1240,23	94,9565	2,1813	1253,73	1230,58	0,3693	0,0994
9	1259,52	95,6905	3,105	1271,09	1253,73	0,1542	0,0666
10	1315,45	91,1764	7,757	1346,31	1284,59	0,9606	0,6731
11	1363,67	97,2426	1,7665	1377,17	1346,31	0,2075	0,0721
12	1419,61	98,4964	0,1011	1421,54	1413,82	0,0475	0,0019
13	1512,19	97,7103	0,7523	1519,91	1508,33	0,0896	0,0164
14	1558,48	98,2702	0,938	1562,34	1550,77	0,0533	0,013
15	1653	98,2968	0,6522	1658,78	1649,14	0,0512	0,0073
16	1718,58	91,9678	6,2265	1737,86	1697,36	0,781	0,4599
17	2515,18	98,0631	0,1788	2532,54	2499,75	0,2671	0,0146
18	2567,25	98,2205	0,03	2582,68	2565,33	0,1256	-0,0001
19	2706,13	98,3824	0,0591	2723,49	2702,27	0,1437	0,0049
20	2754,35	98,442	0,0475	2763,99	2750,49	0,0902	0,0016
21	2873,94	98,5128	0,0318	2875,86	2868,15	0,0496	0,0006
22	3093,82	97,783	1,2141	3107,32	3080,32	0,154	0,0358