

Cyclodextrins initiated ring-opening polymerization of lactide using 4-dimethylaminopyridine (DMAP) as catalyst: study of DMAP/ β -CD inclusion complex and access to new structures

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Nuclear Magnetic Resonance (NMR) analysis

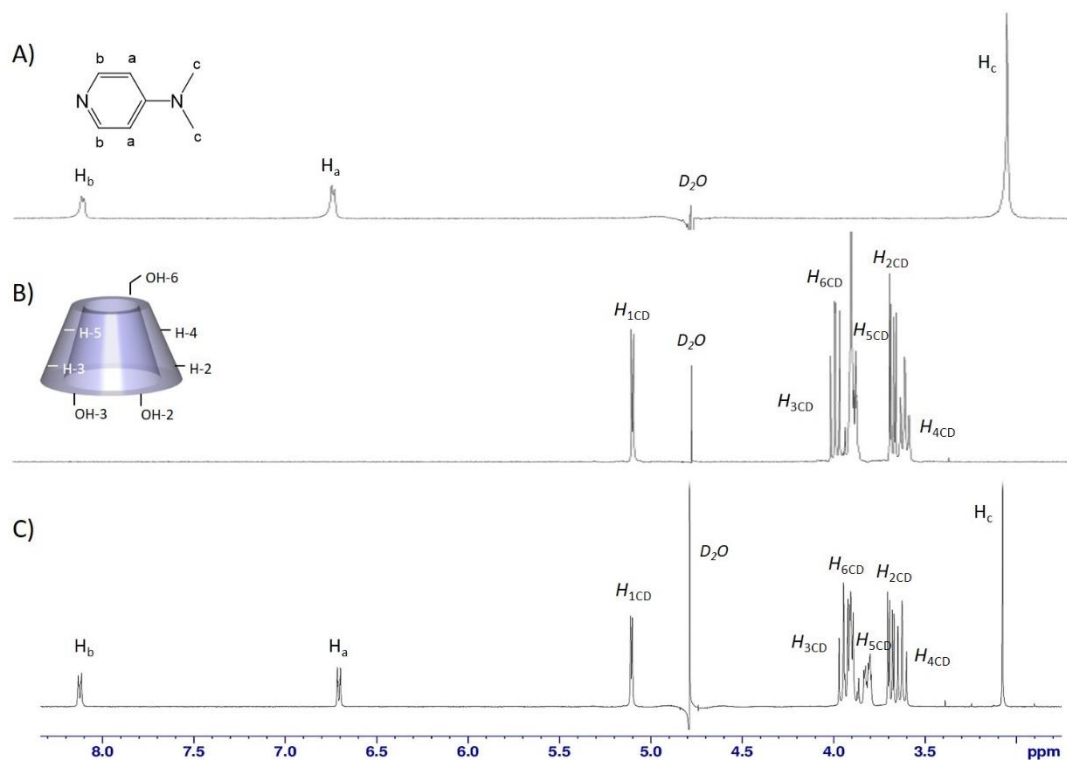


Figure S1. Superposition of ^1H NMR spectra of free DMAP (A), free β -CD (B) and a mixture (1:1) DMAP/ β -CD (C) in D_2O (3.7 mM, 400 MHz, 300 K)

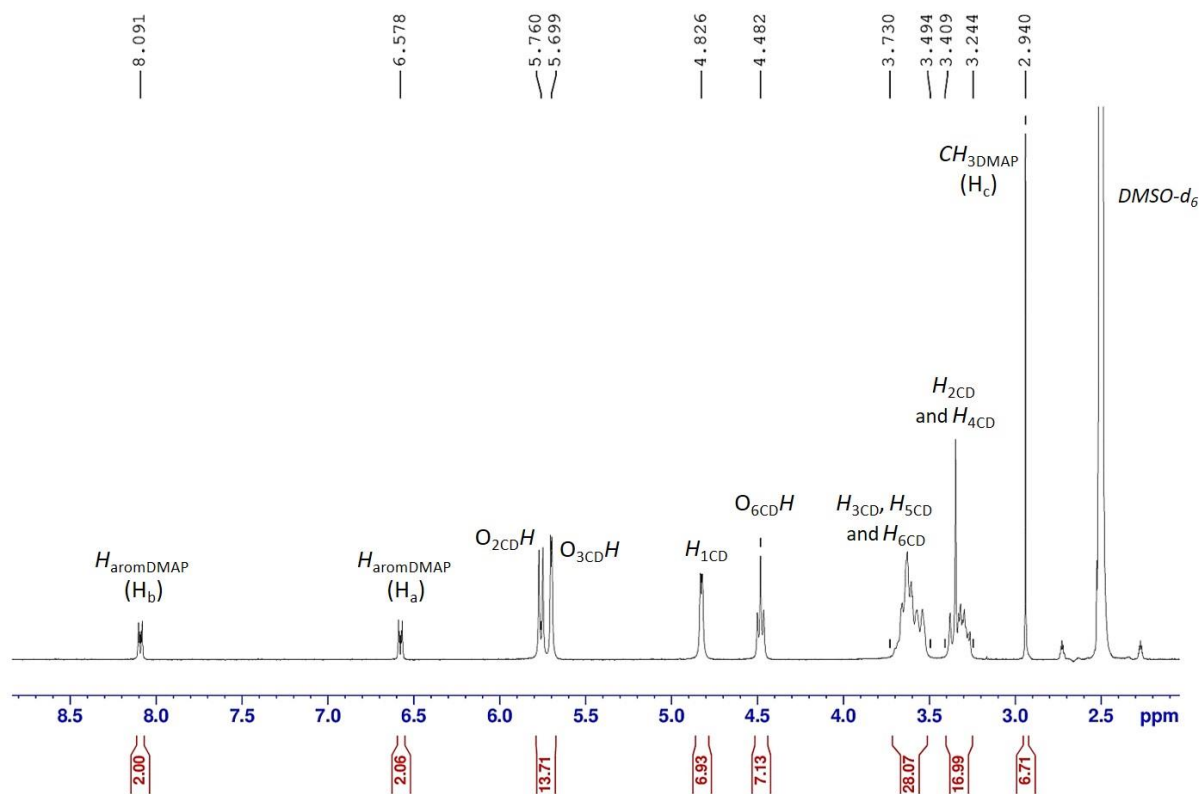


Figure S2. ¹H NMR spectrum of DMAP/β-CD inclusion complex in DMSO-*d*₆ (300 MHz, 298 K)

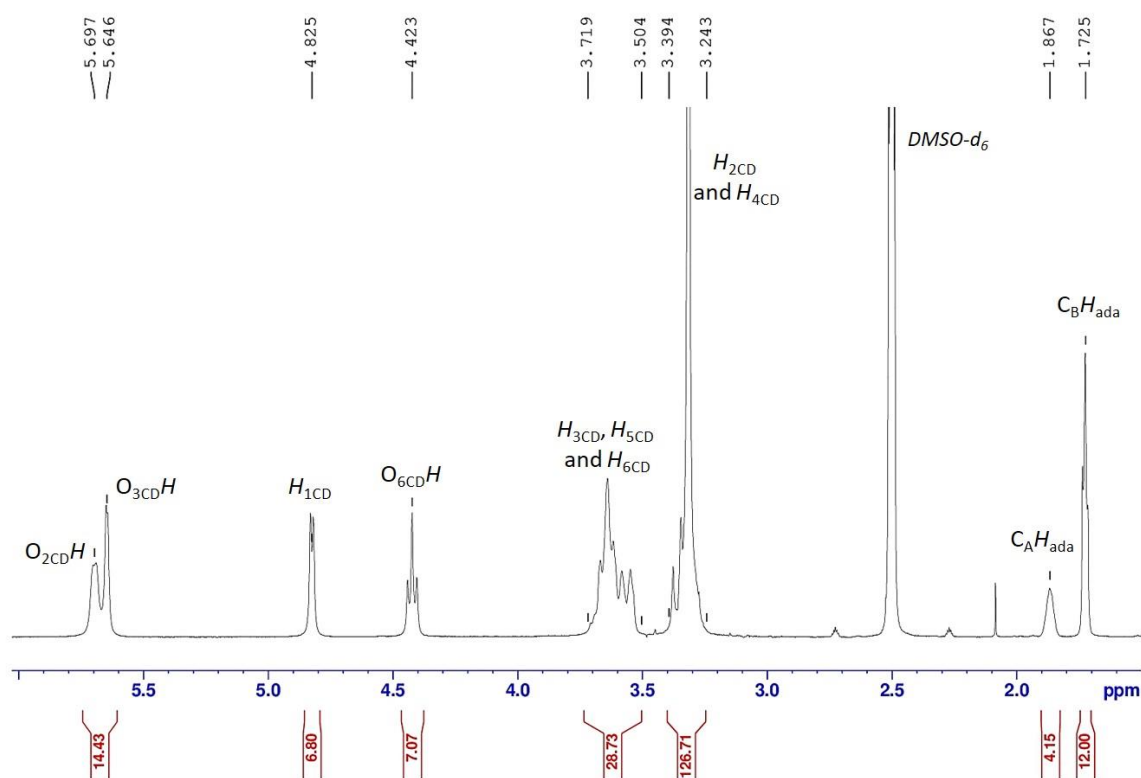


Figure S3. ¹H NMR spectrum of Adamantane/β-CD inclusion complex in DMSO-*d*₆ (300 MHz, 298 K)

Size Exclusion Chromatography (SEC) analysis

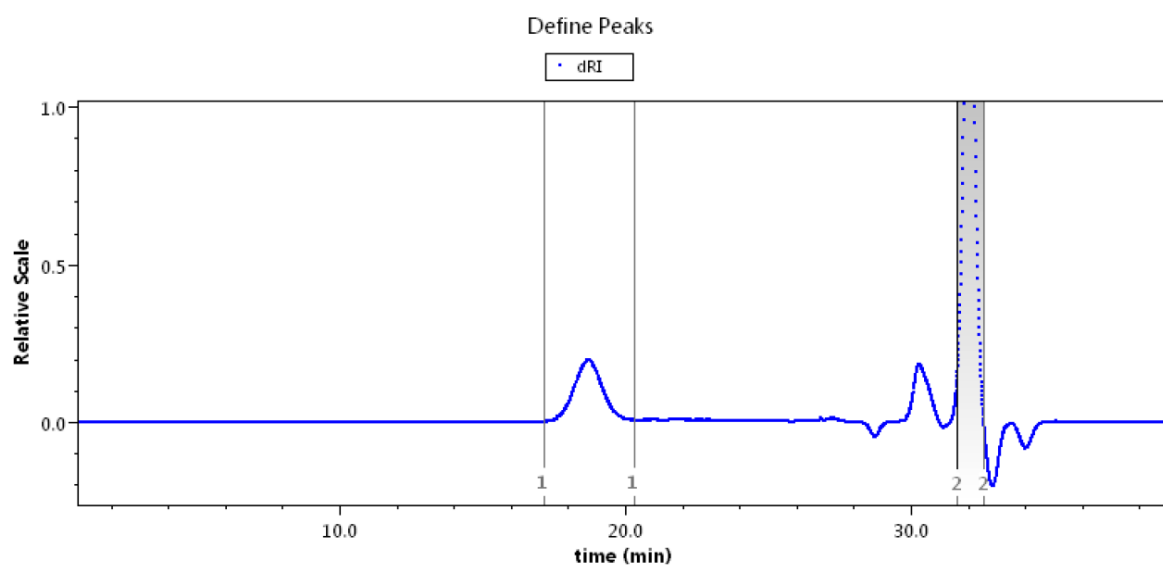


Figure S4. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 2

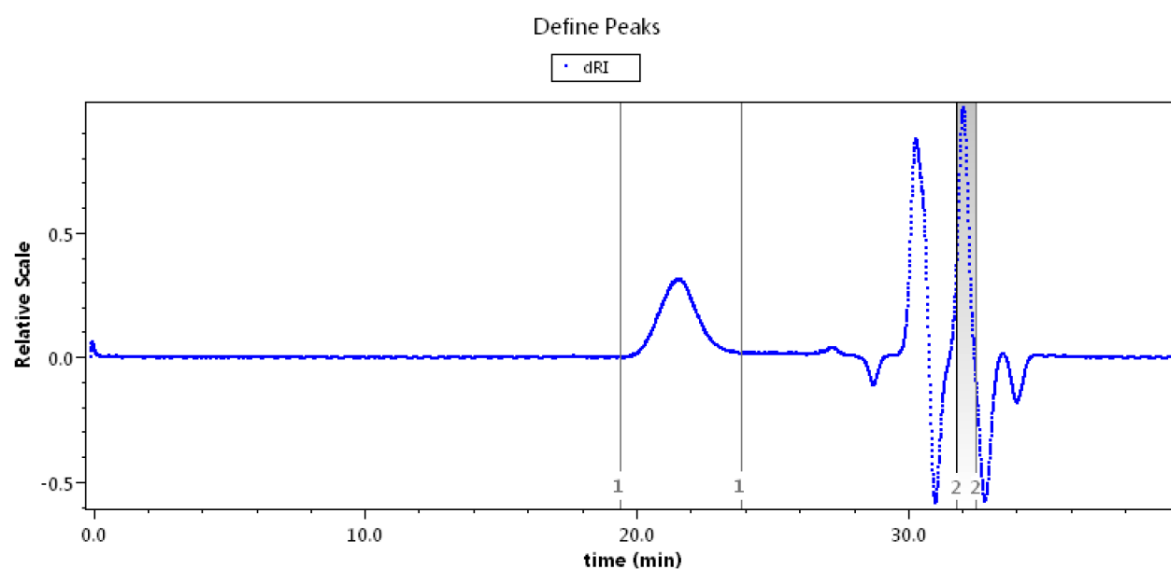


Figure S5. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 4

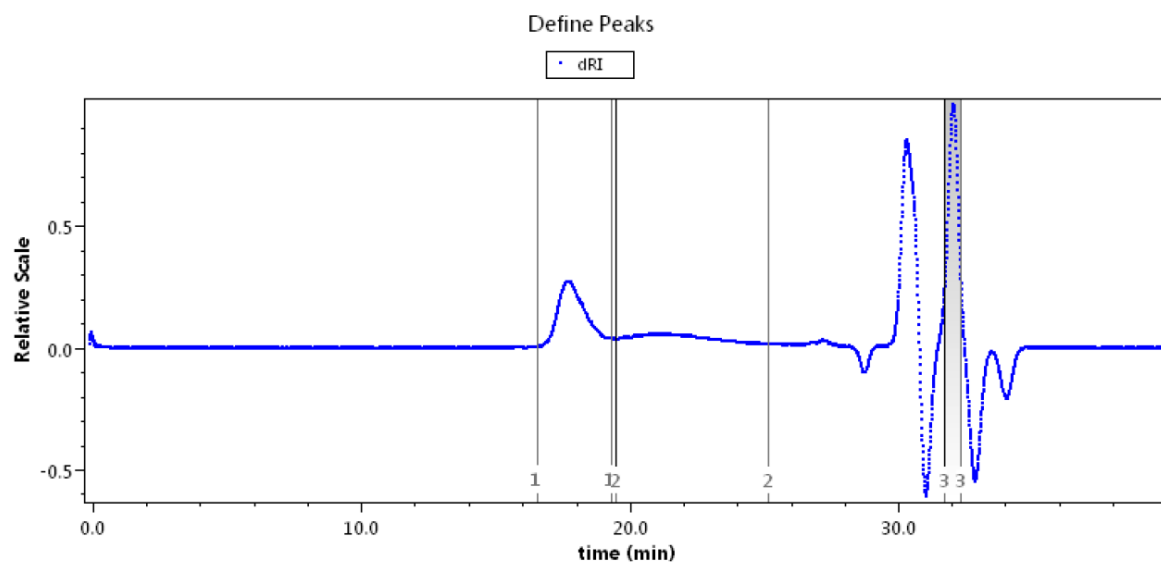


Figure S6. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 5

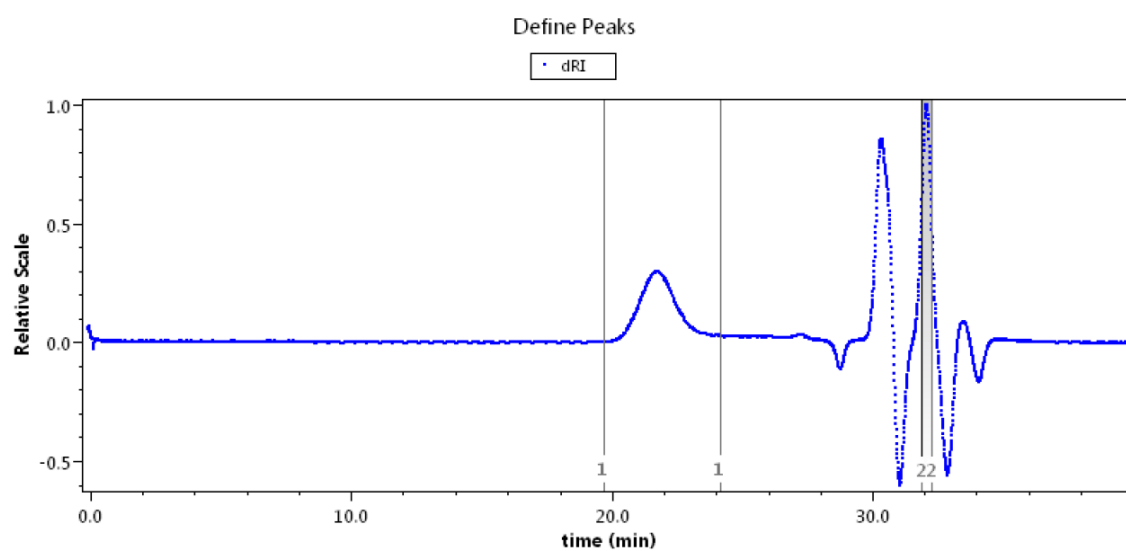


Figure S7. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 6

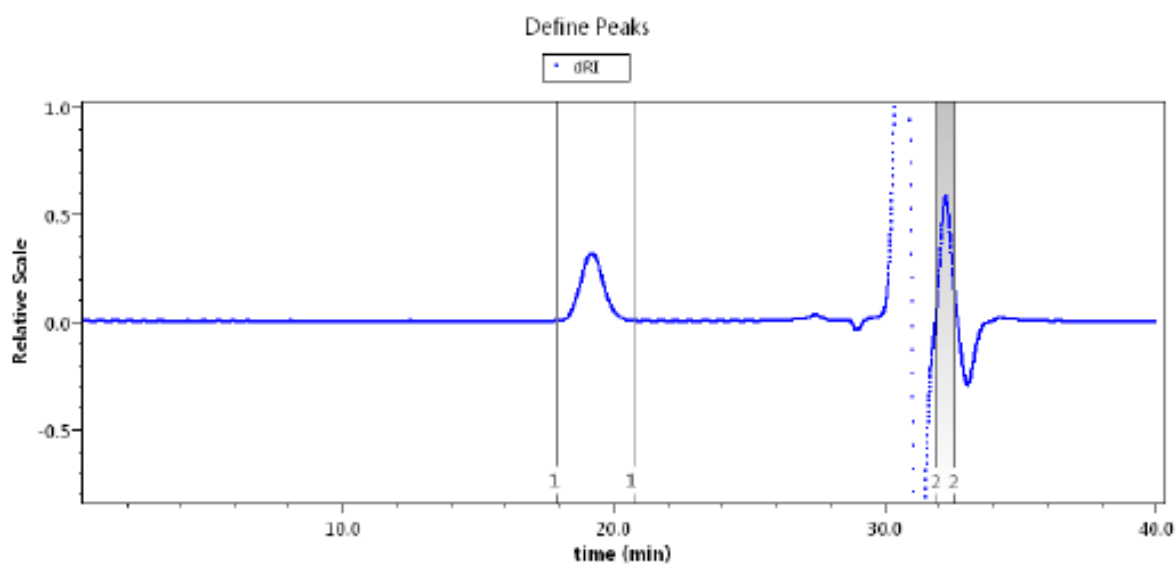


Figure S8. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 7

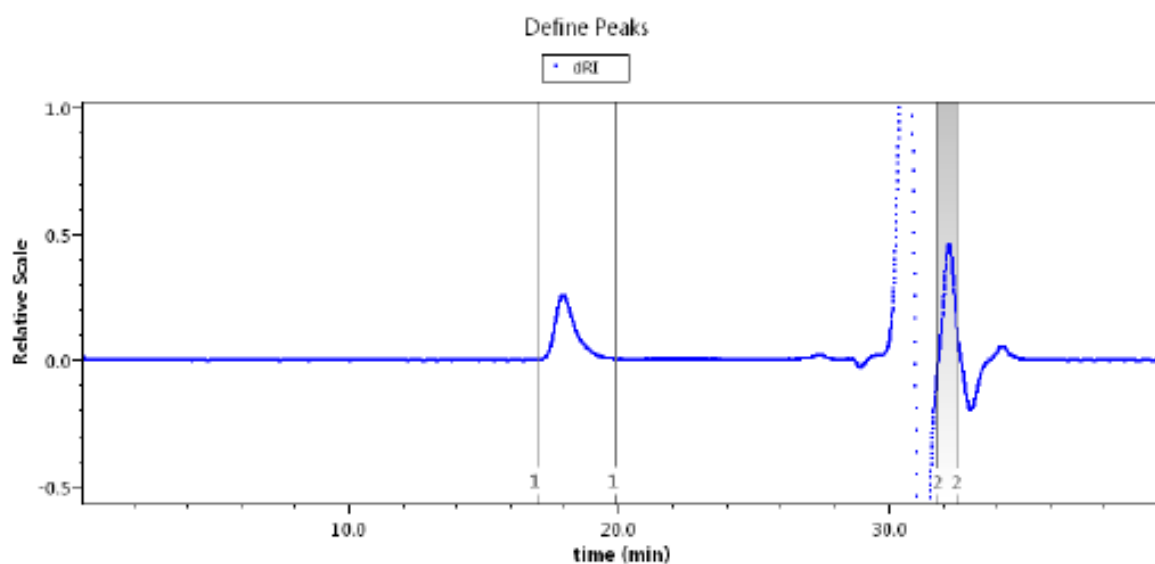


Figure S9. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 8

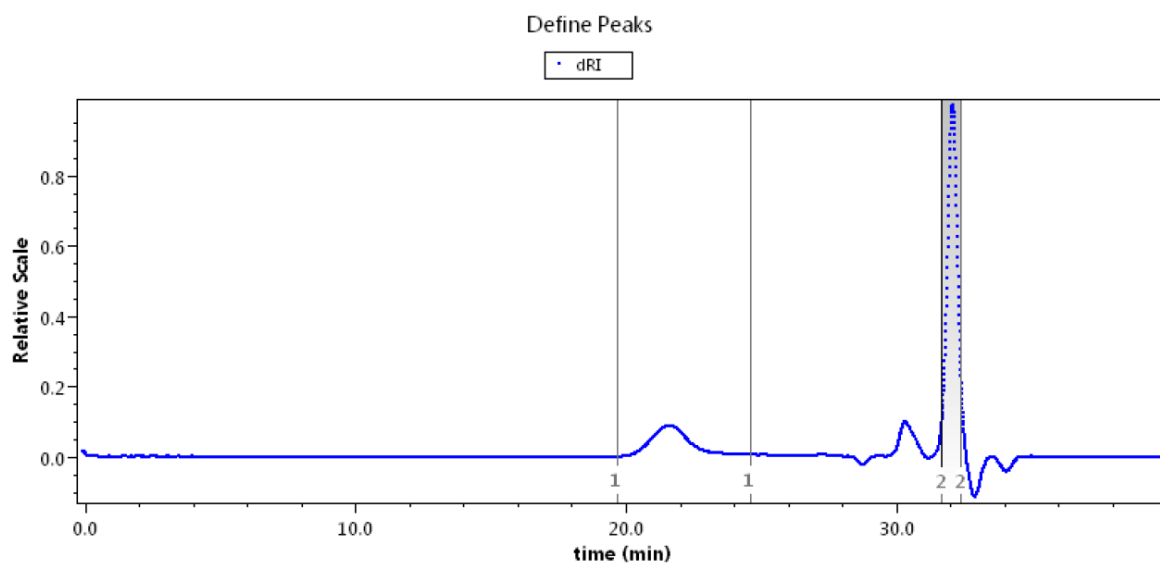


Figure S10. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 9

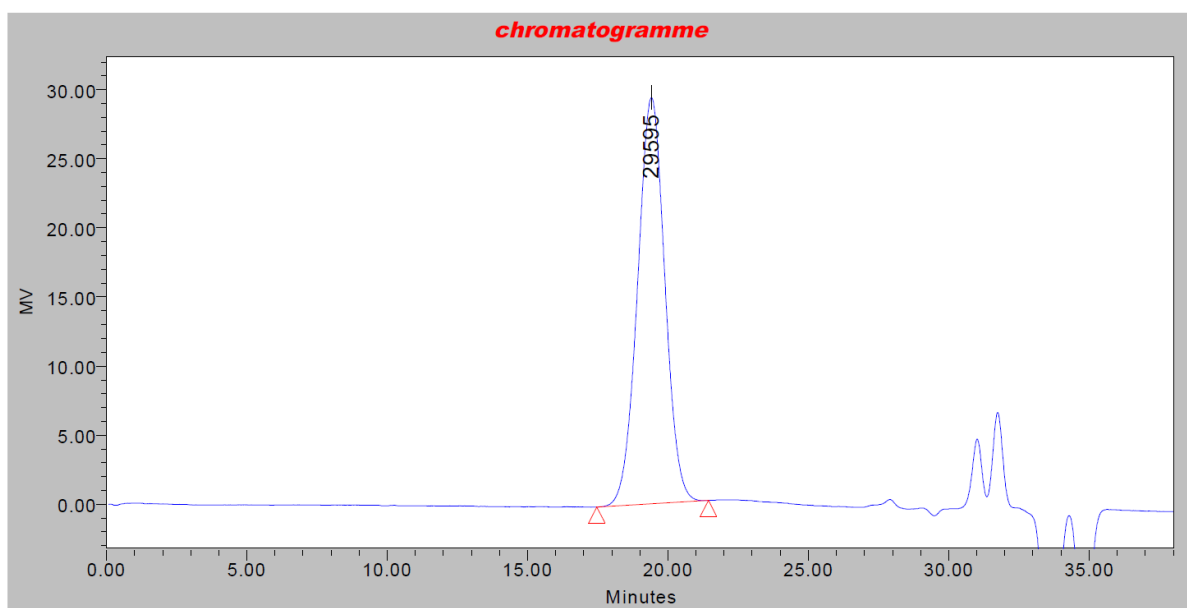


Figure S11. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 10

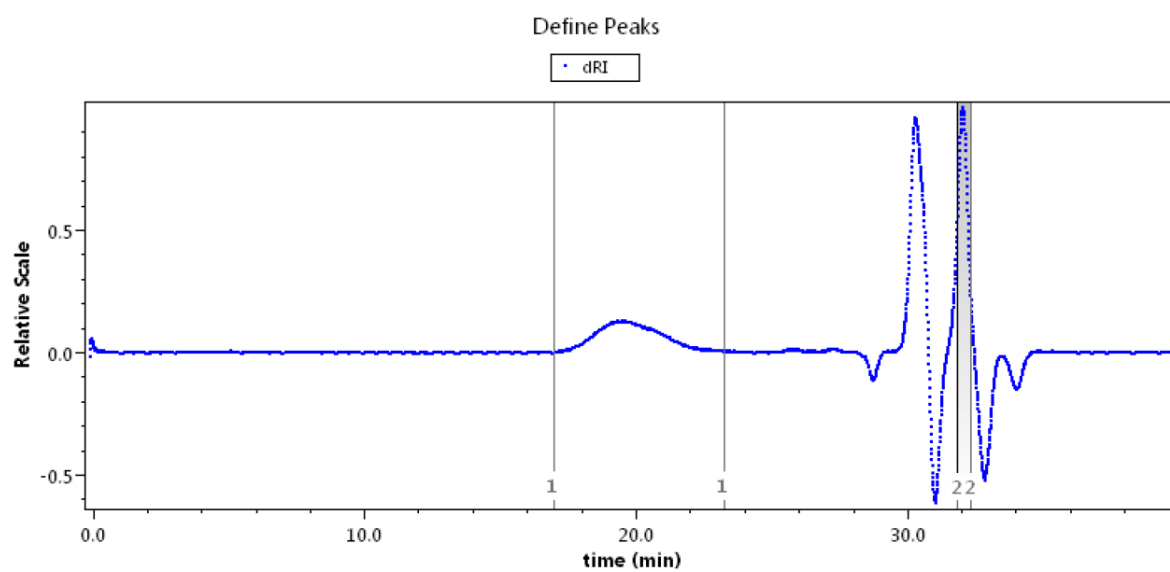


Figure S12. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 11

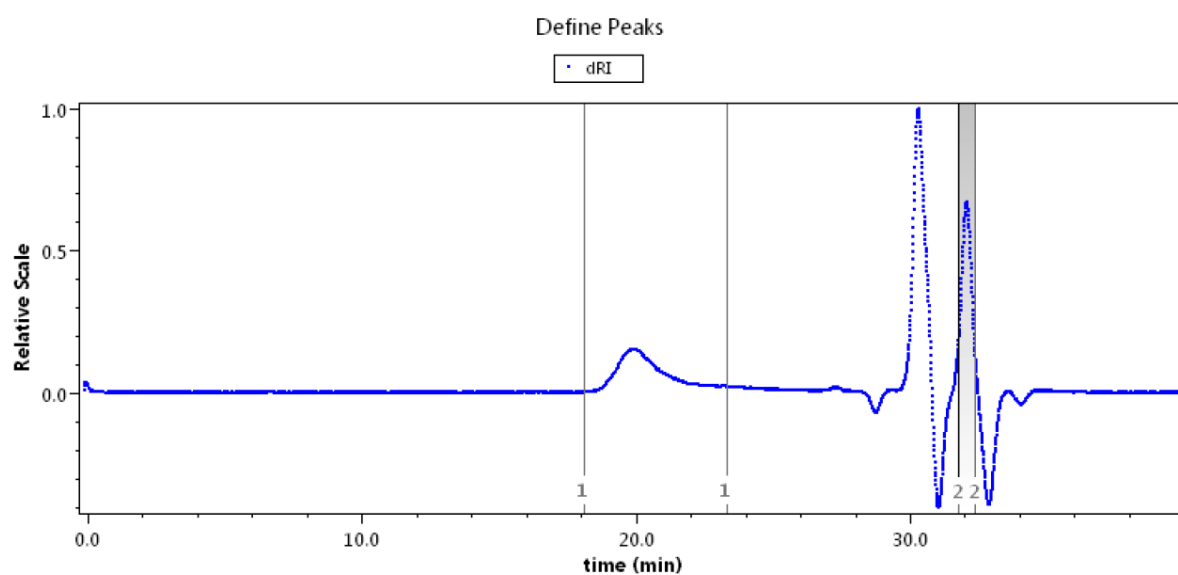
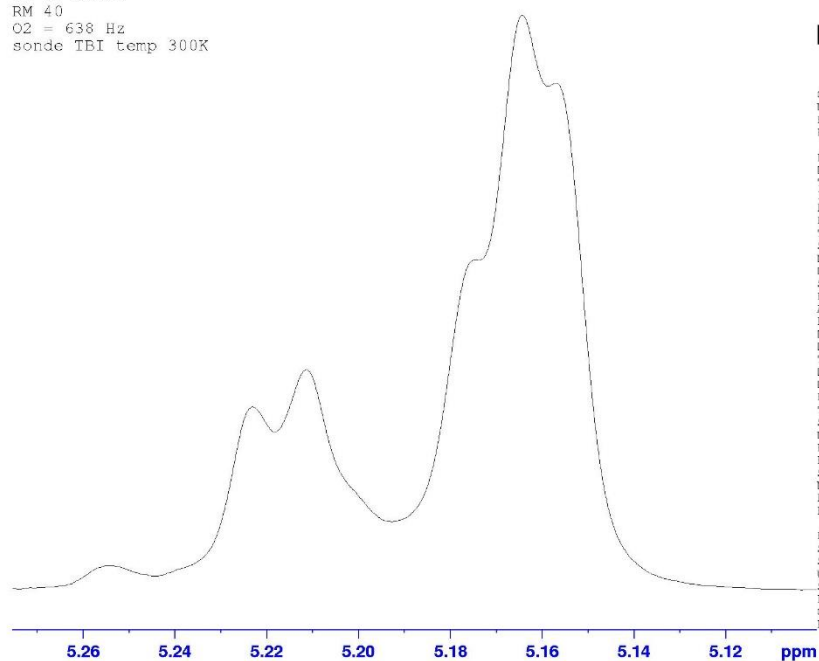


Figure S13. SEC chromatogram (THF, 40°C, polystyrene standards) of entry 12

¹H in CDCl₃
 RM 40
 Q2 = 638 Hz
 sonde TBI temp 300K



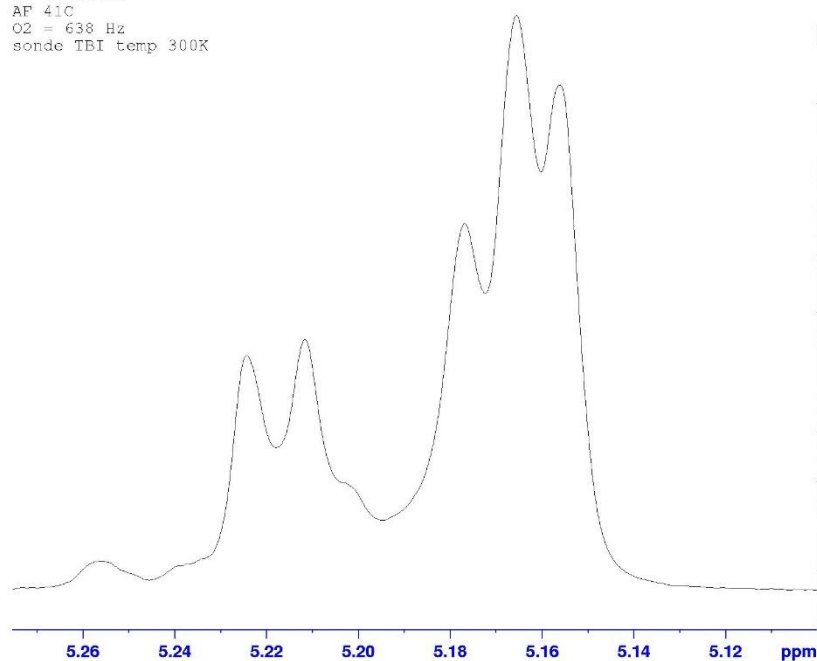
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 EXPNO 112
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220126
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 INSTRUM AvanceNeo
 PROBHD Z8277_0032 (P)
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 3703.704 Hz
 FIDRES 0.113028 Hz
 AQ 0.8473597 sec
 RG 101
 DW 135.000 usec
 DE 10.51 usec
 TE 300.0 K
 D1 1.0000000 sec
 D12 0.0000200 sec
 HODDUTY 20.2 %
 TDC 1
 SFO1 400.3315748 MHz
 NUC1 1H
 FI 10.00 usec
 PLW1 10.7729976 W
 SFO2 400.3306380 MHz
 NUC2 1H
 PLW2 10.7729976 W
 PLW24 0.00068949 W

F2 - Processing parameters
 SI 65536
 SF 400.3300101 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S14. ¹H Homonuclear decoupled NMR of Entry 2

¹H in CDCl₃
 AF 41C
 O2 = 638 Hz
 sonde TBI temp 300K



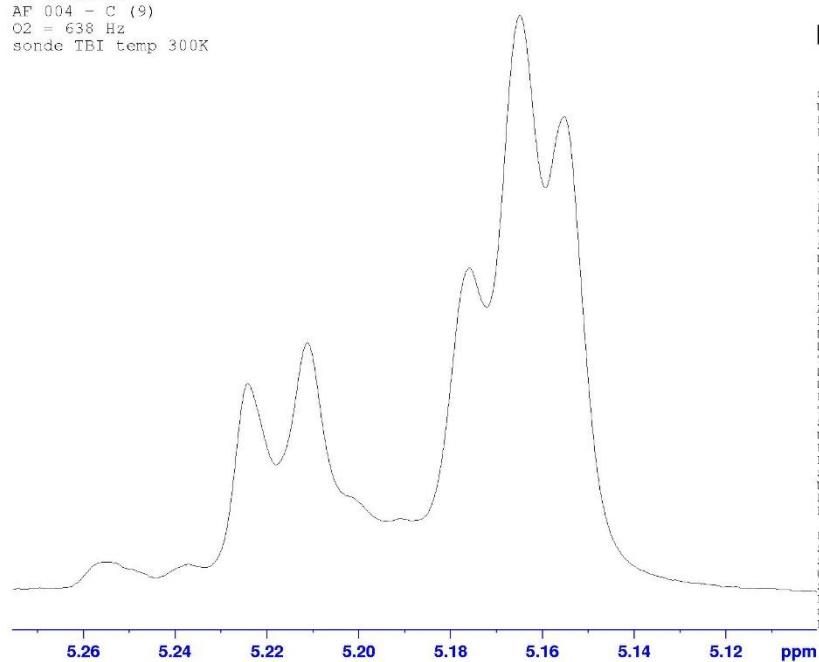
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 EXPNO 111
 PROCNO 1

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 PROBHD Z8277_0032 (PE
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 3703.704 Hz
 FIDRES 0.113028 Hz
 AQ 0.8473597 sec
 RG 101
 DW 135.000 usec
 DE 10.51 usec
 TE 300.2 K
 D1 1.0000000 sec
 D12 0.0000200 sec
 HODDUTY 20.2 %
 TDC 1
 SFO1 400.3315748 MHz
 NUC1 1H
 F1 10.00 usec
 PLW1 10.7729976 W
 SFO2 400.3306380 MHz
 NUC2 1H
 PLW2 10.7729976 W
 PLW24 0.00068949 W

F2 - Processing parameters
 SI 65536
 SF 400.3300103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S15. ¹H Homonuclear decoupled NMR of Entry 5

¹H in CDCl₃
 AF 004 - C (9)
 Q2 = 638 Hz
 sonde TBI temp 300K



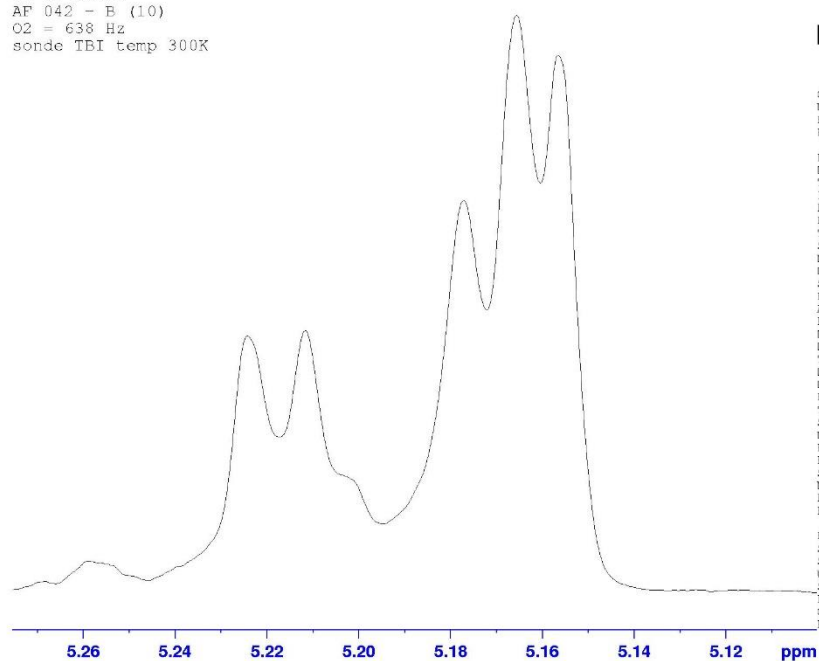
Current Data Parameters
 NAME MB-JM-20222601
 EXPNO 121
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220126
 Time 11.28 h
 INSTRUM AvanceNeo
 PROBHD Z8277_0032 (PE
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 3703.704 Hz
 FIDRES 0.113028 Hz
 AQ 8.8473597 sec
 RG 101
 DW 135.000 usec
 DE 10.51 usec
 TE 300.0 K
 D1 1.00000000 sec
 D12 0.00002000 sec
 HDUTY 20.2 %
 TDC 1
 SFO1 400.3315748 MHz
 NUC1 ¹H
 F1 10.00 usec
 PLW1 10.77299975 W
 SFO2 400.3306380 MHz
 NUC2 ¹H
 PLW2 10.77299975 W
 PLW24 0.00068949 W

F2 - Processing parameters
 SI 65536
 SF 400.3300103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S16. ¹H Homonuclear decoupled NMR of Entry 10

¹H in CDCl₃
 AF 042 - B (10)
 Q2 = 638 Hz
 sonde TBI temp 300K



Current Data Parameters
 NAME MS-GM-20222601
 EXPNO 119
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220126
 Time 11.19 h
 INSTRUM AvanceNeo
 PROBHD Z8277_0032 (PE
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 3703.704 Hz
 FIDRES 0.113028 Hz
 AQ 0.8473597 sec
 RG 101
 DW 135.000 usec
 DE 10.51 usec
 TE 300.2 K
 D1 1.00000000 sec
 D12 0.00002000 sec
 HODDUTY 20.2 %
 TDC 1
 SFO1 400.3315748 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 10.7729976 W
 SFO2 400.3306300 MHz
 NUC2 1H
 PLW2 10.7729976 W
 PLW24 0.00068949 W

F2 - Processing parameters
 SI 65536
 SF 400.3300103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S17. ¹H Homonuclear decoupled NMR of Entry 11