

Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
This journal is (c) The Royal Society of Chemistry 2008

## Supporting information

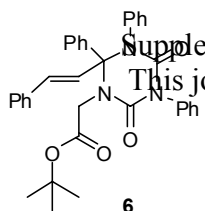
### **Generation of molecular diversity using a complexity-generating MCR-platform towards triazinanediones.**

Bas Groenendaal, Eelco Ruijter, Frans J.J. de Kanter, Martin Lutz, Anthony L. Spek and Romano V.A. Orru\*

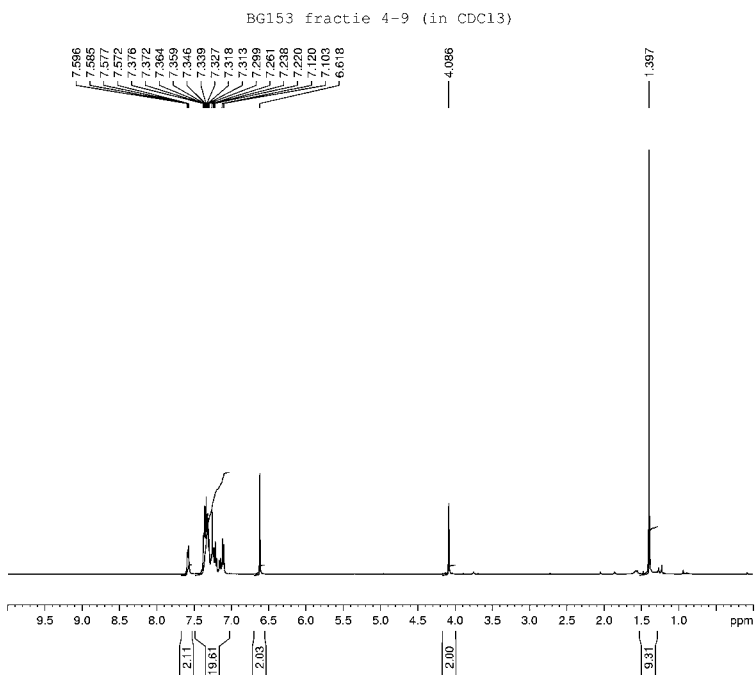
*Department of Chemistry, Vrije Universiteit Amsterdam, De Boelelaan 1083, 1081 HV, Amsterdam, The Netherlands*

[orru@few.vu.nl](mailto:orru@few.vu.nl)

<sup>1</sup>H and <sup>13</sup>C-NMR spectra of all new compounds.



Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008

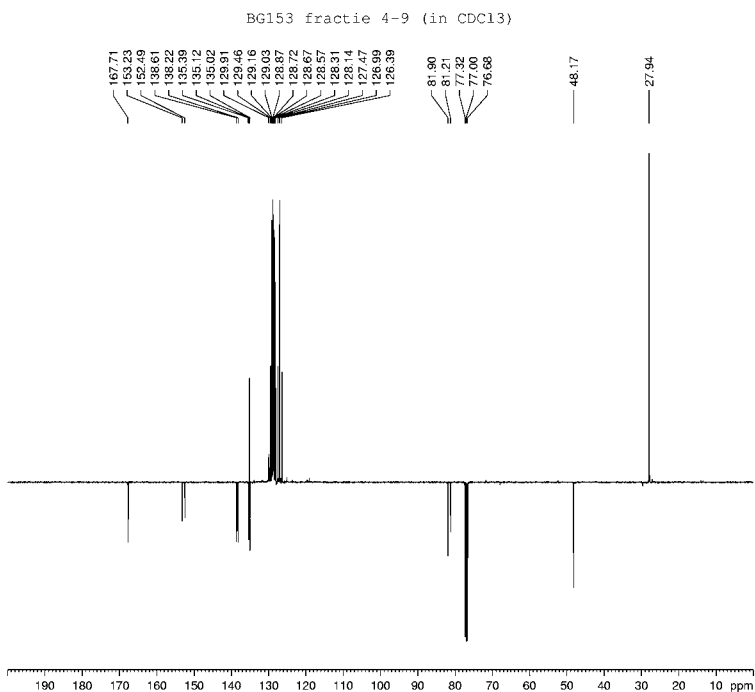


Current Data Parameters  
 NAME: BG153  
 EXNO: 7  
 PRGNO: 1

F2 Acquisitor Parameters  
 Date\_: 20070227  
 Time: 16.42  
 NS: 654  
 DS: 4  
 SWH: 6602.641 Hz  
 FIDRES: 0.085540 Hz  
 AQ: 0.0000000 sec  
 RG: 32.0  
 DW: 09.400 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 D1: 1.0000000 sec  
 D2: 1.0000000 sec  
 D3: 1.0000000 sec

CHANNEL F1  
 NU1: 10  
 P1: 14.00 usec  
 PL1: 0.00 dB  
 SFO1: 400.1324600 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 400.1324600 MHz  
 W-W: 0.00  
 SSI: 0  
 LR: 0.00 Hz  
 GB: 0  
 B0: 2.00



Current Data Parameters  
 NAME: BG153  
 EXNO: 7  
 PRGNO: 1

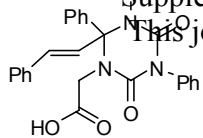
F2 Acquisitor Parameters  
 Date\_: 20070227  
 Time: 16.40  
 NS: 654  
 DS: 4  
 SWH: 20980.814 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 0.0000000 sec  
 RG: 6992.6  
 DW: 20.800 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 D1: 1.0000000 sec  
 D2: 1.0000000 sec  
 D3: 1.0000000 sec  
 D4: 0.0000000 sec  
 D5: 0.0000000 sec  
 D6: 0.0000000 sec  
 D7: 0.0000000 sec

CHANNEL F1  
 NU1: 10  
 P1: 14.00 usec  
 PL1: 0.00 dB  
 SFO1: 100.6228200 MHz

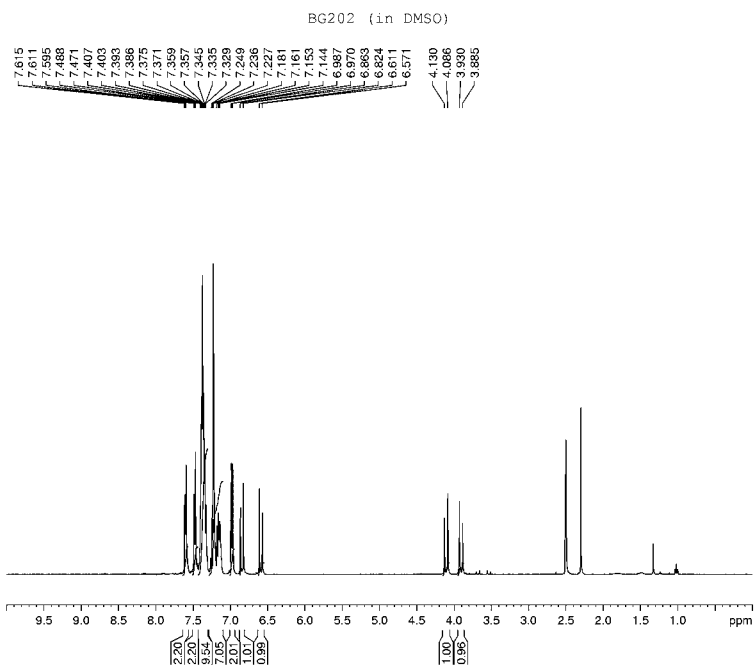
CHANNEL F2  
 NAME: waltz16  
 NU2: 10  
 P2: 20.00 usec  
 PL2: 0.00 dB  
 SFO2: 20.0000000 MHz  
 SFO2: 400.1324600 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 100.6228200 MHz  
 W-W: 0.00  
 SSI: 0  
 LR: 1.00 Hz  
 GB: 0  
 B0: 1.40

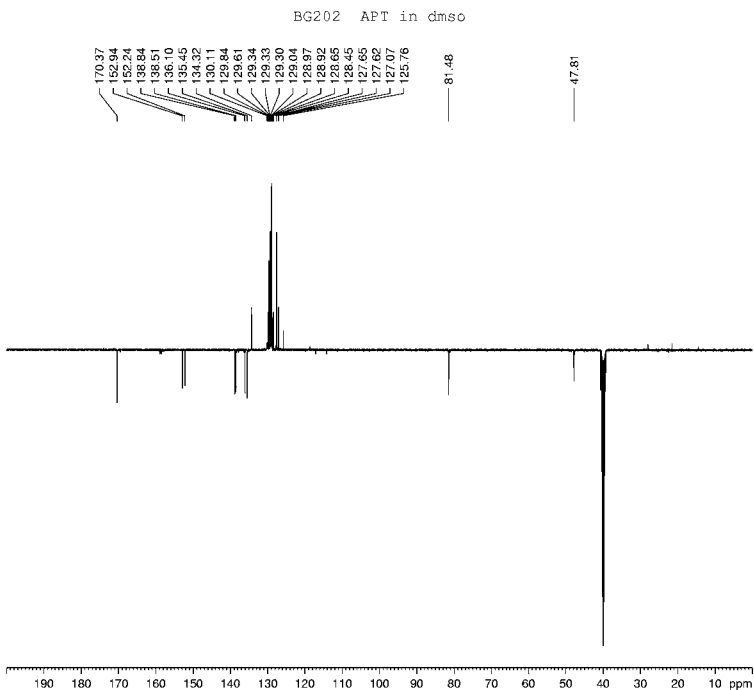
Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008



7

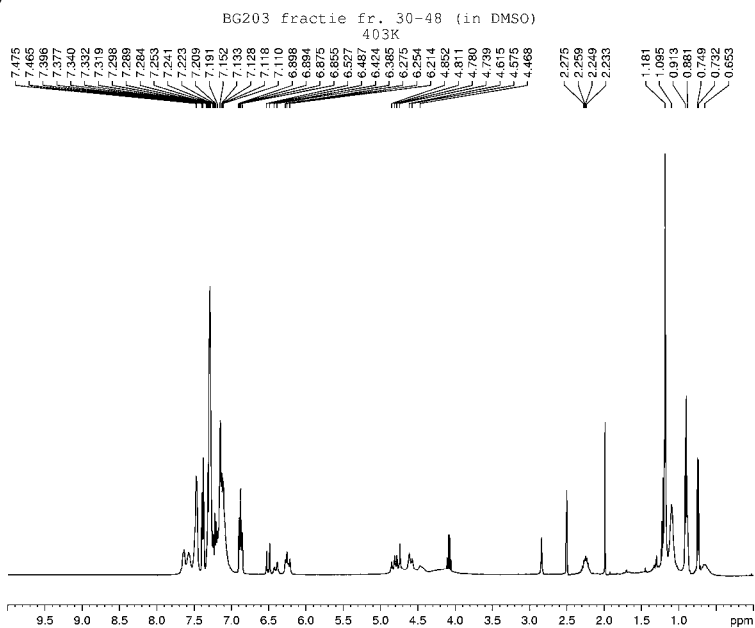
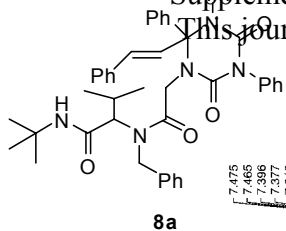


Current Data Parameters  
 NAME: BG202  
 EXPNO: 1  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20070218  
 Time 16:44  
 NS 4000  
 DS 4  
 ANS 400  
 PRGPRD 5 pt Multisat  
 PULPROG zgpg30  
 SOLVENT DMSO  
 NS 4000  
 DS 4  
 SWH 6992.616 Hz  
 FIDRES 0.226919 Hz  
 AQ 2.111749 sec  
 RG 174  
 LW 20.650 Usec  
 LE 6.00 Usec  
 VE 332.4 K  
 ST 1.0000000 sec  
 DQ 1  
 CHANNO 17  
 NUC1 130  
 P1 6.00 Usec  
 PL1 0.00 dB  
 SFO1 400.133209 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 400.133209 MHz  
 W W 64  
 SS 0  
 LB 0.00 Hz  
 GB 0  
 B0 0.00

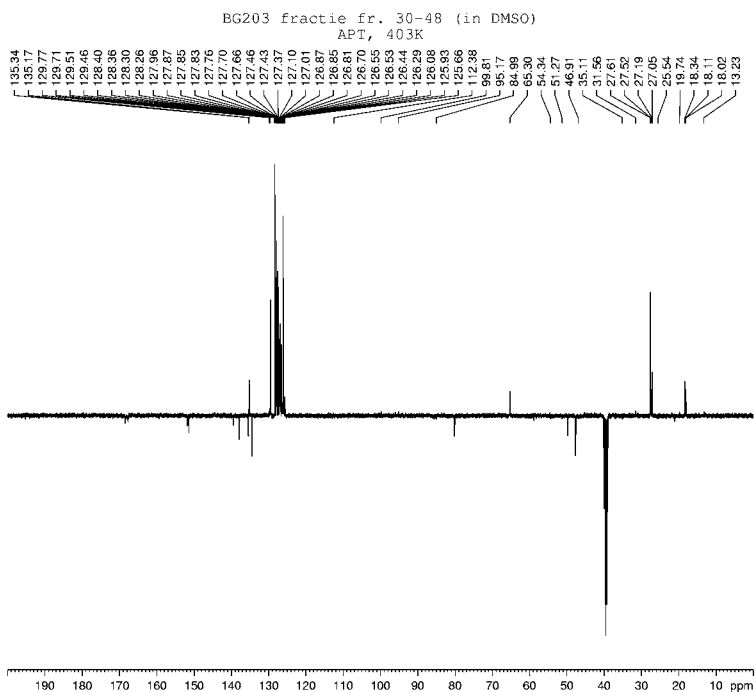


Current Data Parameters  
 NAME: BG202  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20070218  
 Time 17:55  
 NS 4000  
 DS 4  
 ANS 400  
 PRGPRD 5 pt Multisat  
 PULPROG zgpg30  
 SOLVENT DMSO  
 NS 4000  
 DS 4  
 SWH 20980.810 Hz  
 FIDRES 0.226919 Hz  
 AQ 1.3569756 sec  
 RG 174  
 LW 20.650 Usec  
 LE 6.00 Usec  
 VE 332.4 K  
 ST 1.0000000 sec  
 DQ 1  
 CHANNO 17  
 NUC1 130  
 P1 6.00 Usec  
 PL1 0.00 dB  
 SFO1 100.6228298 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 100.6228298 MHz  
 W W 64  
 SS 0  
 LB 1.00 Hz  
 GB 0  
 B0 1.00

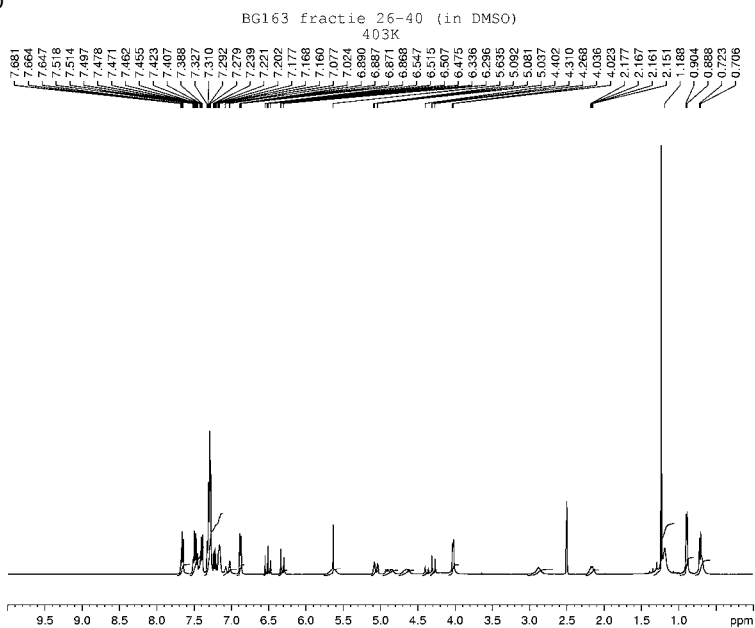
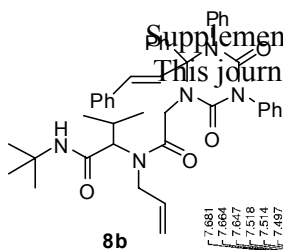
Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008



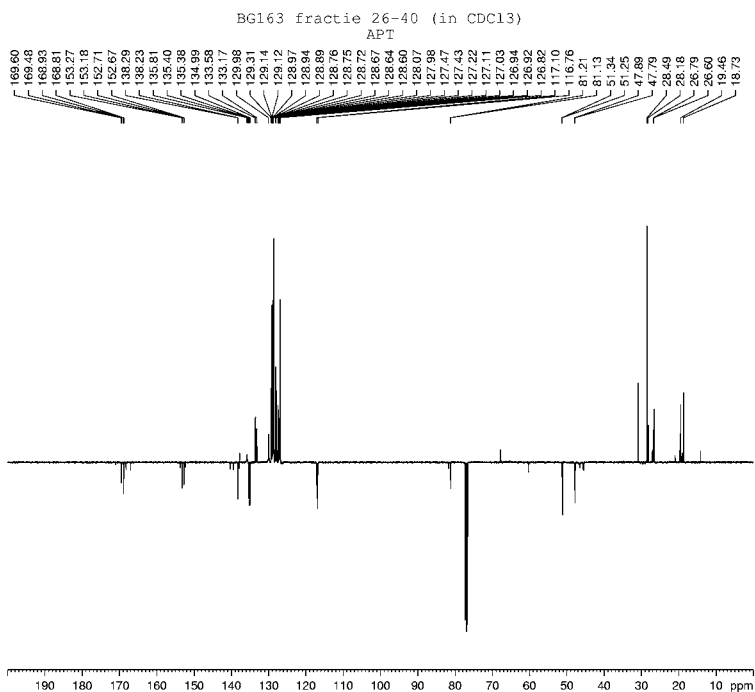
Current Data Parameters  
 NAME: 80203  
 EXPNO: 1  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20080104  
 Time 0.41  
 NS 400  
 DS 2  
 SWH 6993.718 Hz  
 FIDRES 0.2201520 Hz  
 AQ 2.4117169 sec  
 RG 45.5  
 LW 73.600 usec  
 DE 6.00 usec  
 TE 483.4 K  
 DQ 1.0000000 sec  
 TD 1  
 CHANNO: F1  
 NUC1 13C  
 P1 6.00 usec  
 PL 0.00 dB  
 SFO1 400.1326000 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 400.1326000 MHz  
 W W 60  
 SS 0  
 LB 0.00 Hz  
 GB 0  
 PC 0.00



Current Data Parameters  
 NAME: 80203  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20080104  
 Time 0.48  
 NS 400  
 DS 2  
 SWH 21980.810 Hz  
 FIDRES 0.2269198 Hz  
 AQ 1.3564756 sec  
 RG 939.2  
 LW 20.800 usec  
 DE 6.00 usec  
 TE 483.4 K  
 DQ 1.0000000 sec  
 DQ 1.0000000 sec  
 DQ 2.1338888 sec  
 DQ 0.0088963 sec  
 DQ 0.0000167 sec  
 TD 1  
 CHANNO: F1  
 NUC1 13C  
 P1 7.00 usec  
 PL 0.00 dB  
 SFO1 100.6288000 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 100.6288000 MHz  
 W W 60  
 SS 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.00

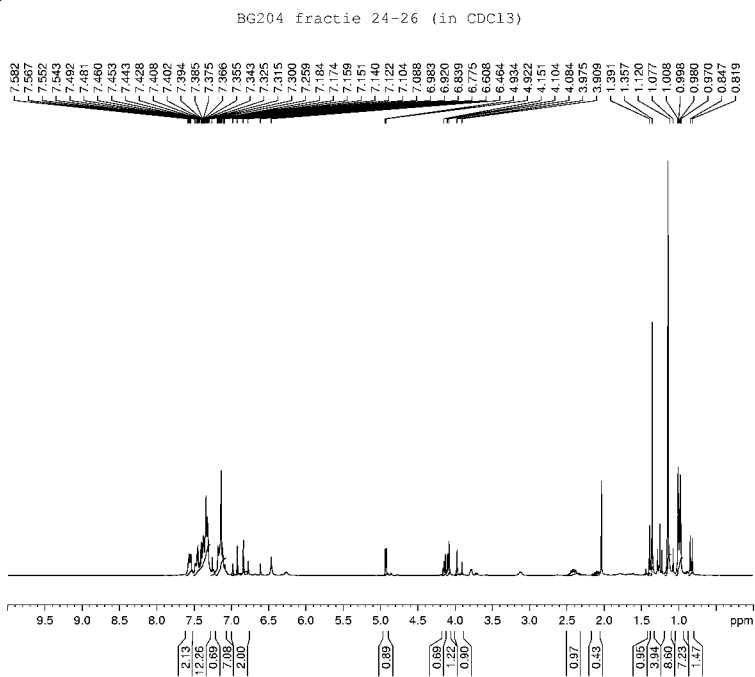
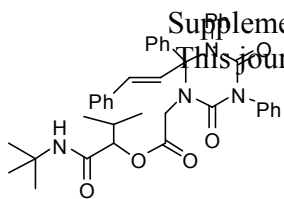


Current Data Parameters  
 NAME: BG163  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20080114  
 Time 13:24  
 NS: 655  
 DS: 4  
 PRG: 1  
 SOLVENT: DMSO  
 NS: 16  
 DS: 2  
 SWH: 6642.641 Hz  
 FIDRES: 0.085540 Hz  
 AQ: 0.000000 sec  
 RG: 64  
 LW: 69.000 usec  
 LE: 6.00 usec  
 FI: 452.4 K  
 CF: 1.000000 sec  
 TD: 1  
 CHAN: F1  
 NUC1: 13  
 P1: 6.00 usec  
 PL1: 0.00 dB  
 SFO1: 400.1324000 MHz  
 F2 Processing parameters  
 SI: 32768  
 SF: 400.1324000 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 2.00

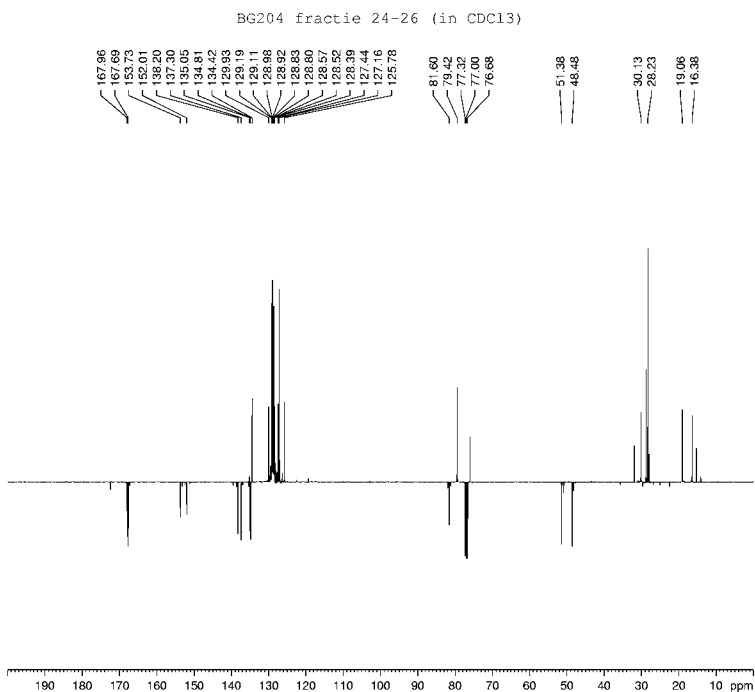


Current Data Parameters  
 NAME: BG163  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20070408  
 Time 2:54  
 NS: 655  
 DS: 4  
 PRG: 1  
 SOLVENT: CDCl3  
 NS: 16  
 DS: 2  
 SWH: 20980.814 Hz  
 FIDRES: 0.266918 Hz  
 AQ: 0.000000 sec  
 RG: 64  
 LW: 20.800 usec  
 LE: 6.00 usec  
 FI: 499.4 K  
 CF: 100.6228000 MHz  
 NUC1: 13  
 P1: 2.00 usec  
 PL1: 0.00 dB  
 SFO1: 100.6228000 MHz  
 F2 Processing parameters  
 SI: 32768  
 SF: 100.6228000 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 1.00

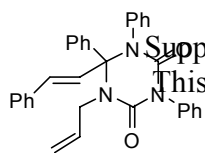
Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008



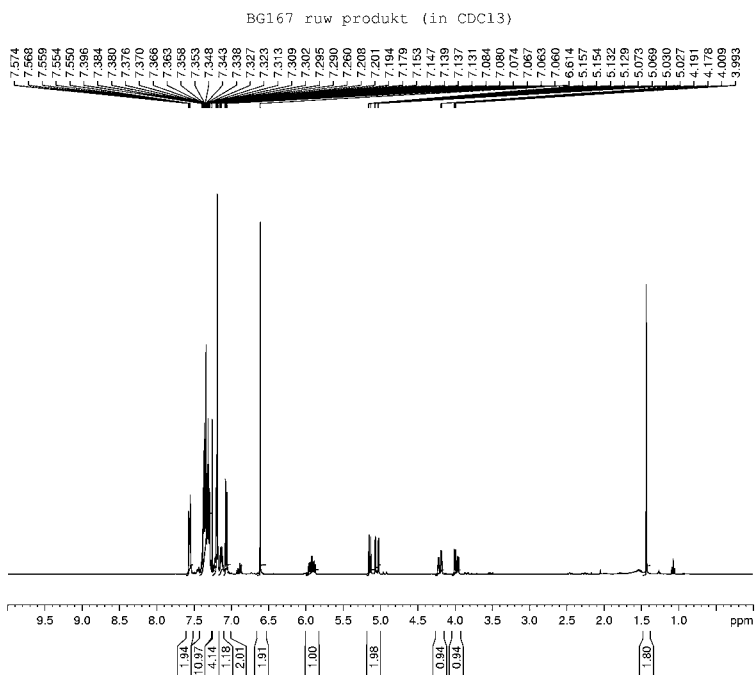
Current Data Parameters  
 NAME: BG204  
 EXPNO: 1  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_: 20071216  
 Time: 16.01  
 NS: 655  
 DS: 4  
 SWH: 5775.495 Hz  
 FIDRES: 0.1078973 Hz  
 AQ: 6.3502777 sec  
 RG: 61.25  
 DW: 94.400 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 SFO: 250.130660 MHz  
 CHANNEL: f1  
 NUC1: 13C  
 P1: 9.00 usec  
 PL1: 0.00 dB  
 SFO1: 250.130660 MHz  
 F2 Processing parameters  
 SI: 32768  
 SF: 250.130660 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 B0: 1.00



Current Data Parameters  
 NAME: BG204  
 EXPNO: 1  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_: 20071216  
 Time: 16.01  
 NS: 655  
 DS: 4  
 SWH: 20980.810 Hz  
 FIDRES: 0.226913 Hz  
 AQ: 1.3564758 sec  
 RG: 4896.0  
 DW: 20.600 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 SFO: 250.130660 MHz  
 CHANNEL: f1  
 NUC1: 13C  
 P1: 2.00 usec  
 PL1: 0.00 dB  
 SFO1: 250.130660 MHz  
 CHANNEL: f2  
 NUC2: 13C  
 P2: 9.00 usec  
 PL2: 0.00 dB  
 SFO2: 250.130660 MHz  
 F2 Processing parameters  
 SI: 65536  
 SF: 100.622769 MHz  
 W: 655  
 SS: 0  
 LB: 1.00 Hz  
 GB: 0  
 B0: 1.00



10

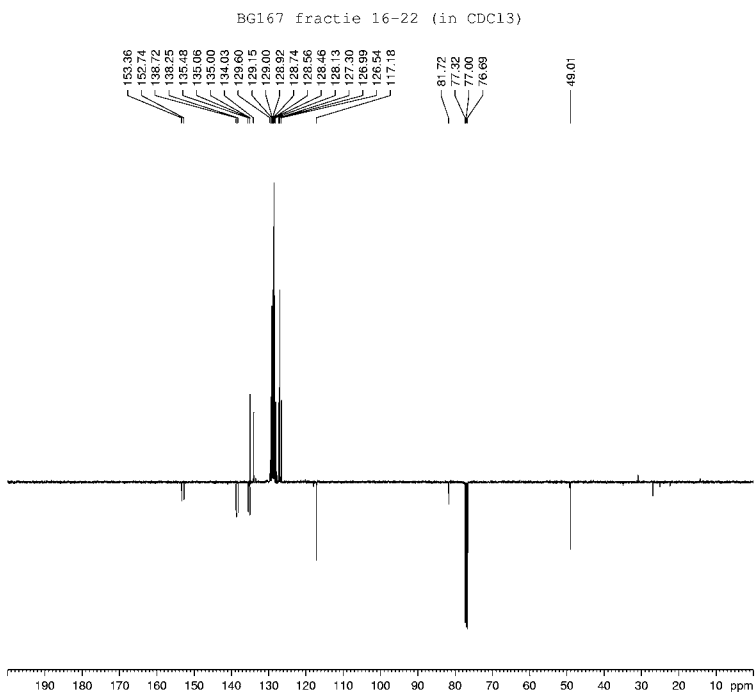


Current Data Parameters  
 NAME: BG167  
 EXPNO: 2  
 PROCNO: 1

F2 Acquisitor Parameters  
 Date\_: 20070613  
 Time: 10.37  
 NS: 655  
 DS: 4  
 SWH: 6602.641 Hz  
 FIDRES: 0.085540 Hz  
 AQ: 0.0559625 sec  
 RG: 327  
 DW: 69.400 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 DD: 1

NUC1: CHANNEL F1  
 P1: 6.20 usec  
 PL1: 0.00 dB  
 SFO1: 400.1324603 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 400.1324603 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 2.00

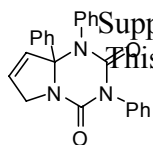


Current Data Parameters  
 NAME: BG167  
 EXPNO: 2  
 PROCNO: 2

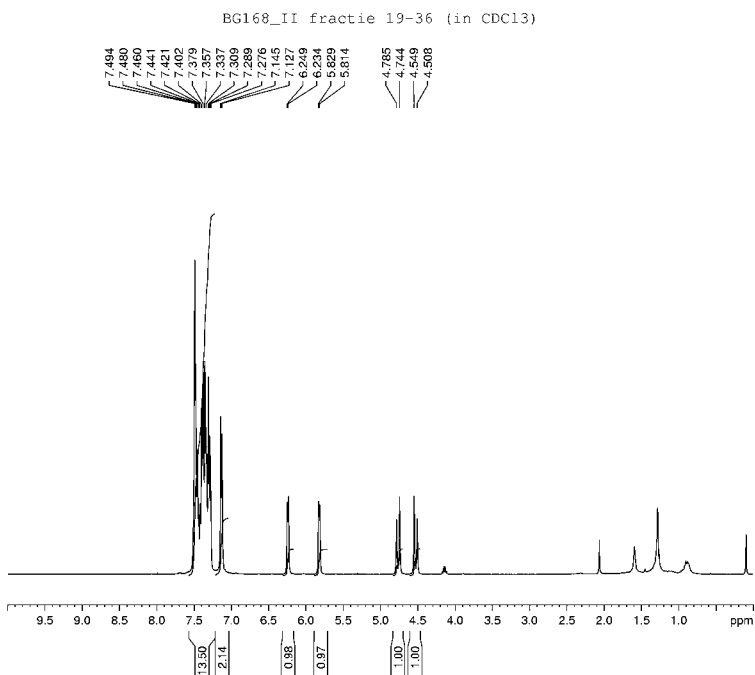
F2 Acquisitor Parameters  
 Date\_: 20070613  
 Time: 10.50  
 NS: 655  
 DS: 4  
 SWH: 20980.814 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3366716 sec  
 RG: 4586  
 DW: 20.650 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 DD: 2.0000000 sec  
 SFO1: 0.0089663 sec  
 SFO2: 0.00001617 sec  
 PC: 0  
 PD: 1

NUC1: CHANNEL F1  
 P1: 1.00 usec  
 PL1: 21.70 dB  
 PL2: 6.00 dB  
 SFO1: 100.6228295 MHz

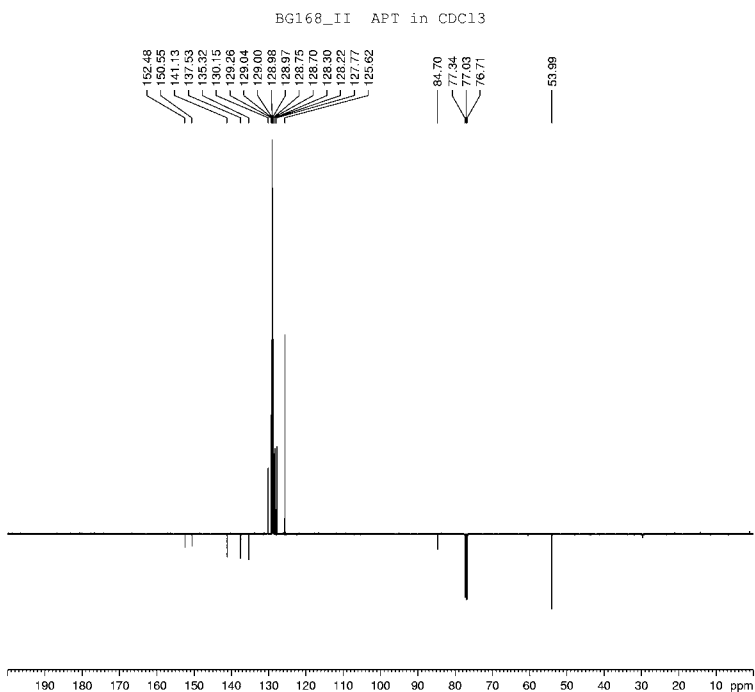
CHANNEL F2  
 W: 4586  
 SI: 4586  
 SF: 100.6227712 MHz  
 W: 655  
 SS: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 1.00



11

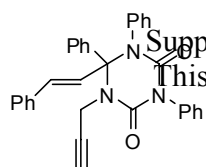


Current Data Parameters  
 NAME: BG168\_II  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acq: 20071219  
 Date\_ 20071219  
 Time 16:25  
 NS: 600  
 DS: 4  
 SWH: 6993.616 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 2.411765 sec  
 RG: 52.4  
 LW: 73.600 usec  
 LE: 6.00 usec  
 VE: 382.4 K  
 DT: 1.0000000 sec  
 DQ: 1  
 CHANNEL: f1  
 NUC1: 13C  
 P1: 6.00 usec  
 PL1: 0.00 dB  
 SFO1: 400.132619 MHz  
 F2 Processing parameters  
 SI: 32768  
 SF: 400.132619 MHz  
 W: 65536  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 0.00



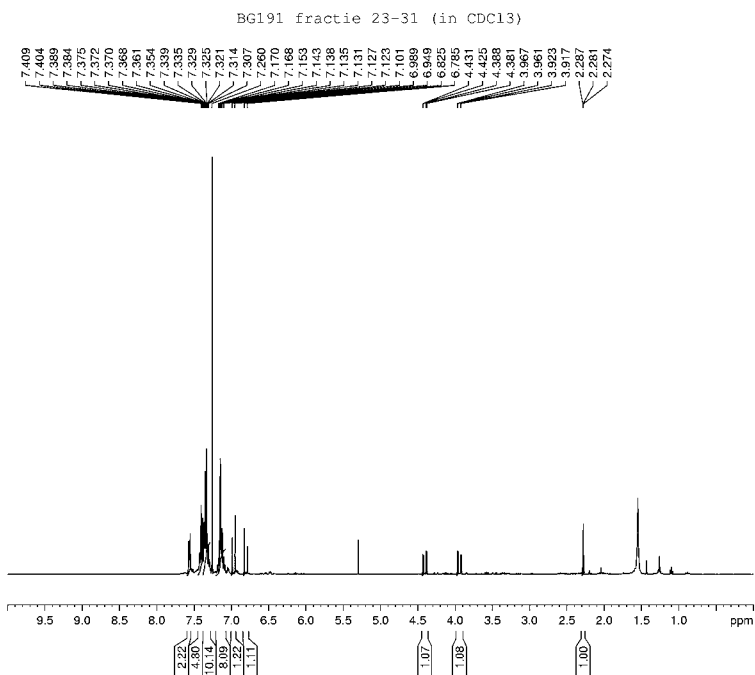
Current Data Parameters  
 NAME: BG168\_II  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acq: 20071219  
 Date\_ 20071219  
 Time 17:30  
 NS: 600  
 DS: 4  
 SWH: 20980.810 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3569156 sec  
 RG: 5992.6  
 LW: 20.800 usec  
 LE: 6.00 usec  
 VE: 382.4 K  
 DT: 1.0000000 sec  
 DQ: 1  
 CHANNEL: f1  
 NUC1: 13C  
 P1: 2.00 usec  
 PL1: 20.00 dB  
 SFO1: 100.6228295 MHz  
 CHANNEL: f2  
 NUC2: 13C  
 P2: 80.00 usec  
 PL2: 0.00 dB  
 SFO2: 400.132619 MHz  
 F2 Processing parameters  
 SI: 32768  
 SF: 100.6228295 MHz  
 W: 65536  
 SS: 0  
 LB: 0.20 Hz  
 GB: 0  
 PC: 1.00





12

Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008

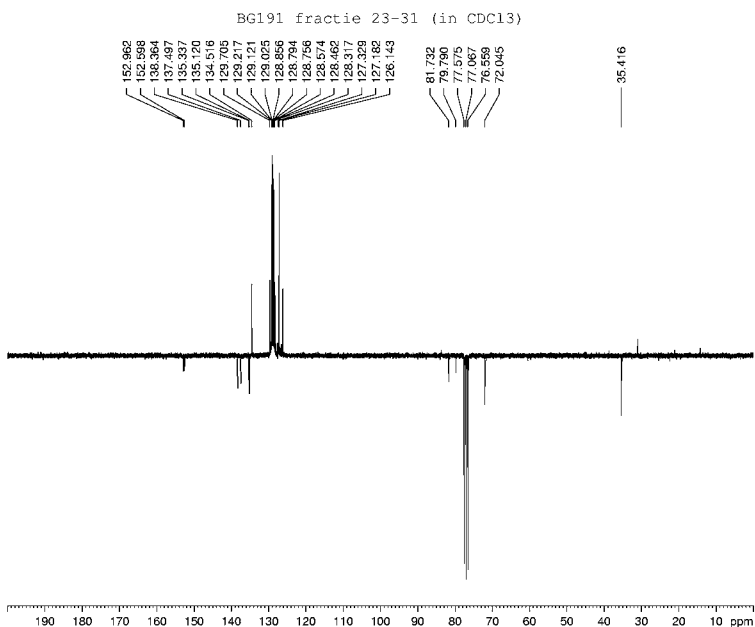


Current Data Parameters  
 NAME: BG191  
 EXPNO: 1  
 PROCNO: 1

F2 Acquisitor Parameters  
 Date\_: 20080109  
 Time: 11.05  
 NS: 655  
 DS: 4  
 ANS: 655  
 PRG: 500  
 PULPROG: zgpg30  
 SOLVENT: CDCl3  
 NS2: 2  
 DS2: 2  
 SWH: 6998.718 Hz  
 FIDRES: 0.221520 Hz  
 AQ: 2.111145 sec  
 RG: 456.4  
 LW: 73.600 usec  
 LE: 6.00 usec  
 FI: 855.4 K  
 CD: 1.0000000 sec  
 DD: 1

CHANNEL F1  
 NU1: 10  
 F1: 6.20 usec  
 P1: 0.00 dB  
 SFO1: 400.1500000 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 400.1500000 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 0.00



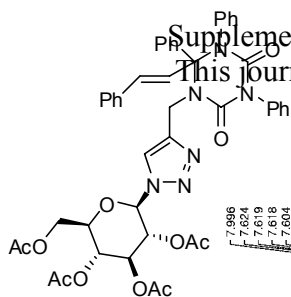
Current Data Parameters  
 NAME: BG191  
 EXPNO: 1  
 PROCNO: 1

F2 Acquisitor Parameters  
 Date\_: 20070917  
 Time: 17.57  
 NS: 655  
 DS: 4  
 ANS: 655  
 PRG: 500  
 PULPROG: zgpg30  
 SOLVENT: CDCl3  
 NS2: 2  
 DS2: 2  
 SWH: 16063.247 Hz  
 FIDRES: 0.228601 Hz  
 AQ: 2.118845 sec  
 RG: 458.6  
 LW: 35.220 usec  
 LE: 6.00 usec  
 FI: 296.2 K  
 CD: 1.0000000 sec  
 DD: 1.0000000 sec  
 SFO1: 101.6250000 MHz  
 SFO2: 0.0089663 MHz  
 SFO3: 0.0089663 MHz  
 SFO4: 0.0089663 MHz  
 SFO5: 0.0089663 MHz  
 SFO6: 0.0089663 MHz

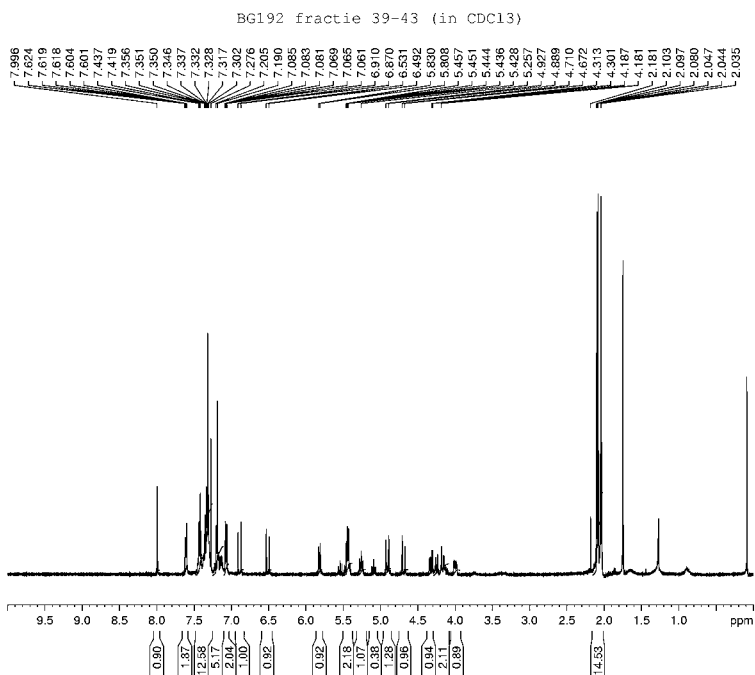
CHANNEL F1  
 NU1: 10  
 F1: 6.75 usec  
 P1: 15.00 dB  
 SFO1: 0.00 dB  
 SFO2: 62.9018250 MHz

CHANNEL F2  
 W: 1.0  
 NS2: 2  
 DS2: 2  
 SWH2: 80.00 usec  
 FIDRES2: 0.00 dB  
 AQ2: 0.00 dB  
 RG2: 22.00 dB  
 LW2: 230.1500000 MHz

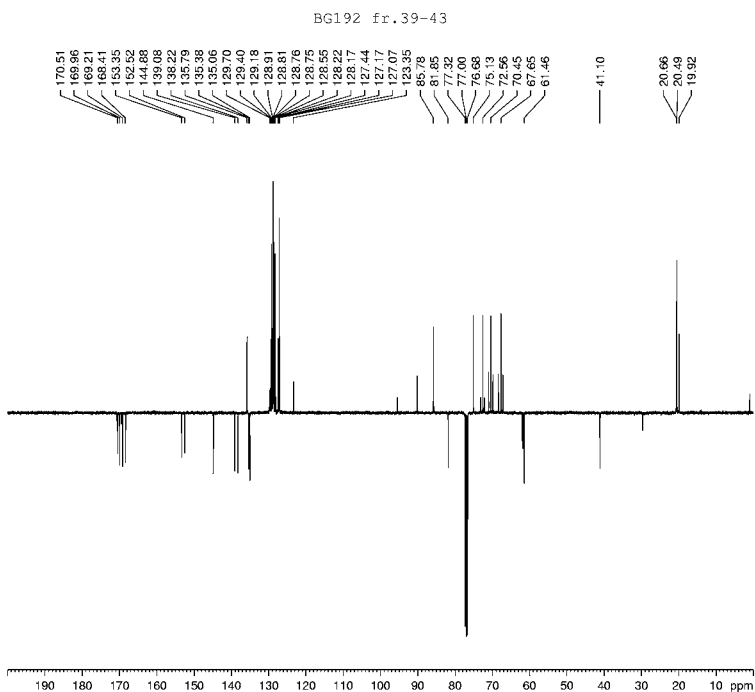
F2 Processing parameters  
 SI: 32768  
 SF: 62.9025000 MHz  
 W: 655  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 1.00



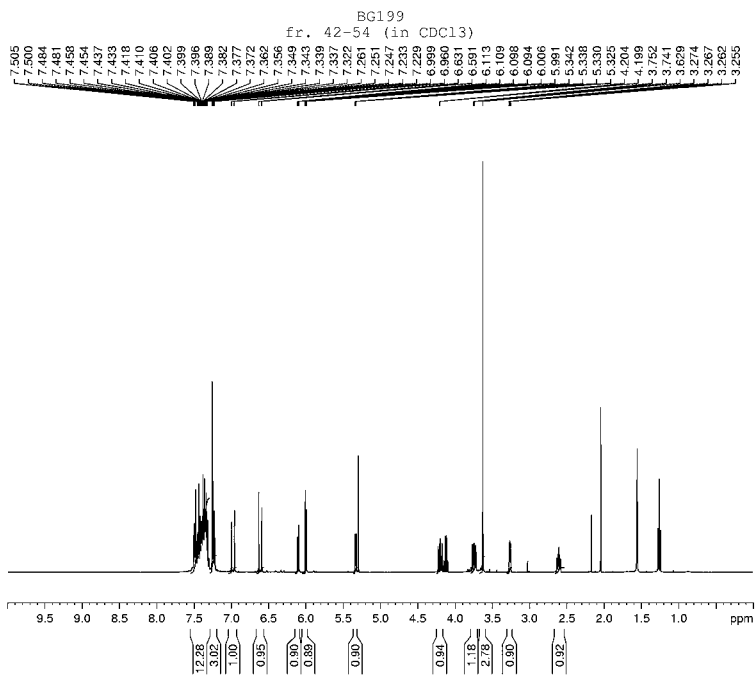
14



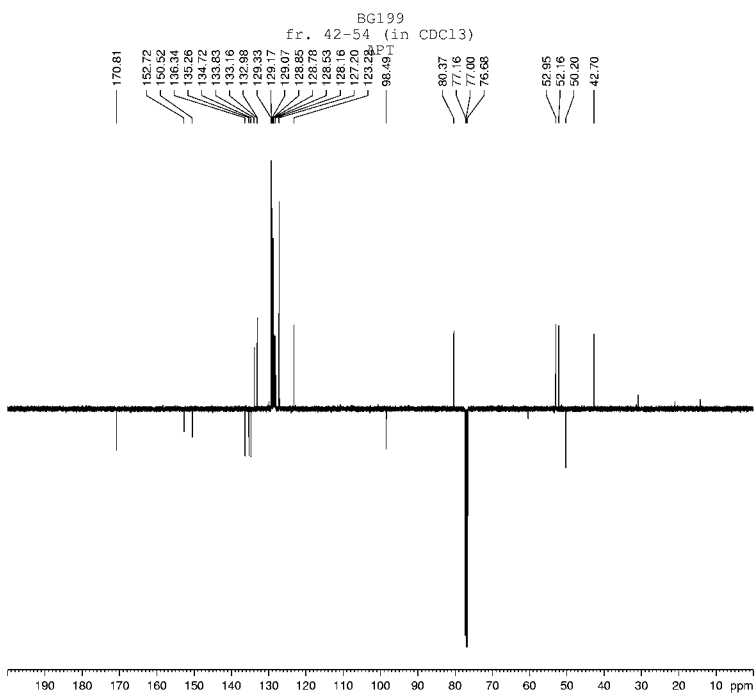
Current Data Parameters  
 NAME: BG192  
 EXPNO: 4  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_: 20080104  
 Time: 9.24  
 NS: 655  
 DS: 4  
 PRB: 9.00 MHz  
 PULPROG: zgpg30  
 PC: 12.00  
 SOLVENT: CDCl3  
 NS: 16  
 DS: 2  
 SWH: 6993.618 Hz  
 FIDRES: 0.2201520 Hz  
 AQ: 2.4117149 sec  
 RG: 52.4  
 LW: 73.400 Usec  
 LE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 DD: 1  
 CHAN: F1  
 NUC1: 13C  
 P1: 6.20 Usec  
 PL1: 0.00 dB  
 SFO1: 400.1326100 MHz  
 F2 Processing parameters  
 SI: 62536  
 SF: 400.1326100 MHz  
 W W: 60  
 SSI: 0  
 LR: 0.00 Hz  
 CR: 0  
 CD: 0.00



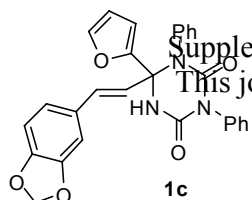
Current Data Parameters  
 NAME: BG192  
 EXPNO: 4  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_: 20071221  
 Time: 15.18  
 NS: 655  
 DS: 4  
 PRB: 9.00 MHz  
 PULPROG: zgpg30  
 PC: 12.00  
 SOLVENT: CDCl3  
 NS: 2560  
 DS: 4  
 SWH: 20980.810 Hz  
 FIDRES: 0.2209118 Hz  
 AQ: 1.3664758 sec  
 RG: 468.6  
 LW: 20.800 Usec  
 LE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000  
 DD: 1.0000000  
 DD2: 2.0000000 sec  
 DD3: 0.0000000 sec  
 DD4: 0.0000000 sec  
 DD5: 0  
 DD6: 0  
 CHAN: F2  
 NUC1: 13C  
 P1: 2.70 Usec  
 PL1: 20.40 dB  
 SFO1: 100.6228200 MHz  
 F2 Processing parameters  
 SI: 62536  
 SF: 100.6228200 MHz  
 W W: 60  
 SSI: 0  
 LR: 1.00 Hz  
 CR: 0  
 CD: 1.40



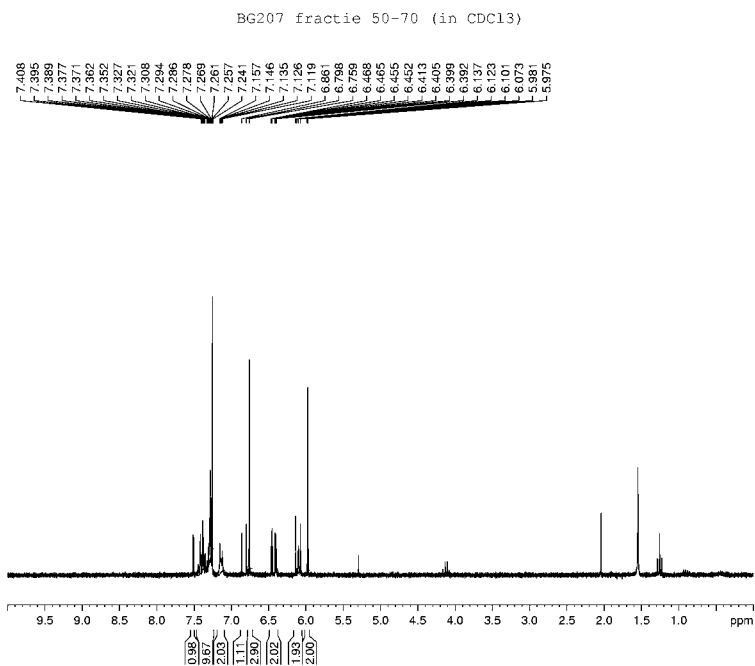
Current Data Parameters  
 NAME: BG199  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20071029  
 Time 14:56  
 NS 400  
 DS 2  
 SWH 6410.246 Hz  
 FIDRES 0.196628 Hz  
 AQ 2.5559540 sec  
 RG 204  
 DW 78.000 Usec  
 DE 6.00 Usec  
 TE 300.2 K  
 DQ 1.0000000 sec  
 SFO 400.136093 MHz  
 CHANNO1 F1  
 NUC1 13C  
 P1 6.20 Usec  
 PL 0.00 dB  
 SFO1 100.626395 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 400.136093 MHz  
 W W 64  
 SS 0  
 LR 0.00 Hz  
 GR 0  
 PD 0.00



Current Data Parameters  
 NAME: BG199  
 EXPNO: 2  
 PROCNO: 1  
 F2 Acquisitor Parameters  
 Date\_ 20071029  
 Time 17:39  
 NS 400  
 DS 2  
 SWH 20980.814 Hz  
 FIDRES 0.226918 Hz  
 AQ 1.3664756 sec  
 RG 425.6  
 DW 20.800 Usec  
 DE 6.00 Usec  
 TE 300.2 K  
 DQ 1.0000000 sec  
 SFO 100.626395 MHz  
 CHANNO1 F1  
 NUC1 13C  
 P1 2.70 Usec  
 PL 0.00 dB  
 SFO1 100.626395 MHz  
 F2 Processing parameters  
 SI 32768  
 SF 100.626395 MHz  
 W W 64  
 SS 0  
 LR 0.00 Hz  
 GR 0  
 PD 1.40



Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008

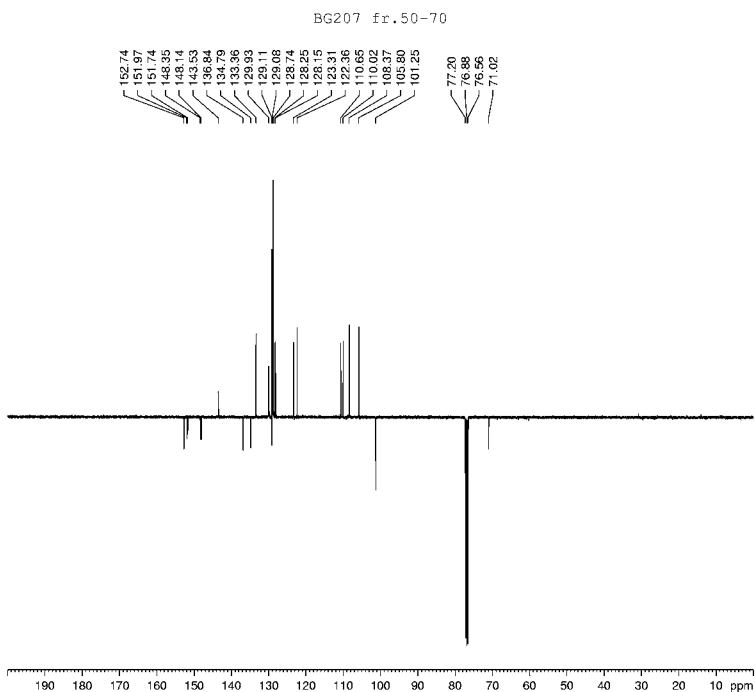


Current Data Parameters  
 NAME: BG207  
 EXNO: 1  
 PRGNO: 1

F2 Acquisition Parameters  
 Date\_: 20071127  
 Time: 8.57  
 NS: 400  
 PROBR: 9.00 MHz  
 PULPROG: zgpg30  
 CH: 62936  
 SOLVENT: CDCl<sub>3</sub>  
 NS: 16  
 DS: 2  
 SWH: 5775.995 Hz  
 FIDRES: 0.078979 Hz  
 AQ: 6.5882777 sec  
 RG: 1425.5  
 DW: 96.600 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 D1: 1.0000000 sec  
 D2: 1

CHANNEL F1  
 NU1: 10  
 P1: 9.00 usec  
 PL1: 0.00 dB  
 SFO1: 250.1352667 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 250.1352667 MHz  
 W W: 60  
 SSI: 0  
 LB: 0.50 Hz  
 GB: 0.0  
 B0: 1.00



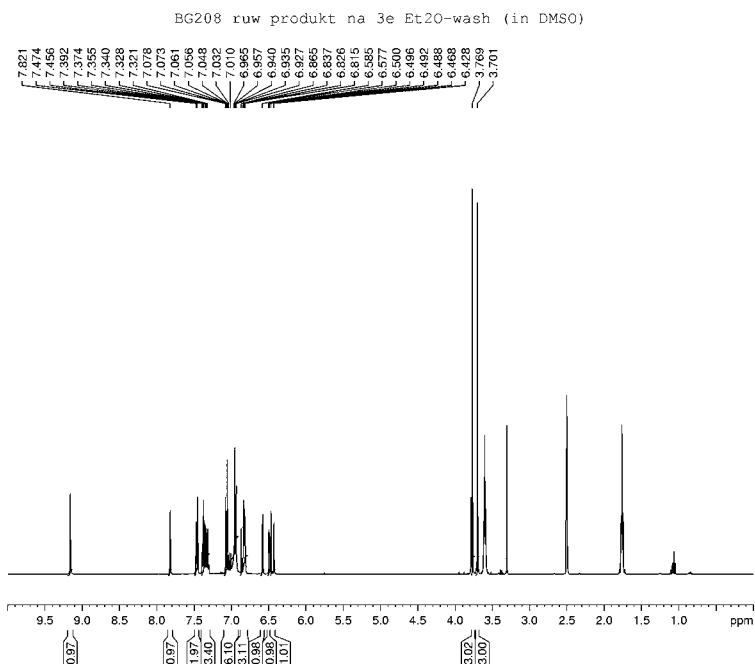
Current Data Parameters  
 NAME: BG207  
 EXNO: 2  
 PRGNO: 2

F2 Acquisition Parameters  
 Date\_: 20071223  
 Time: 9.45  
 NS: 400  
 PROBR: 9.00 MHz  
 PULPROG: zgpg30  
 CH: 62936  
 SOLVENT: CDCl<sub>3</sub>  
 NS: 2560  
 DS: 4  
 SWH: 25983.810 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3566736 sec  
 RG: 245.6  
 DW: 20.850 usec  
 DE: 6.00 usec  
 TE: 300.2 K  
 DMSD: 149.0000000  
 DMSD1: 1.0000000  
 D1: 2.0000000 sec  
 D2: 0.0000000 sec  
 D3: 0.0000000 sec  
 D4: 20  
 D5: 1

CHANNEL F1  
 NU1: 150  
 P1: 20.00 usec  
 PL1: 20.00 dB  
 SFO1: 100.6228225 MHz

CHANNEL F2  
 PULPROG: waltz16  
 NU2: 10  
 P2: 80.00 usec  
 PL2: 0.00 dB  
 SFO2: 27.27 MHz  
 SFO3: 400.1352667 MHz

F2 Processing parameters  
 SI: 40960  
 SF: 100.6228225 MHz  
 W W: 60  
 SSI: 0  
 LB: 1.00 Hz  
 GB: 0  
 B0: 1.00

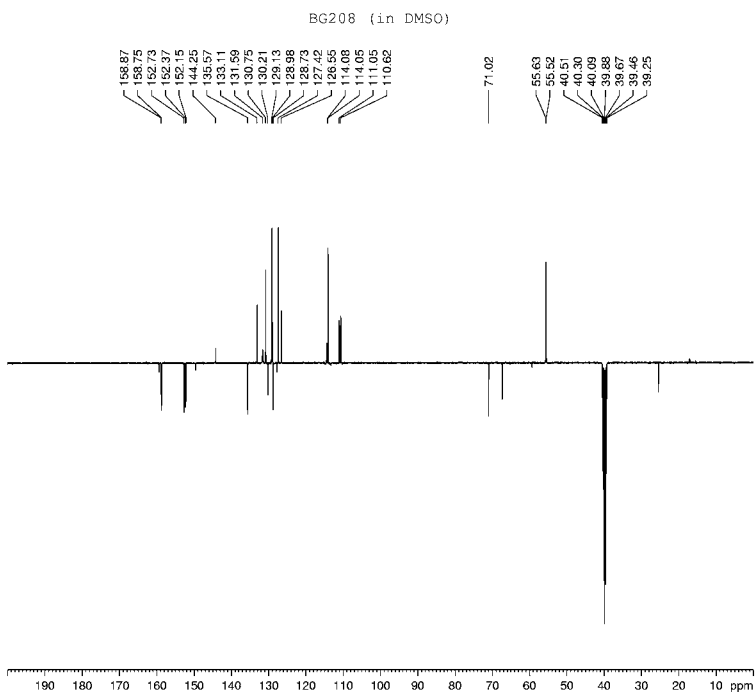


Current Data Parameters  
 NAME: BG208  
 EXPNO: 1  
 PROCNO: 1

F2 Acquisitor Parameters  
 Date\_: 20071127  
 Time: 14.03  
 NS: 655  
 DS: 4  
 SWH: 6410.246 Hz  
 FIDRES: 0.196625 Hz  
 AQ: 2.5559240 sec  
 RG: 174  
 DW: 75.000 Usec  
 DE: 6.00 Usec  
 TE: 300.2 K  
 D1: 1.0000000 sec  
 D11: 0.0000000 sec  
 D12: 0.0000000 sec  
 D13: 0.0000000 sec

NAME: CHANNEL F1  
 P1: 6.20 Usec  
 P2: 0.00 Usec  
 SFO1: 400.1360000 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 400.1360000 MHz  
 W: 655  
 SSB: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 0.00



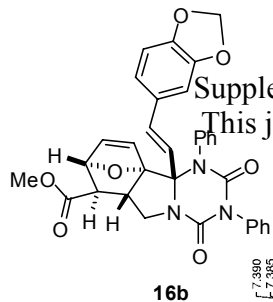
Current Data Parameters  
 NAME: BG208  
 EXPNO: 2  
 PROCNO: 1

F2 Acquisitor Parameters  
 Date\_: 20071228  
 Time: 14.49  
 NS: 655  
 DS: 4  
 SWH: 25980.810 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3569756 sec  
 RG: 5792.6  
 DW: 20.600 Usec  
 DE: 6.00 Usec  
 TE: 300.2 K  
 DMS12: 149.0000000  
 DMS11: 1.0000000  
 D1: 2.0000000 sec  
 D2: 0.0000000 sec  
 D11A: 0.0000000 sec  
 D12: 0.0000000 sec  
 D13: 0.0000000 sec

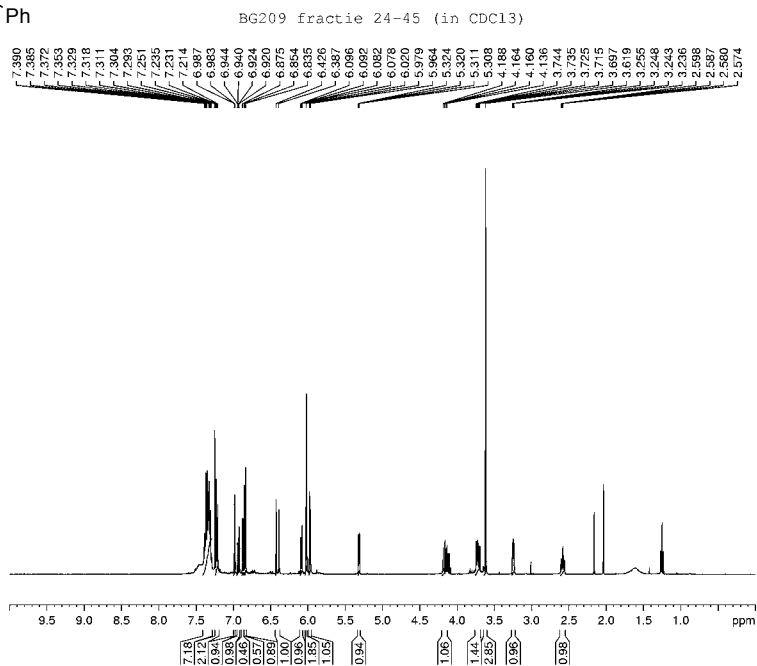
NAME: CHANNEL F1  
 P1: 1.00 Usec  
 P2: 21.40 Usec  
 P3: 6.00 Usec  
 SFO1: 100.6228205 MHz

NAME: CHANNEL F2  
 P1: 80.00 Usec  
 P2: 0.00 Usec  
 P3: 27.20 Usec  
 SFO2: 400.1360000 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 100.6228205 MHz  
 W: 655  
 SSB: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 1.40



Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008

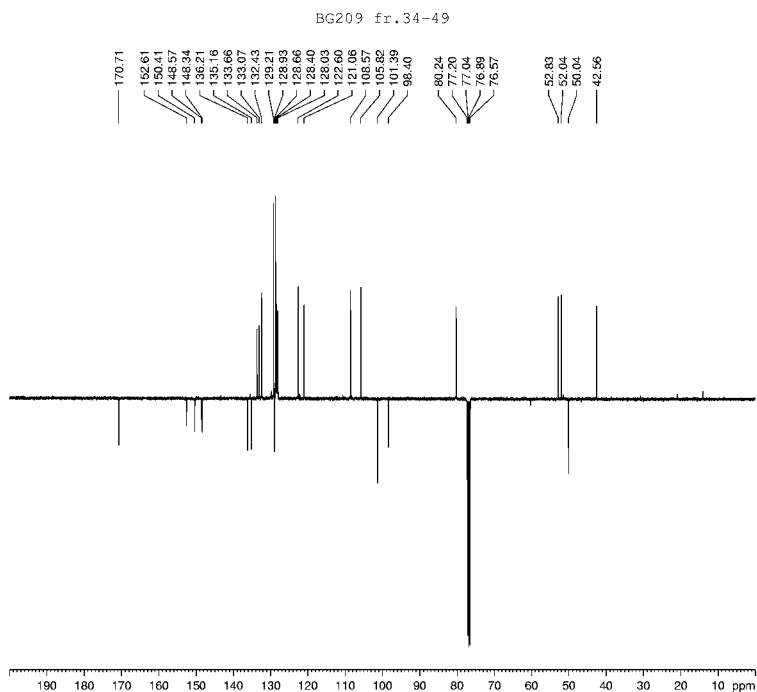


Current Data Parameters  
 NAME: BG209  
 EXPNO: 2  
 PROCNO: 1

F2 Acquisition Parameters  
 Date\_: 20080111  
 Time: 16.01  
 NS: 654  
 DS: 4  
 SWH: 6410.246 Hz  
 FIDRES: 0.196626 Hz  
 AQ: 2.5559740 sec  
 RG: 123  
 DW: 78.000 Usec  
 DE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 TD: 1

NUC1 CHANNEL F1  
 P1: 6.20 Usec  
 PL1: 0.00 dB  
 SFO1: 400.1360000 MHz

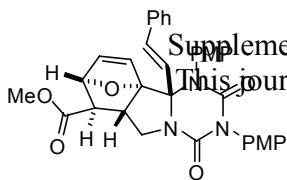
F2 Processing parameters  
 SI: 32768  
 SF: 400.1360000 MHz  
 W: 65536  
 SS: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 0.00



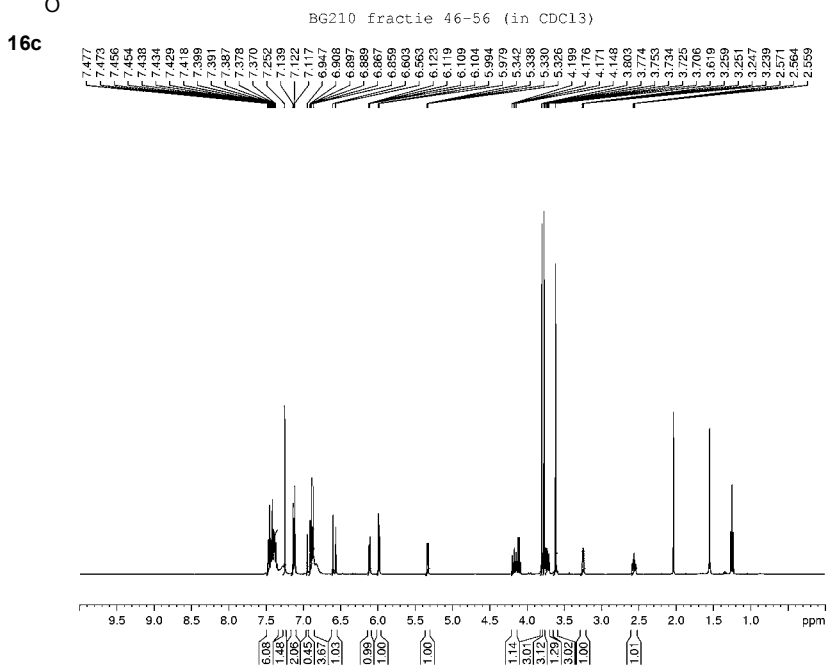
Current Data Parameters  
 NAME: BG209  
 EXPNO: 2  
 PROCNO: 1

F2 Acquisition Parameters  
 Date\_: 20071226  
 Time: 8.56  
 NS: 654  
 DS: 4  
 SWH: 25980.810 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3566176 sec  
 RG: 2298.8  
 DW: 20.800 Usec  
 DE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000  
 SFO1: 100.6228000 MHz  
 SFO2: 201.2456000 MHz  
 SFO3: 201.2456000 MHz  
 SFO4: 201.2456000 MHz  
 SFO5: 201.2456000 MHz  
 SFO6: 201.2456000 MHz  
 SFO7: 201.2456000 MHz  
 SFO8: 201.2456000 MHz  
 SFO9: 201.2456000 MHz  
 SFO10: 201.2456000 MHz  
 SFO11: 201.2456000 MHz  
 SFO12: 201.2456000 MHz  
 SFO13: 201.2456000 MHz  
 SFO14: 201.2456000 MHz  
 SFO15: 201.2456000 MHz  
 SFO16: 201.2456000 MHz  
 SFO17: 201.2456000 MHz  
 SFO18: 201.2456000 MHz  
 SFO19: 201.2456000 MHz  
 SFO20: 201.2456000 MHz  
 SFO21: 201.2456000 MHz  
 SFO22: 201.2456000 MHz  
 SFO23: 201.2456000 MHz  
 SFO24: 201.2456000 MHz  
 SFO25: 201.2456000 MHz  
 SFO26: 201.2456000 MHz  
 SFO27: 201.2456000 MHz  
 SFO28: 201.2456000 MHz  
 SFO29: 201.2456000 MHz  
 SFO30: 201.2456000 MHz  
 SFO31: 201.2456000 MHz  
 SFO32: 201.2456000 MHz  
 SFO33: 201.2456000 MHz  
 SFO34: 201.2456000 MHz  
 SFO35: 201.2456000 MHz  
 SFO36: 201.2456000 MHz  
 SFO37: 201.2456000 MHz  
 SFO38: 201.2456000 MHz  
 SFO39: 201.2456000 MHz  
 SFO40: 201.2456000 MHz  
 SFO41: 201.2456000 MHz  
 SFO42: 201.2456000 MHz  
 SFO43: 201.2456000 MHz  
 SFO44: 201.2456000 MHz  
 SFO45: 201.2456000 MHz  
 SFO46: 201.2456000 MHz  
 SFO47: 201.2456000 MHz  
 SFO48: 201.2456000 MHz  
 SFO49: 201.2456000 MHz  
 SFO50: 201.2456000 MHz  
 SFO51: 201.2456000 MHz  
 SFO52: 201.2456000 MHz  
 SFO53: 201.2456000 MHz  
 SFO54: 201.2456000 MHz  
 SFO55: 201.2456000 MHz  
 SFO56: 201.2456000 MHz  
 SFO57: 201.2456000 MHz  
 SFO58: 201.2456000 MHz  
 SFO59: 201.2456000 MHz  
 SFO60: 201.2456000 MHz  
 SFO61: 201.2456000 MHz  
 SFO62: 201.2456000 MHz  
 SFO63: 201.2456000 MHz  
 SFO64: 201.2456000 MHz  
 SFO65: 201.2456000 MHz  
 SFO66: 201.2456000 MHz  
 SFO67: 201.2456000 MHz  
 SFO68: 201.2456000 MHz  
 SFO69: 201.2456000 MHz  
 SFO70: 201.2456000 MHz  
 SFO71: 201.2456000 MHz  
 SFO72: 201.2456000 MHz  
 SFO73: 201.2456000 MHz  
 SFO74: 201.2456000 MHz  
 SFO75: 201.2456000 MHz  
 SFO76: 201.2456000 MHz  
 SFO77: 201.2456000 MHz  
 SFO78: 201.2456000 MHz  
 SFO79: 201.2456000 MHz  
 SFO80: 201.2456000 MHz  
 SFO81: 201.2456000 MHz  
 SFO82: 201.2456000 MHz  
 SFO83: 201.2456000 MHz  
 SFO84: 201.2456000 MHz  
 SFO85: 201.2456000 MHz  
 SFO86: 201.2456000 MHz  
 SFO87: 201.2456000 MHz  
 SFO88: 201.2456000 MHz  
 SFO89: 201.2456000 MHz  
 SFO90: 201.2456000 MHz  
 SFO91: 201.2456000 MHz  
 SFO92: 201.2456000 MHz  
 SFO93: 201.2456000 MHz  
 SFO94: 201.2456000 MHz  
 SFO95: 201.2456000 MHz  
 SFO96: 201.2456000 MHz  
 SFO97: 201.2456000 MHz  
 SFO98: 201.2456000 MHz  
 SFO99: 201.2456000 MHz  
 SFO100: 201.2456000 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 100.6228000 MHz  
 W: 65536  
 SS: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 1.40



Supplementary Material (ESI) for Organic & Biomolecular Chemistry  
 This journal is (c) The Royal Society of Chemistry 2008

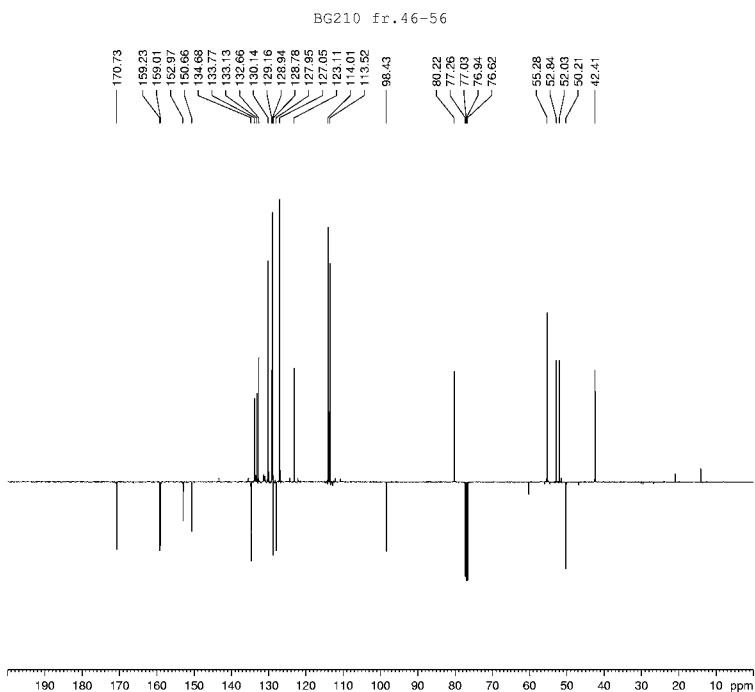


Current Data Parameters  
 NAME: BG210  
 EXNO: 7  
 PRGNO: 1

F2 Acquisitor Parameters  
 Date\_: 20071228  
 Time: 16:10  
 NS: 400  
 PRGPRG: 9 pp Maximal  
 PULPROG: zgpg30  
 CH: 132143  
 SOLVENT: CDCl<sub>3</sub>  
 NS: 16  
 DS: 2  
 SWH: 6410.246 Hz  
 FIDRES: 0.196626 Hz  
 AQ: 2.5559640 sec  
 RG: 225.1  
 LW: 75.000 Usec  
 LE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000 sec  
 TD: 1

CHANNEL: F1  
 NU1: 10  
 P1: 6.00 Usec  
 PL1: 0.00 dB  
 SFO1: 400.136093 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 400.136093 MHz  
 W W: 60  
 SSI: 0  
 LB: 0.00 Hz  
 GB: 0  
 B0: 0.00



Current Data Parameters  
 NAME: BG210  
 EXNO: 7  
 PRGNO: 1

F2 Acquisitor Parameters  
 Date\_: 20071228  
 Time: 7:50  
 NS: 400  
 PRGPRG: 9 pp Maximal  
 PULPROG: zgpg30  
 CH: 132143  
 SOLVENT: CDCl<sub>3</sub>  
 NS: 2560  
 DS: 4  
 SWH: 25980.814 Hz  
 FIDRES: 0.226918 Hz  
 AQ: 1.3569756 sec  
 RG: 6792.6  
 LW: 20.800 Usec  
 LE: 6.00 Usec  
 TE: 300.2 K  
 DQ: 1.0000000  
 CHAN: 149.0000000  
 CHAN: 1.0000000  
 DQ: 2.0000000 sec  
 SFO1: 100.6228295 MHz  
 SFO2A: 0.00001617 sec  
 TD: 20  
 TD0: 1

CHANNEL: F1  
 NU1: 130  
 P1: 2.70 Usec  
 PL1: 20.00 dB  
 SFO1: 6.00 MHz  
 SFO2: 100.6228295 MHz

CHANNEL: F2  
 NS: 16  
 P1: 80.00 Usec  
 PL1: 0.00 dB  
 SFO1: 27.27 MHz  
 SFO2: 400.136093 MHz

F2 Processing parameters  
 SI: 32768  
 SF: 100.6228295 MHz  
 W W: 60  
 SSI: 0  
 LB: 1.00 Hz  
 GB: 0  
 B0: 1.40