

Parameter	Value
1 Data File Name	/ Users/ rebeccaakande/ OneDrive - University of Pretoria/ NMR2/ Rebecca-CPD-55/ 10/ fid
2 Title	55
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Instrument	spect
6 Author	Rebecca Akande
7 Solvent	CDCl3
8 Temperature	297.4
9 Pulse Sequence	zg30
10 Experiment	1D
11 Probe	Z820201_0164 (PA BBI 400S1 H-BB-D-05 Z)
12 Number of Scans	128
13 Receiver Gain	181.0
14 Relaxation Delay	1.0000
15 Pulse Width	9.0000
16 Presaturation Frequency	
17 Acquisition Time	4.0894
18 Acquisition Date	2020-08-29T10:48:25
19 Modification Date	2020-08-29T10:48:26
20 Purity	98.37 %
21 Spectrum Quality	-0.229
22 Spectrometer Frequency	400.21
23 Spectral Width	8012.8
24 Lowest Frequency	-1544.8
25 Nucleus	¹ H
26 Acquired Size	32768
27 Spectral Size	65536
28 Digital Resolution	0.12

¹H NMR (400 MHz, CDCl₃) δ 5.35 (d, *J* = 5.0 Hz, 1H), 3.52 (tt, *J* = 10.6, 4.7 Hz, 1H), 2.34 – 2.17 (m, 2H), 2.09 – 1.91 (m, 3H), 1.91 – 1.77 (m, 3H), 1.76 – 1.41 (m, 13H), 1.41 – 1.30 (m, 4H), 1.29 (d, *J* = 7.2 Hz, 4H), 1.25 (s, 7H), 1.24 – 1.07 (m, 9H), 1.02 (d, *J* = 7.9 Hz, 8H), 0.93 – 0.86 (m, 6H), 0.86 – 0.82 (m, 5H), 0.82 – 0.72 (m, 5H), 0.69 (d, *J* = 7.5 Hz, 3H).

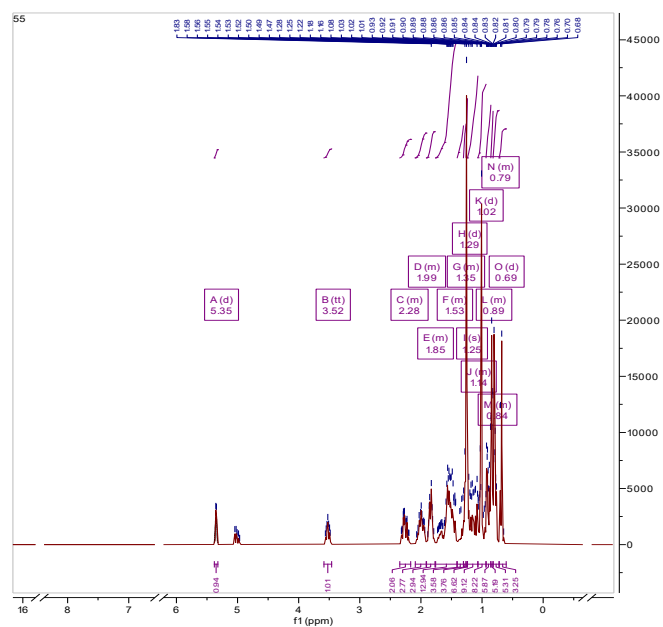


Fig. 3. ¹H NMR of Stigmasterol

¹³C NMR (101 MHz, CDCl₃) δ 140.77, 121.73, 71.82, 50.14, 42.32, 37.26, 36.52, 31.92, 31.68, 29.71, 21.10, 19.41, 11.87.

Parameter	Value
1 Data File Name	/ Users/ rebeccaakande/ OneDrive - University of Pretoria/ NMR2/ Rebecca-CPD-55/ 11/ fid
2 Title	55
3 Origin	Bruker BioSpin GmbH
4 Owner	nmsu
5 Instrument	spect
6 Author	Rebecca Akande
7 Solvent	CDCl ₃
8 Temperature	297.6
9 Pulse Sequence	zgpg30
10 Experiment	1D
11 Probe	Z820201_0164 (PA BBI 400S1 H-BB-D-05 Z)
12 Number of Scans	3000
13 Receiver Gain	362.0
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Presaturation Frequency	
17 Acquisition Time	1.3631
18 Acquisition Date	2020-08-29T13:41:42
19 Modification Date	2020-08-29T13:41:44
20 Purity	100.00 %
21 Spectrum Quality	0.269
22 Spectrometer Frequency	100.64
23 Spectral Width	24038.5
24 Lowest Frequency	-1956.4
25 Nucleus	13C
26 Acquired Size	32768
27 Spectral Size	65536
28 Digital Resolution	0.37

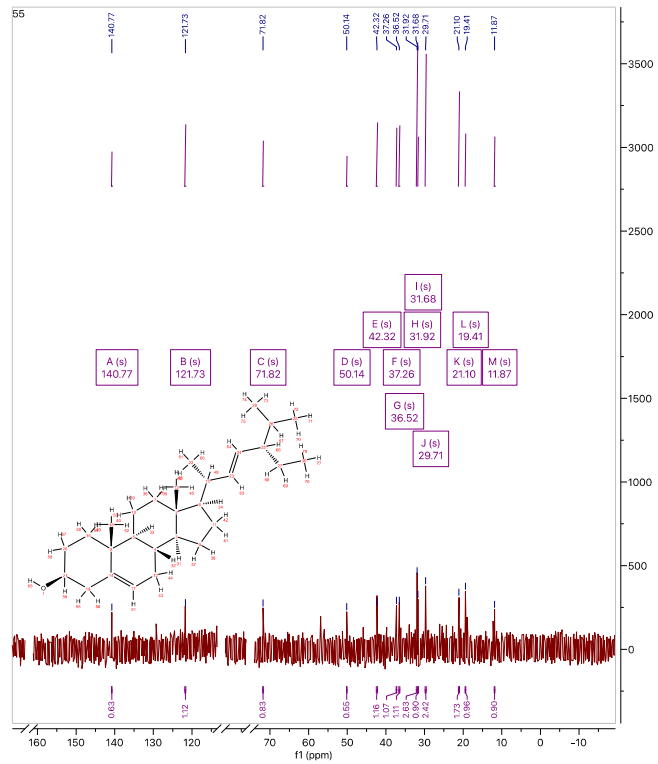


Fig. 4. ¹³CNMR of Stigmasterol

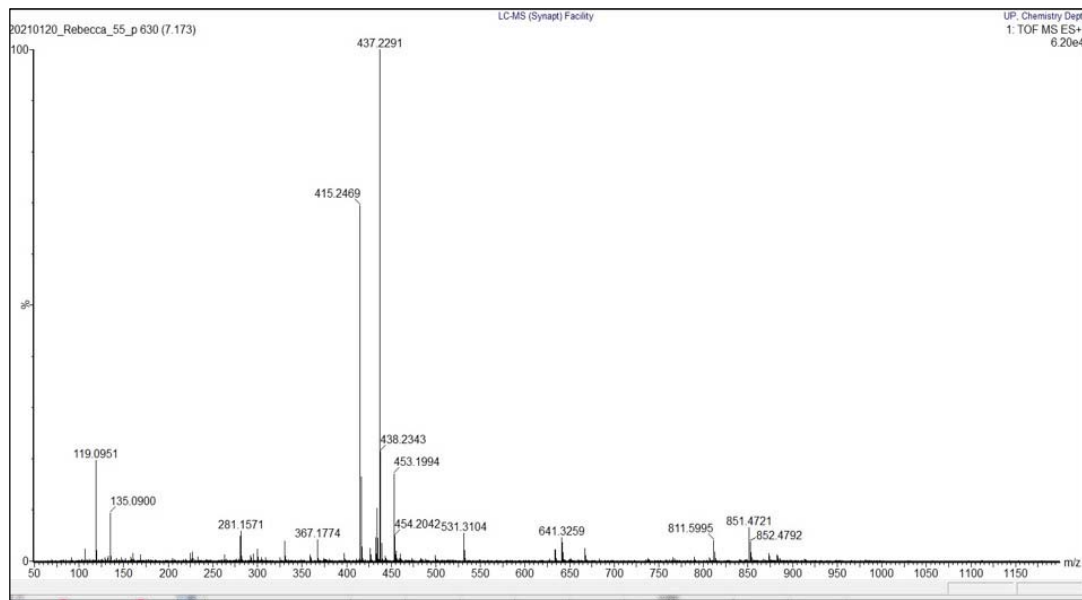


Fig. 5. LCMS of stigmasterol

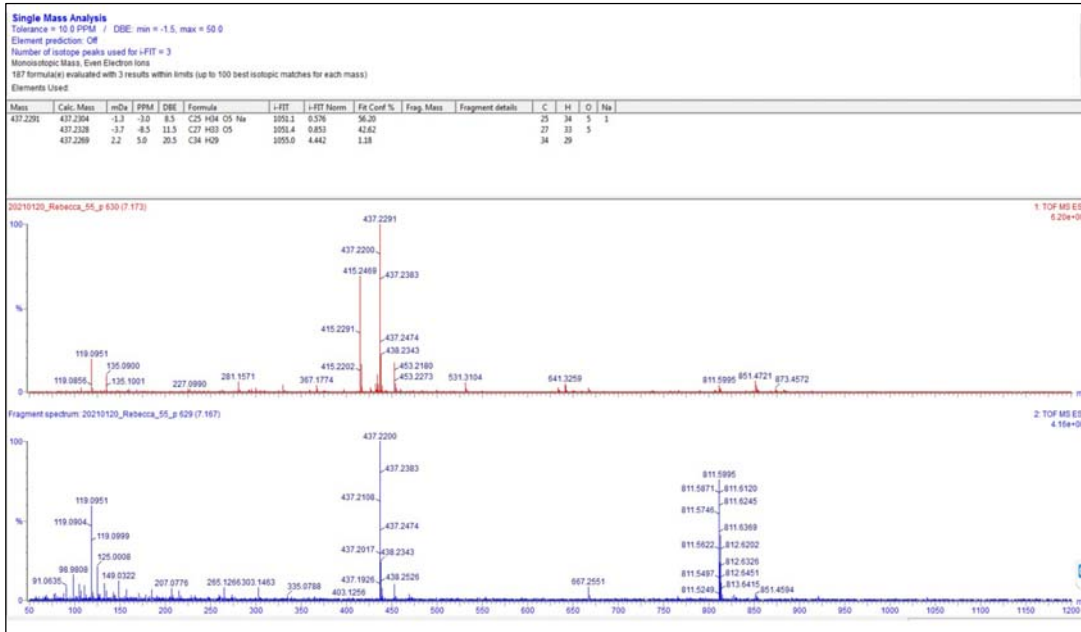


Fig. 6. LCMS of stigmasterol

Peak True - sample "20210305F Rebecca 50:1", peak 181, at 2120.4 s

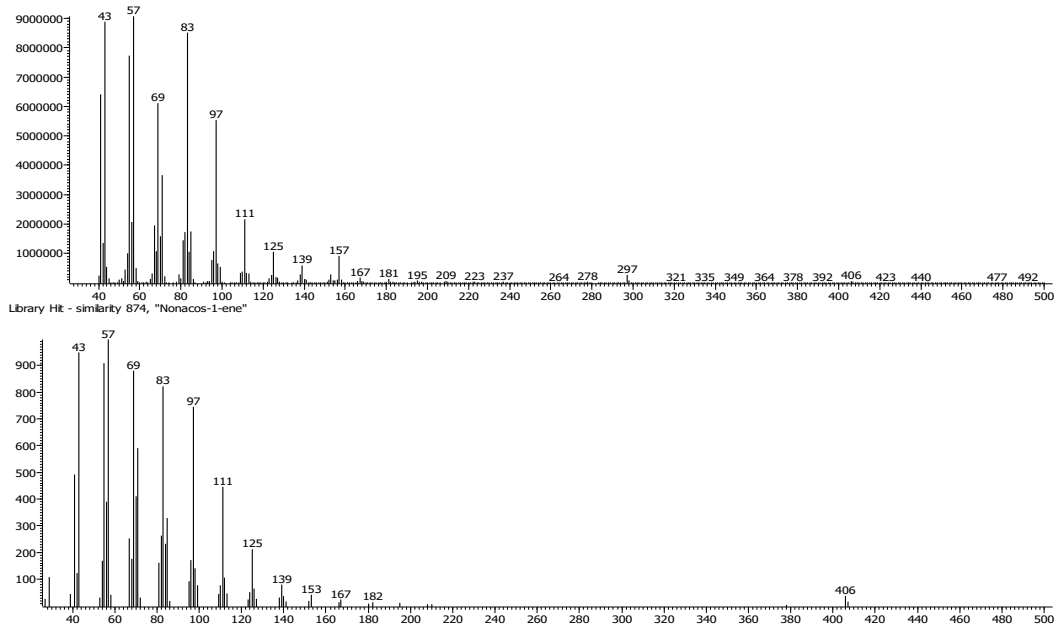


Fig 7. MS of Nonacosene

Peak True - sample "20210305G Rebecca 124 (4):1", peak 263, at 1854.3 s

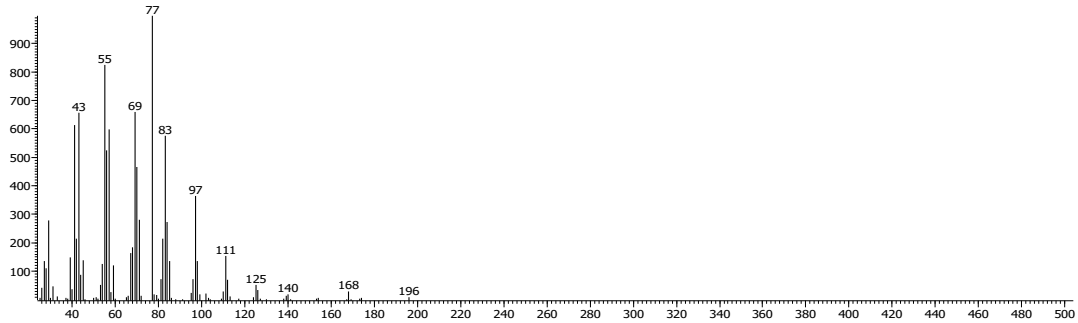
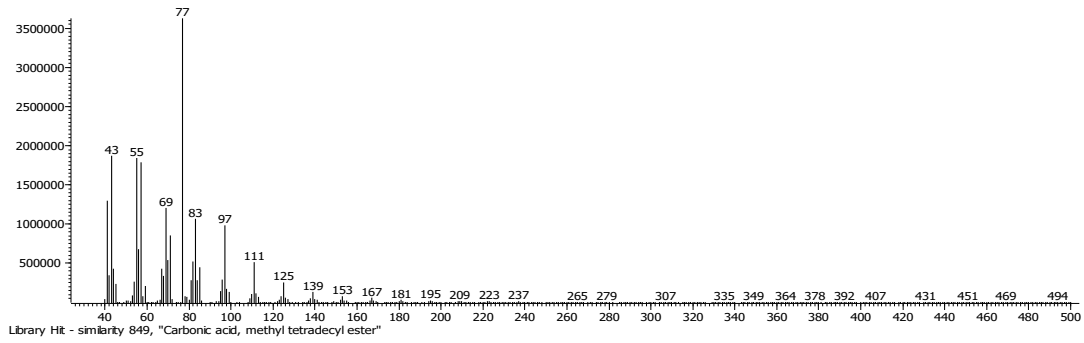


Fig. 8. MS of Carbonic acid

Peak True - sample "20210305E Rebecca 63:1", peak 67, at 1960.8 s

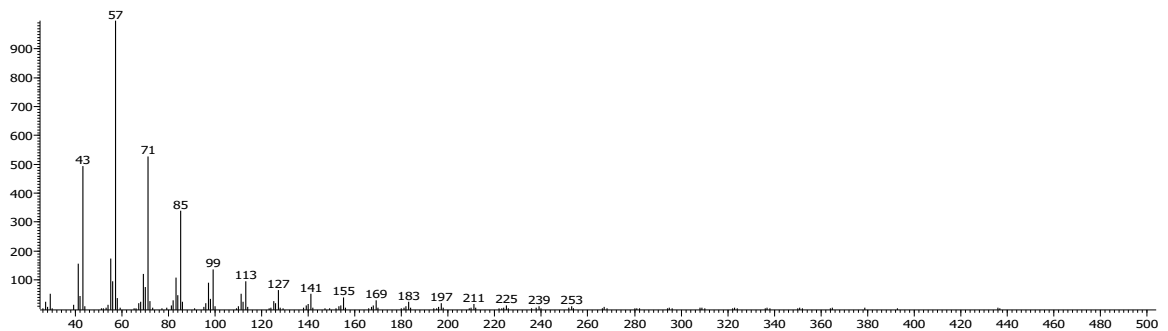
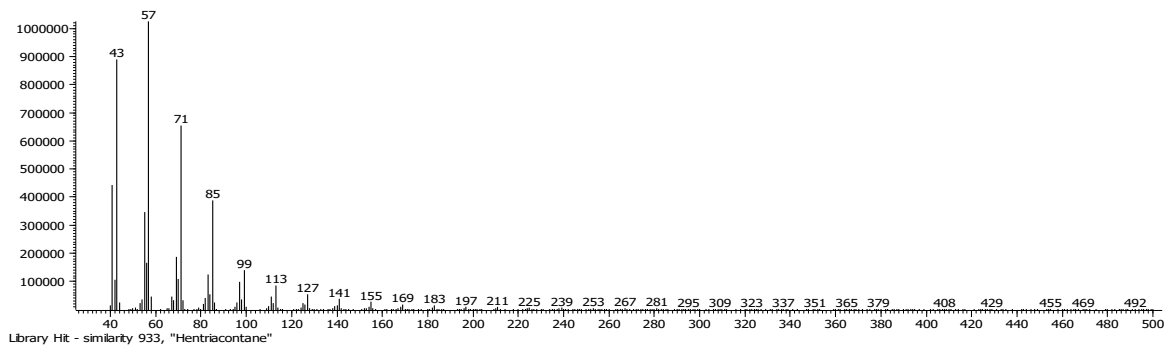
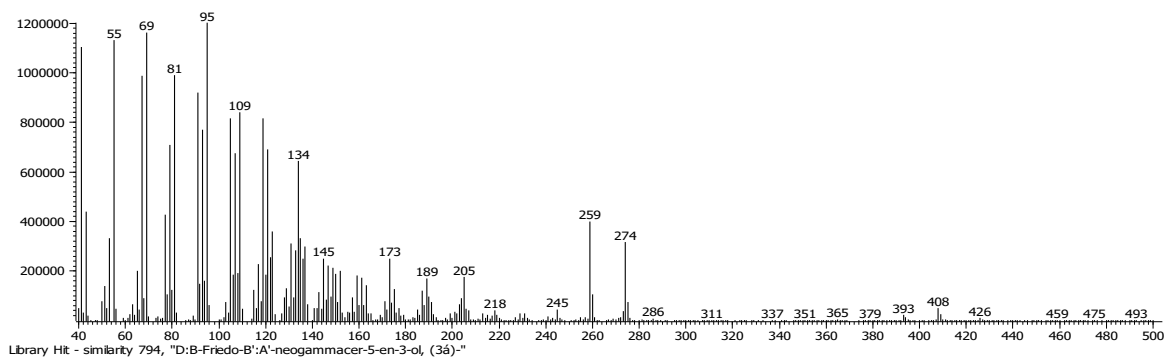


Fig. 9. MS of Hentriacontane

Peak True - sample "20210305D Rebecca 124(3):1", peak 167, at 1922.5 s



Library Hit - similarity 794, "D:B-Friedo-B':A'-neogammacer-5-en-3-ol, (3 α)"

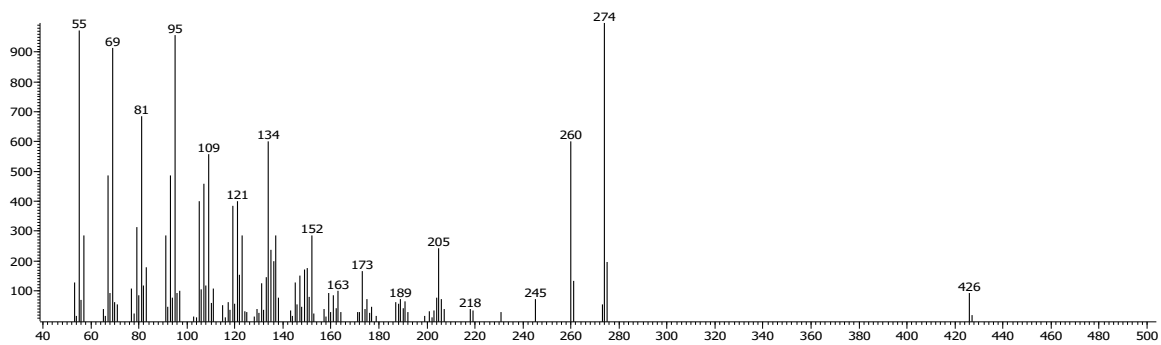


Fig 10. MS of D:B-Friedo-B':A'-neogammacer-5-en-3-ol, (3 α)