

Searching for Novel Sources of Hydrogen Sulfide Donors: Chemical Profiling of *Polycarpa aurata* Extract and Evaluation of the Anti-inflammatory Effects

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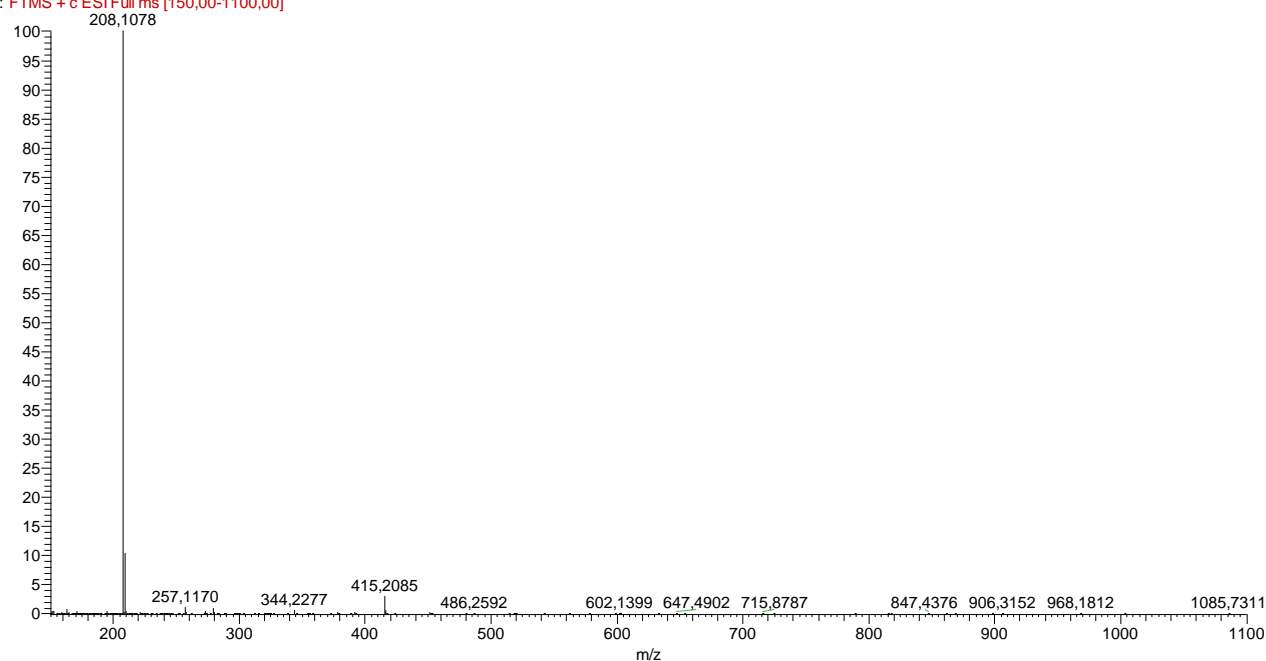
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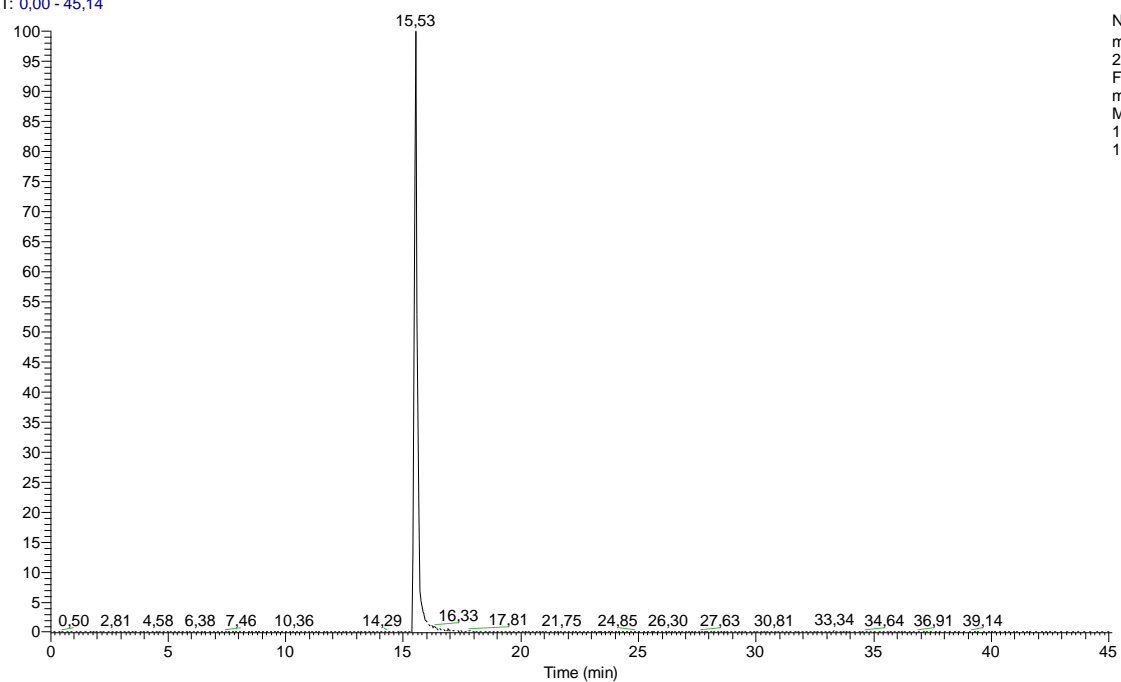
Table of content

Figure S1. LC-HRMS of 1 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	2
Figure S2. LC-HRMS of 2 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	4
Figure S3. LC-HRMS of 3 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	5
Figure S4. LC-HRMS of 4 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	7
Figure S5. LC-HRMS of 5 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	8
Figure S6. LC-HRMS of 6 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	11
Figure S7. LC-HRMS of 7 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	13
Figure S8. LC-HRMS of 8 : (A) Extracted ion Chromatogram (XIC) at the selected ion, (B) relevant HRMS and (C) relevant HRMS ² spectra	14
Figure S9. ¹ H NMR spectrum (700 MHz) in CDCl ₃ of PAB2	16
Figure S10. COSY spectrum in CDCl ₃ of PAB2	16
Figure S11. Downfield region enlargement of COSY spectrum in CDCl ₃ of PAB2	17
Figure S12. HSQC spectrum in CDCl ₃ of PAB2;	17
Figure S13. HMBC spectrum in CDCl ₃ of PAB2	18
Figure S14. Downfield region enlargement of HMBC spectrum in CDCl ₃ of PAB2	18

18052023PABMEOH10 #1627 RT: 15.53 AV: 1 NL: 2,98E7
F: FTMS + c ESI Full ms [150,00-1100,00]



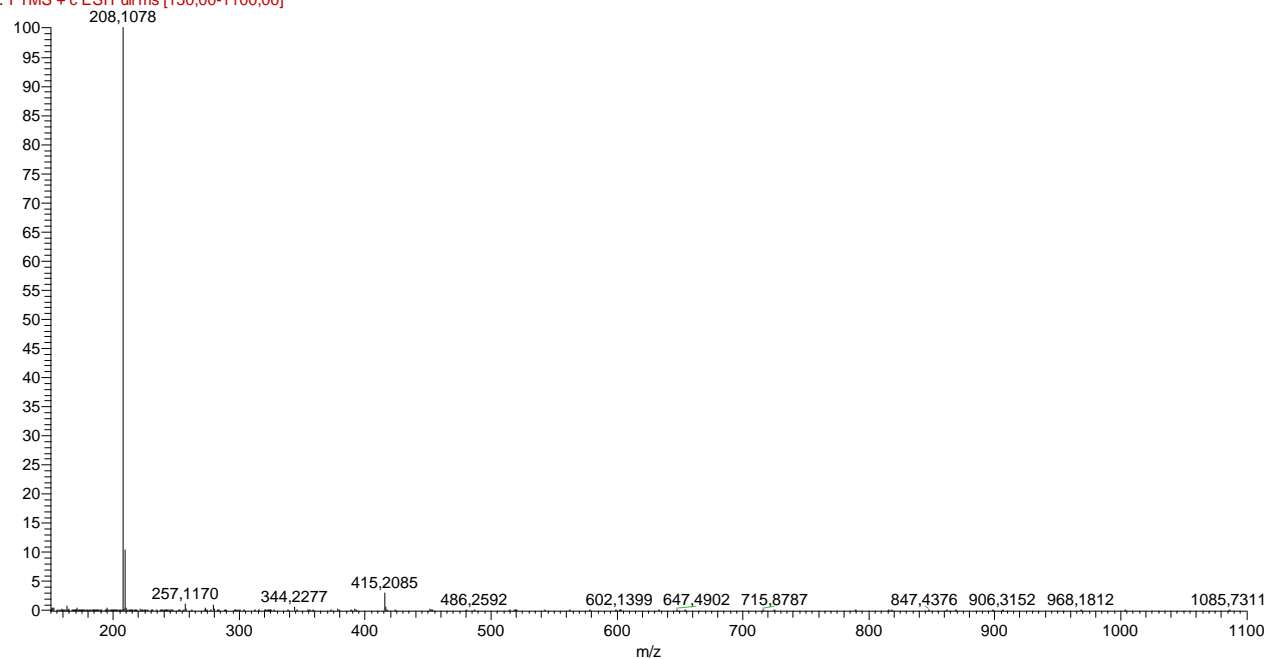
RT: 0,00 - 45,14



NL: 2,98E7
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F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #1627 RT: 15,53 AV: 1 NL: 2,98E7

F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #1646 RT: 15,72 AV: 1 NL: 7,74E5

T: FTMS + c ESI d Full ms2 208,11@cid25,00 [50,00-220,

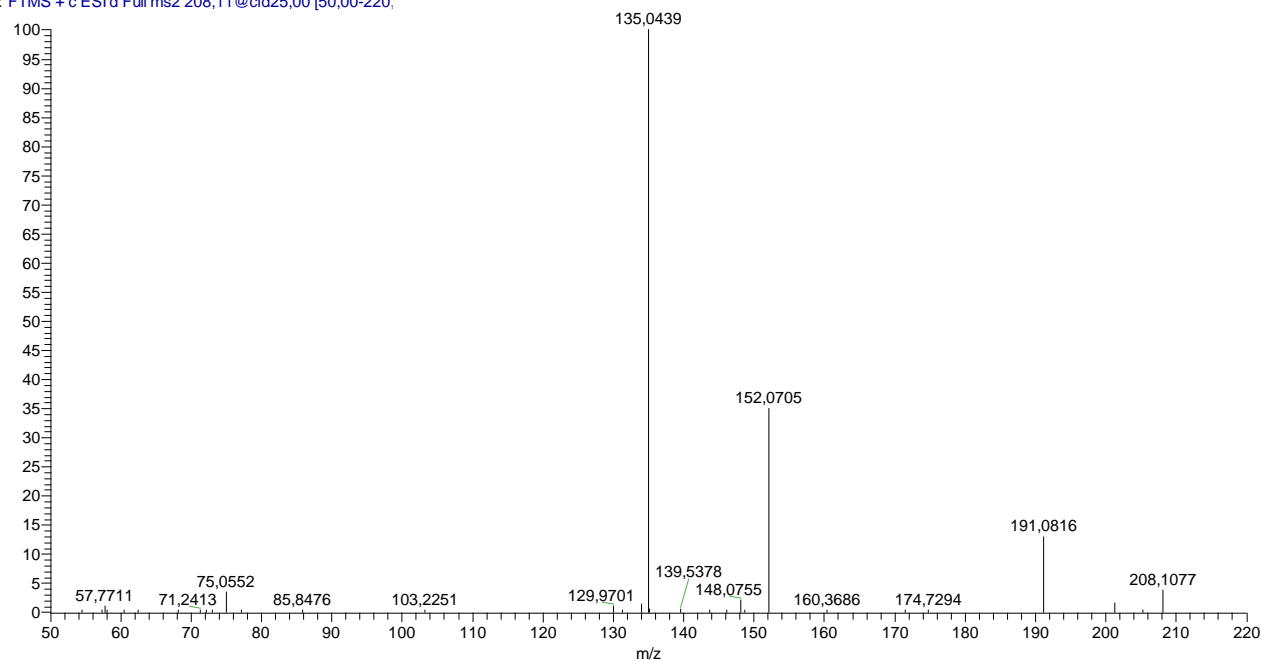
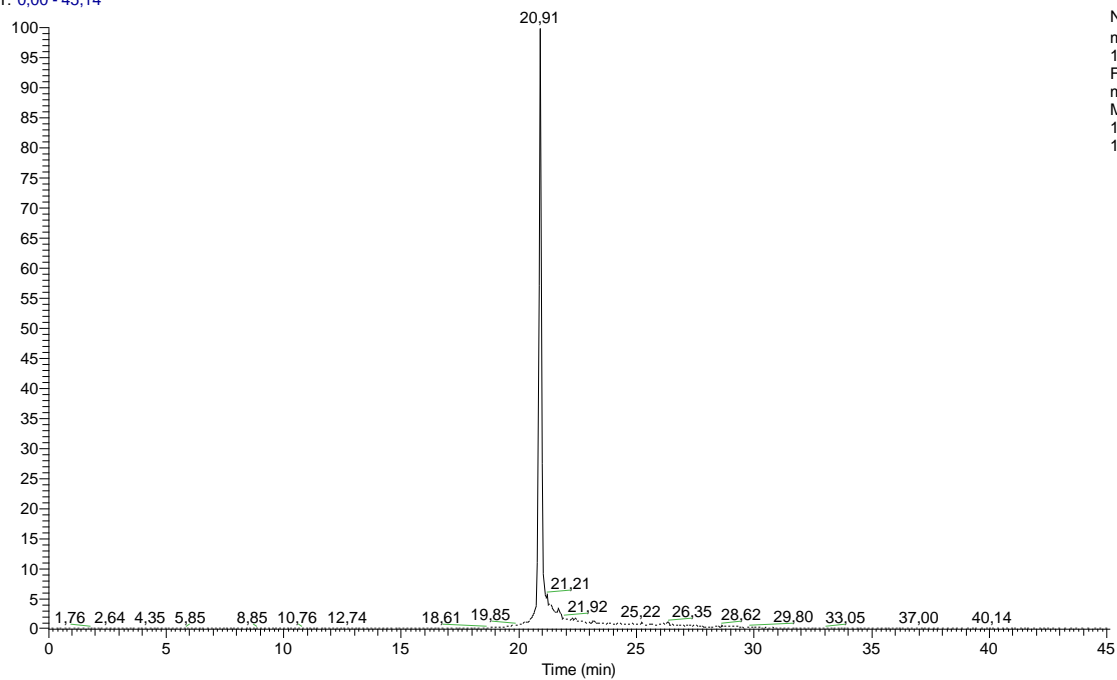


Figure S1. LC-HRMS analyses of **1** on an LTQ Orbitrap XLTM Hybrid FT Mass Spectrometer system: (A) Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 208.1078, (B) relevant HRMS spectrum and (C) relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 208.1 as precursor.

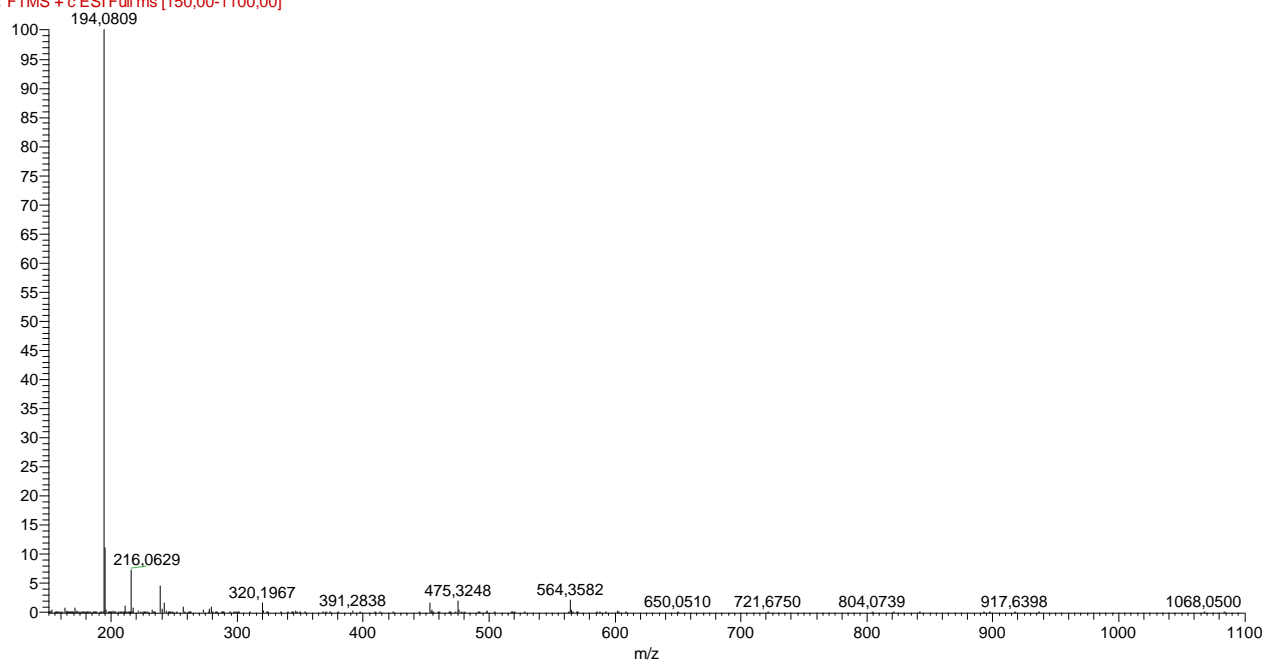
RT: 0,00 - 45,14



NL: 6,22E7
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ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #2185 RT: 20,84 AV: 1 NL: 3,56E7

F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #2228 RT: 21,28 AV: 1 NL: 2,38E6
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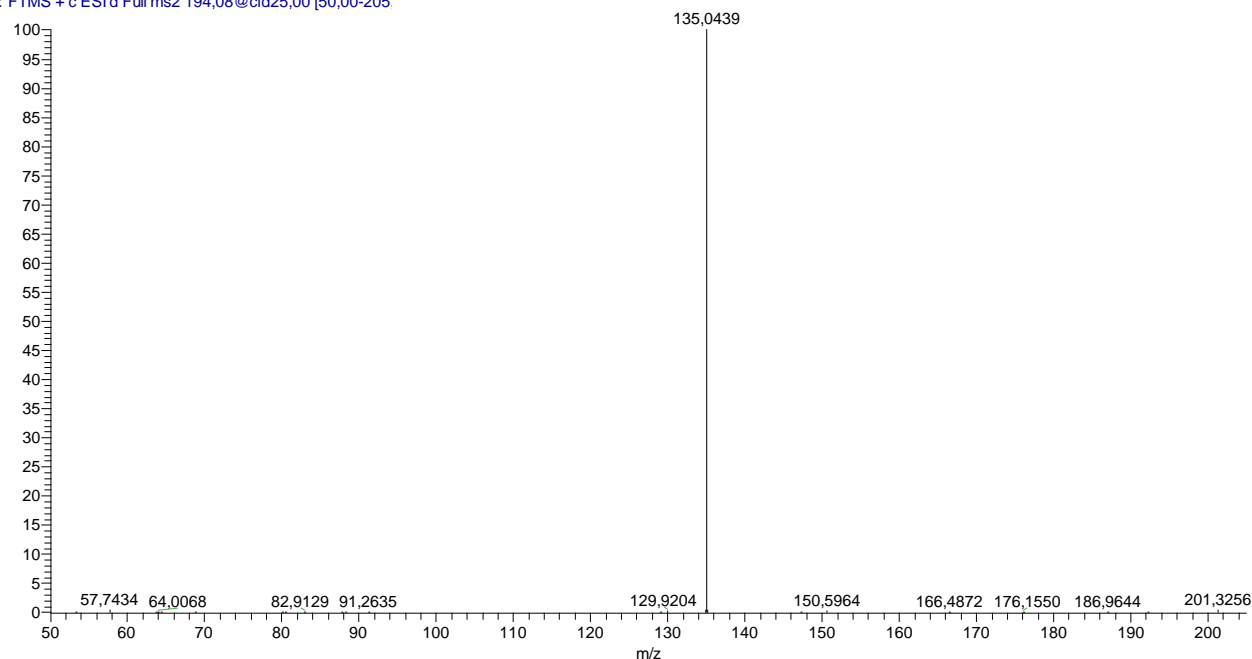
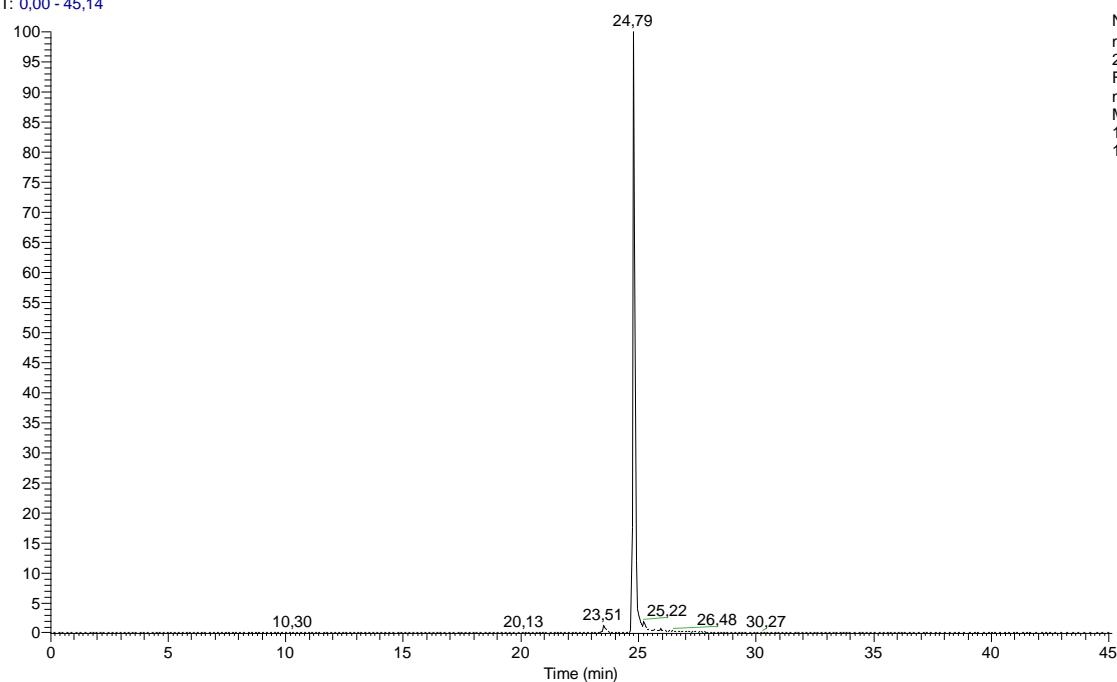


Figure S2. LC-HRMS analyses of **2** on an LTQ Orbitrap XLTM Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 194.0809, **(B)** relevant HRMS spectrum and **(C)** relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 194.1 as precursor.

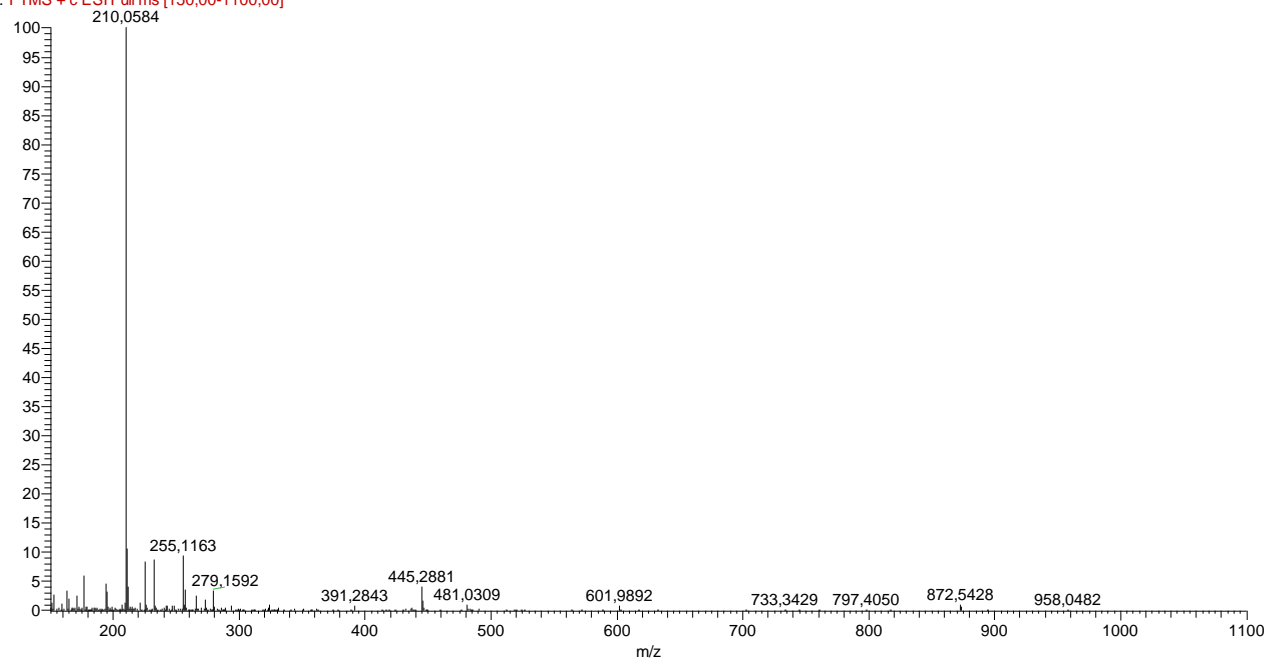
RT: 0,00 - 45,14



NL: 9,37E6
 m/z =
210,0562-210,0604
F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #2587 RT: 24,79 AV: 1 NL: 9,37E6

F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #2613 RT: 25,04 AV: 1 NL: 1,96E5

T: FTMS + c ESI d Full ms2 210,06@cid25,00 [50,00-225]

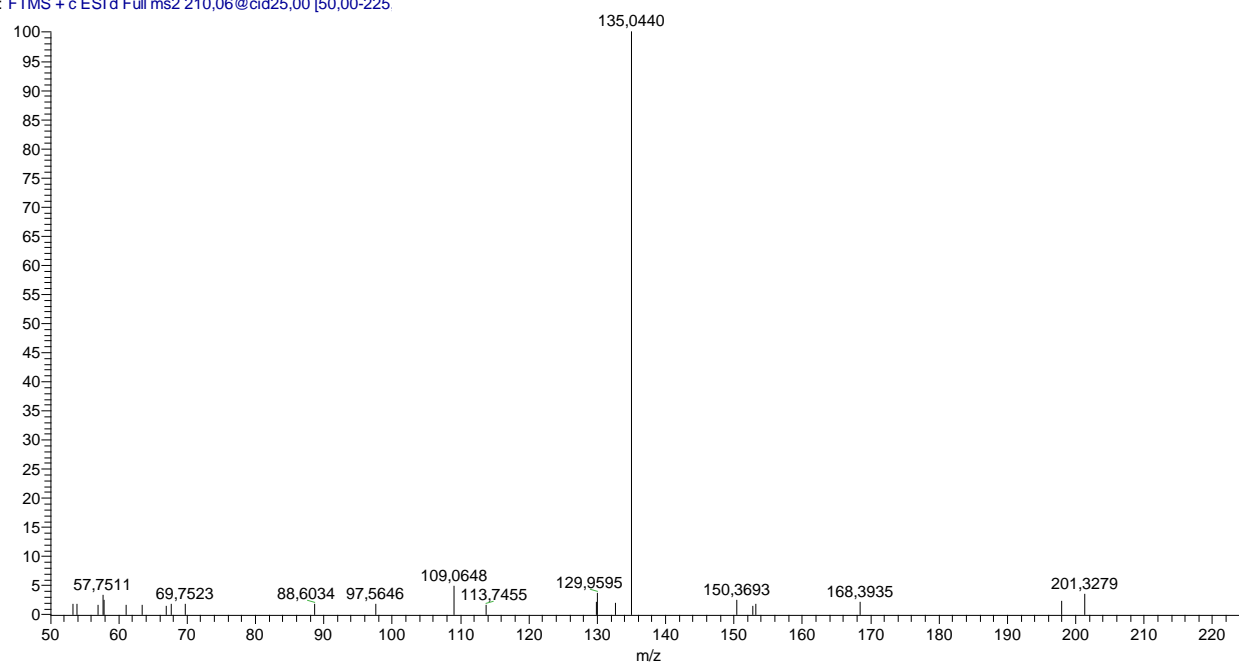
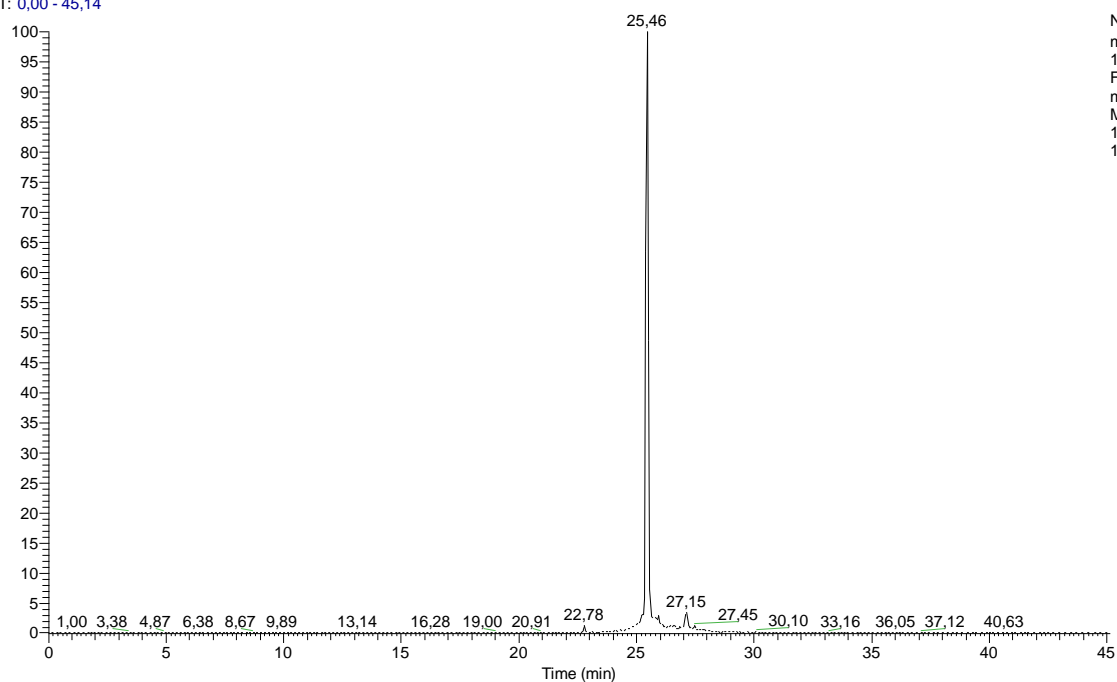


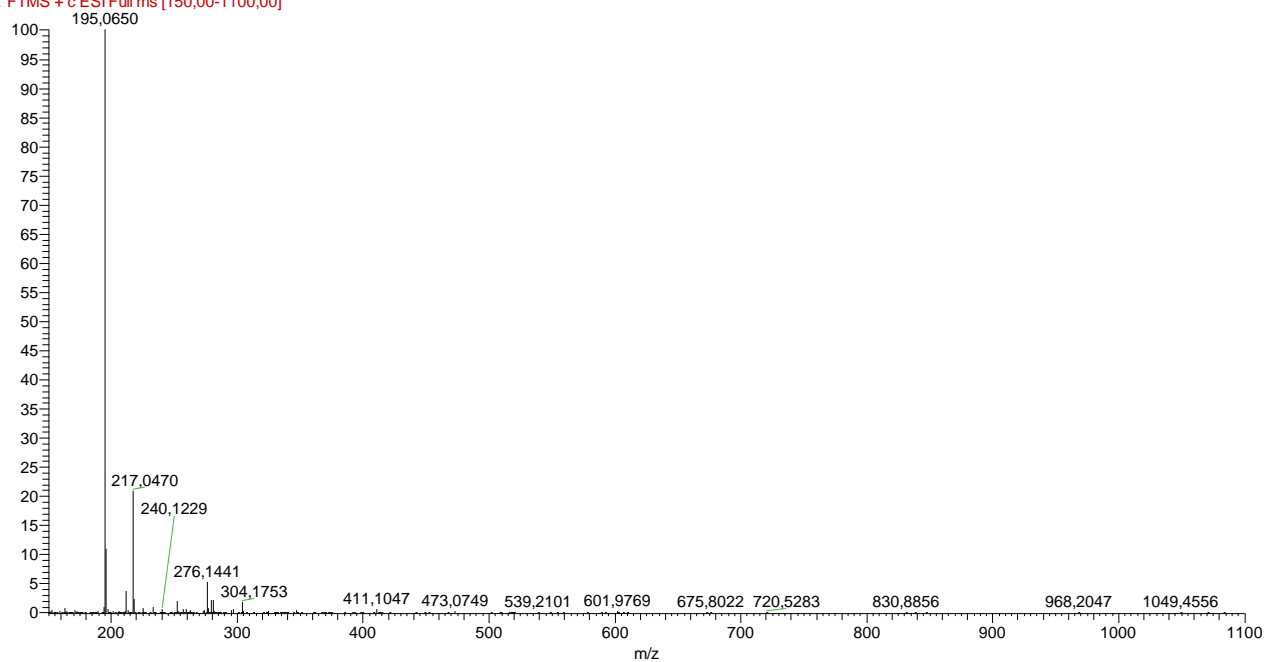
Figure S3. LC-HRMS analyses of **3** on an LTQ Orbitrap XL™ Hybrid FT Mass Spectrometer system: (A) Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 210.0584, (B) relevant HRMS spectrum and (C) relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 210.1 as precursor.

RT: 0,00 - 45,14



NL: 3,48E7
m/z=
195,0640-195,0660
F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #2659 RT: 25,46 AV: 1 NL: 3,48E7
F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #2672 RT: 25,59 AV: 1 NL: 1,36E6
T: FTMS + c ESI d Full ms2 195,07@cid25,00 [50,00-210]

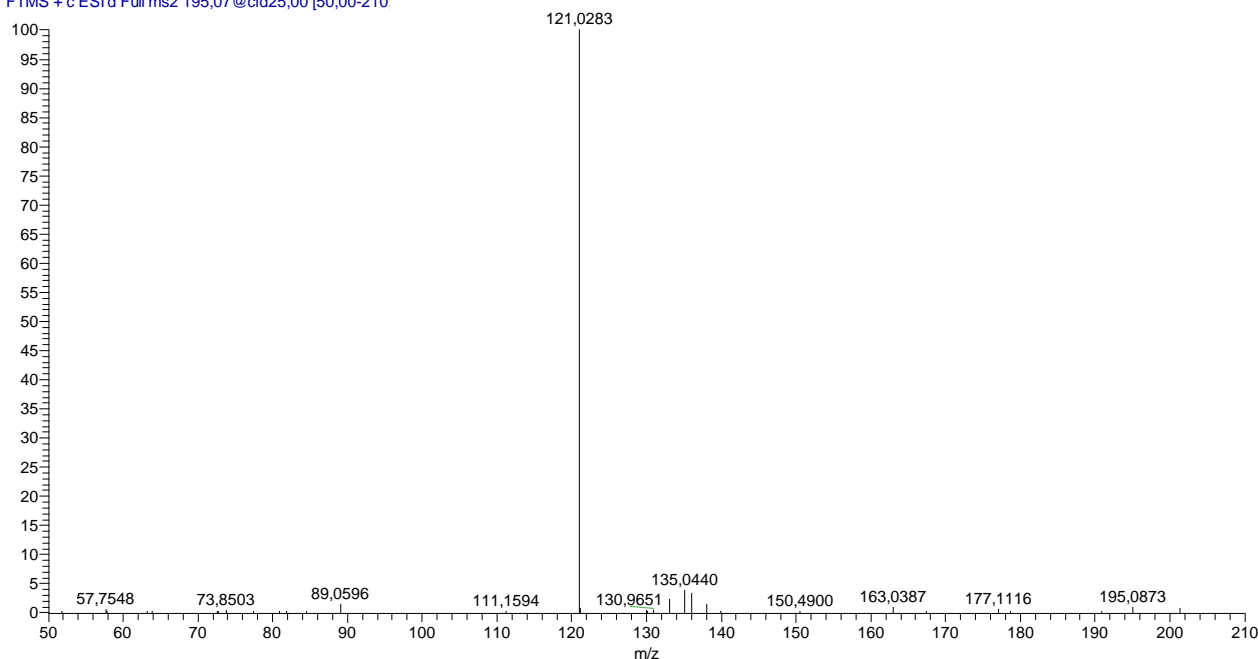
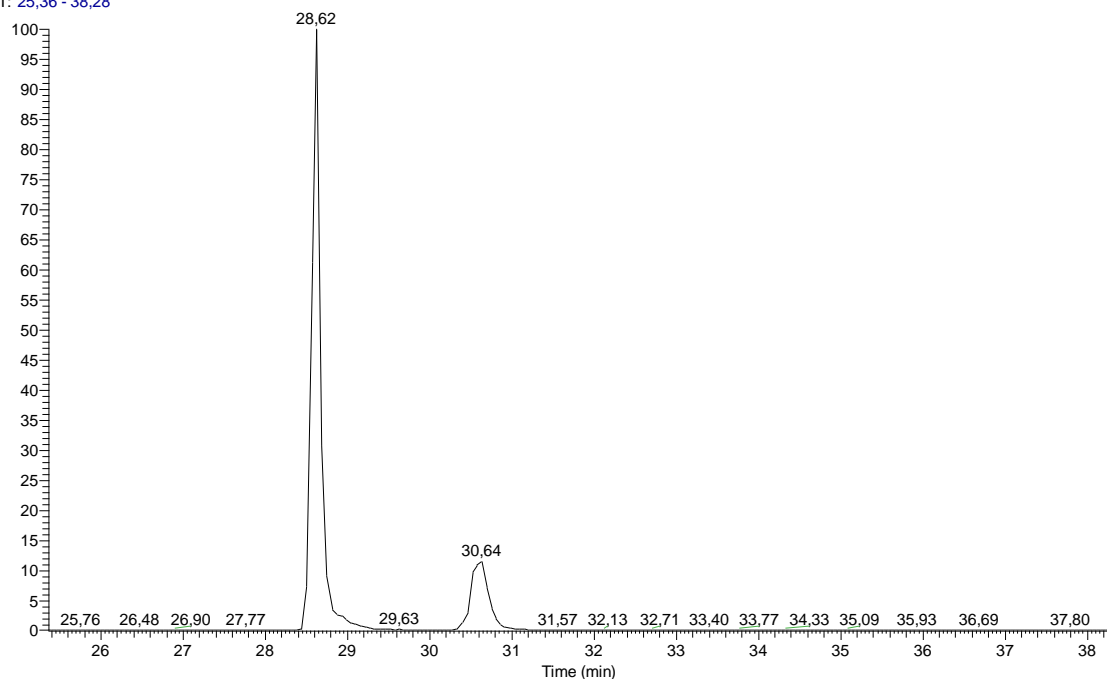


Figure S4. LC-HRMS analyses of **4** on an LTQ Orbitrap XLTM Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 195.0650, **(B)** relevant HRMS spectrum and **(C)** relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 195.1 as precursor.

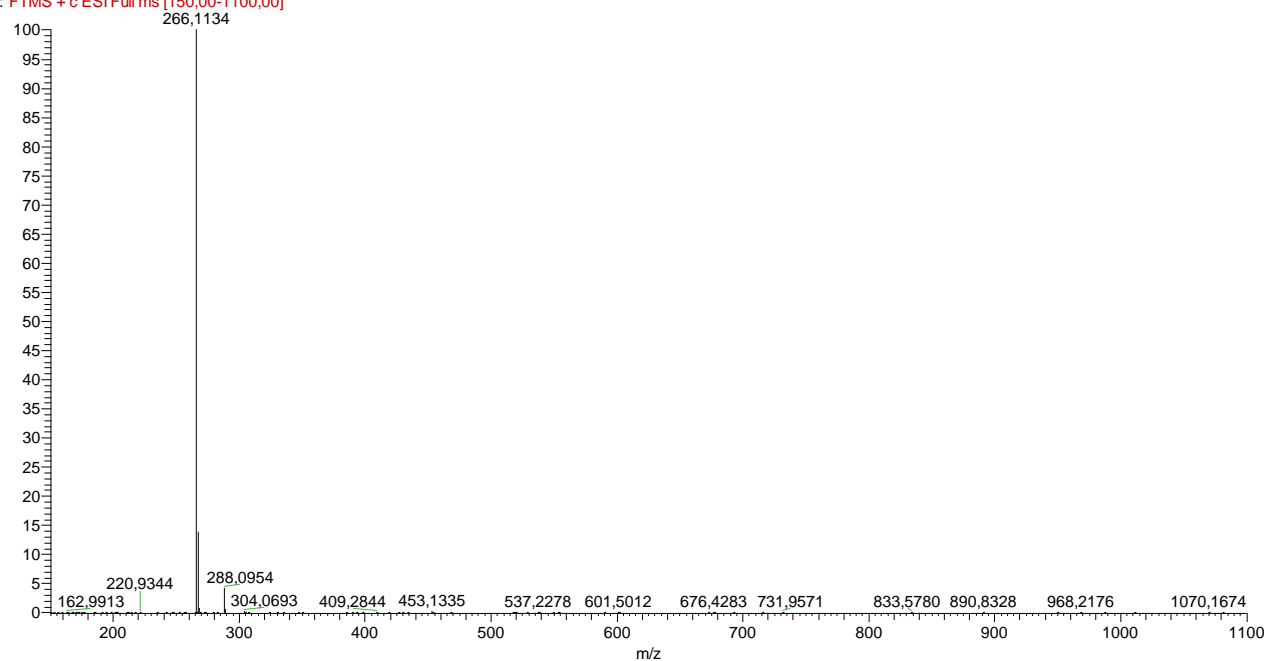
RT: 25,36 - 38,28



NL: 3,63E8
 m/z =
266,1119-266,1145
F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

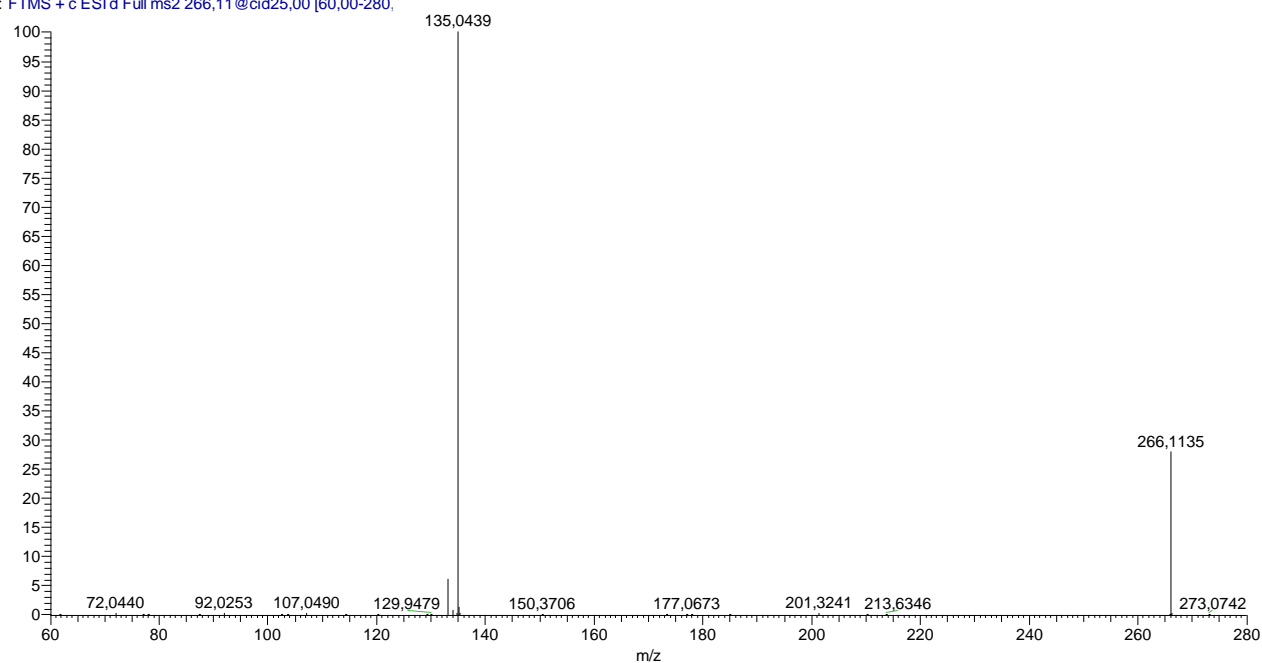
18052023PABMEOH10 #2965 RT: 28,57 AV: 1 NL: 2,23E8

F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #2996 RT: 28,90 AV: 1 NL: 4,08E6

T: FTMS + c ESI d Full ms2 266,11 @cid25,00 [60,00-280,



18052023PABMEOH10 #3205 RT: 30.94 AV: 1 NL: 7.36E5
T: FTMS + c ESI d Full ms2 266,11 @cid25,00 [60,00-280]

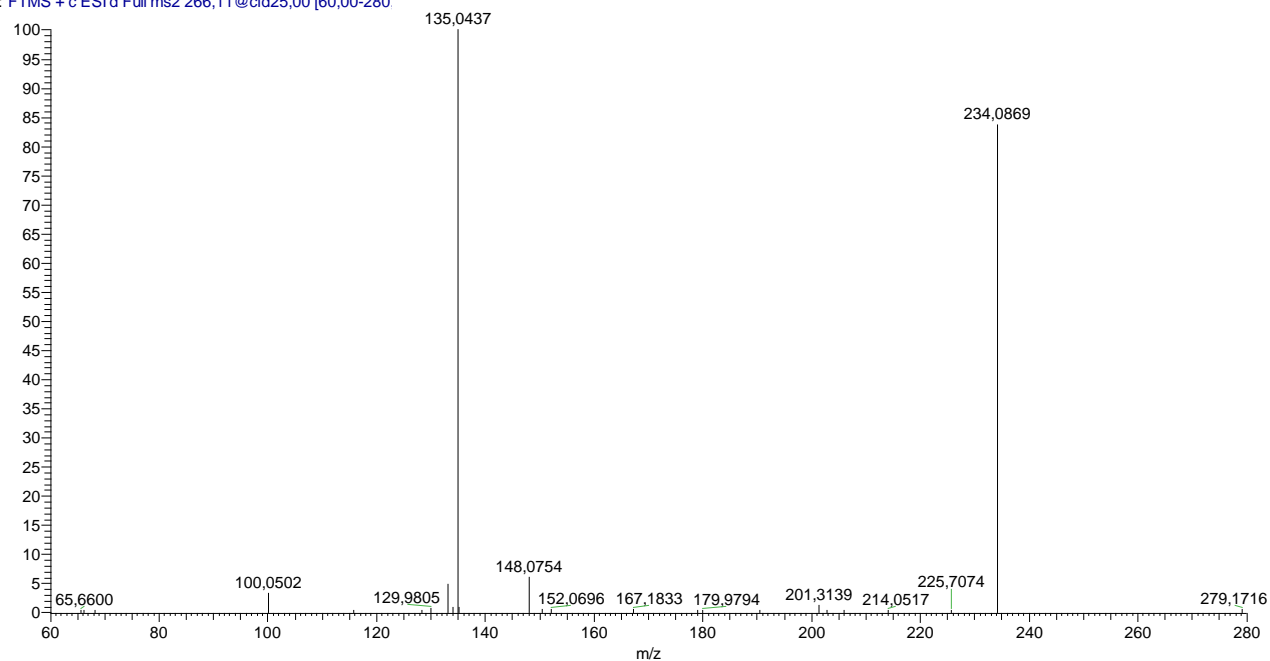
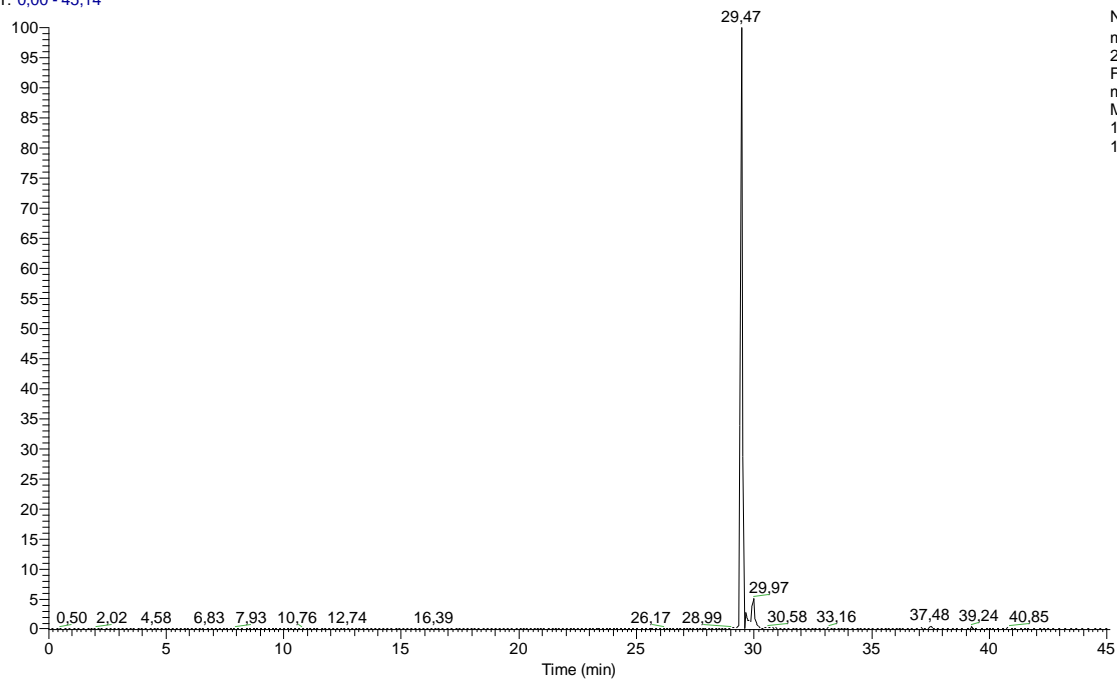


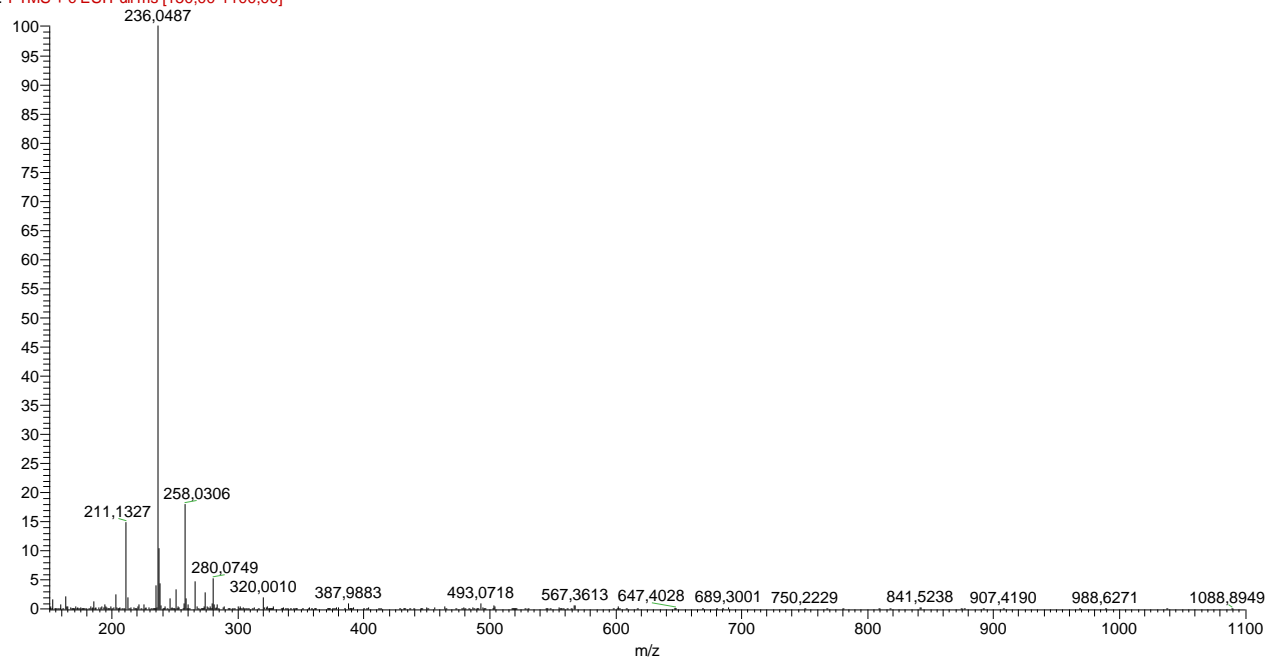
Figure S5. LC-HRMS analyses of **5** on an LTQ Orbitrap XLTM Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 266.1134, **(B)** relevant HRMS spectrum and **(C)** relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 266.1 as precursor.

RT: 0,00 - 45,14

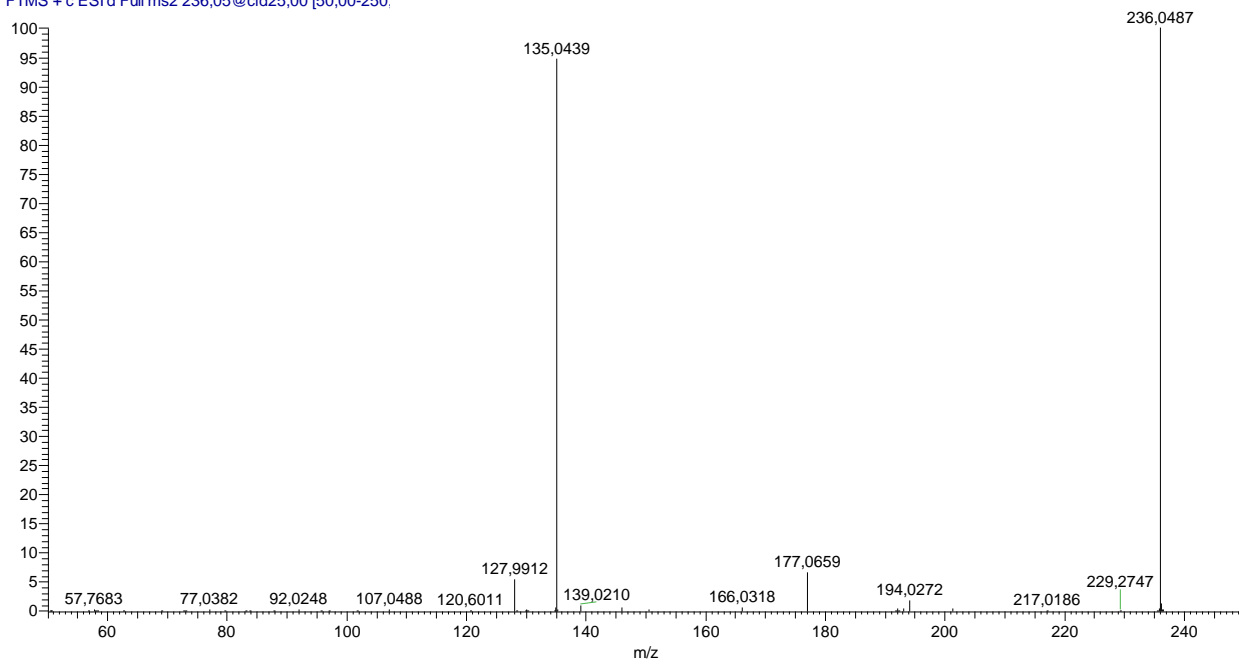


NL: 1,65E7
m/z= 236,0475-236,0499
F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #3055 RT: 29.47 AV: 1 NL: 1,65E7
F: FTMS + c ESI Full ms [150,00-1100,00]



18052023PABMEOH10 #3050 RT: 29.43 AV: 1 NL: 3,04E6
T: FTMS + c ESI d Full ms2 236,05@cid25,00 [50,00-250,



18052023PABMEOH10 #3092 RT: 29.82 AV: 1 NL: 1,43E5
T: FTMS + c ESI d Full ms2 236,05@cid25,00 [50,00-250,

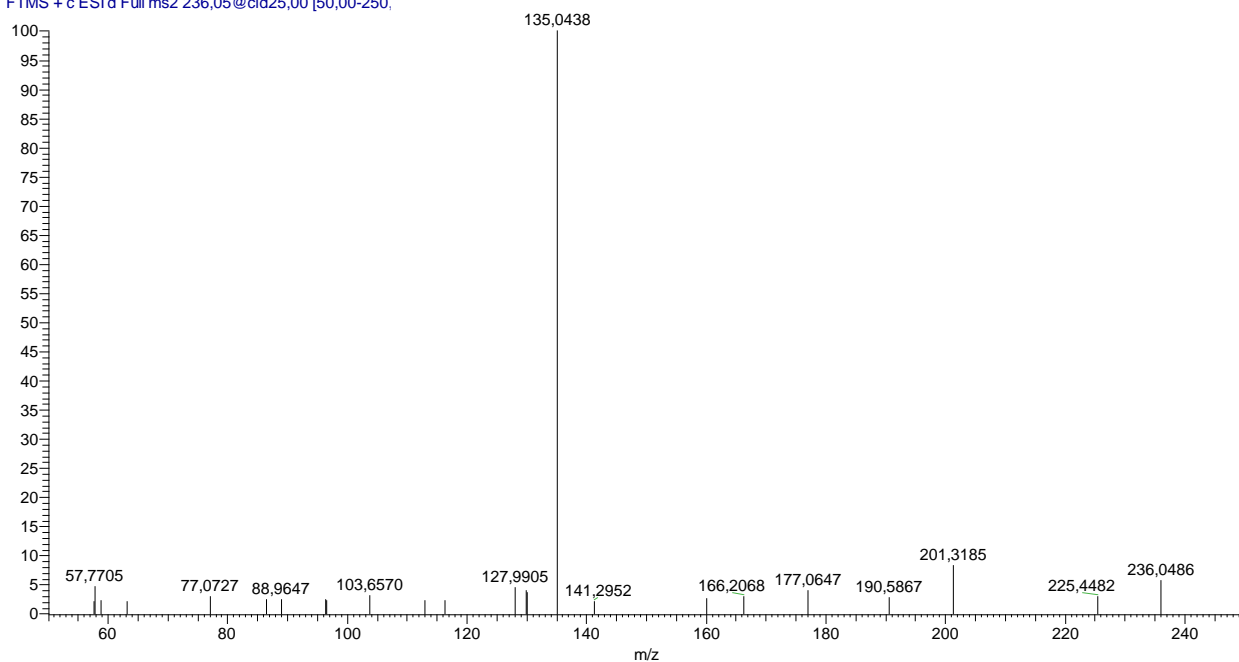


Figure S6. LC-HRMS analyses of **6** on an LTQ Orbitrap XL™ Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 236.0487, **(B)** relevant HRMS spectrum and **(C)** relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 236.0 as precursor.

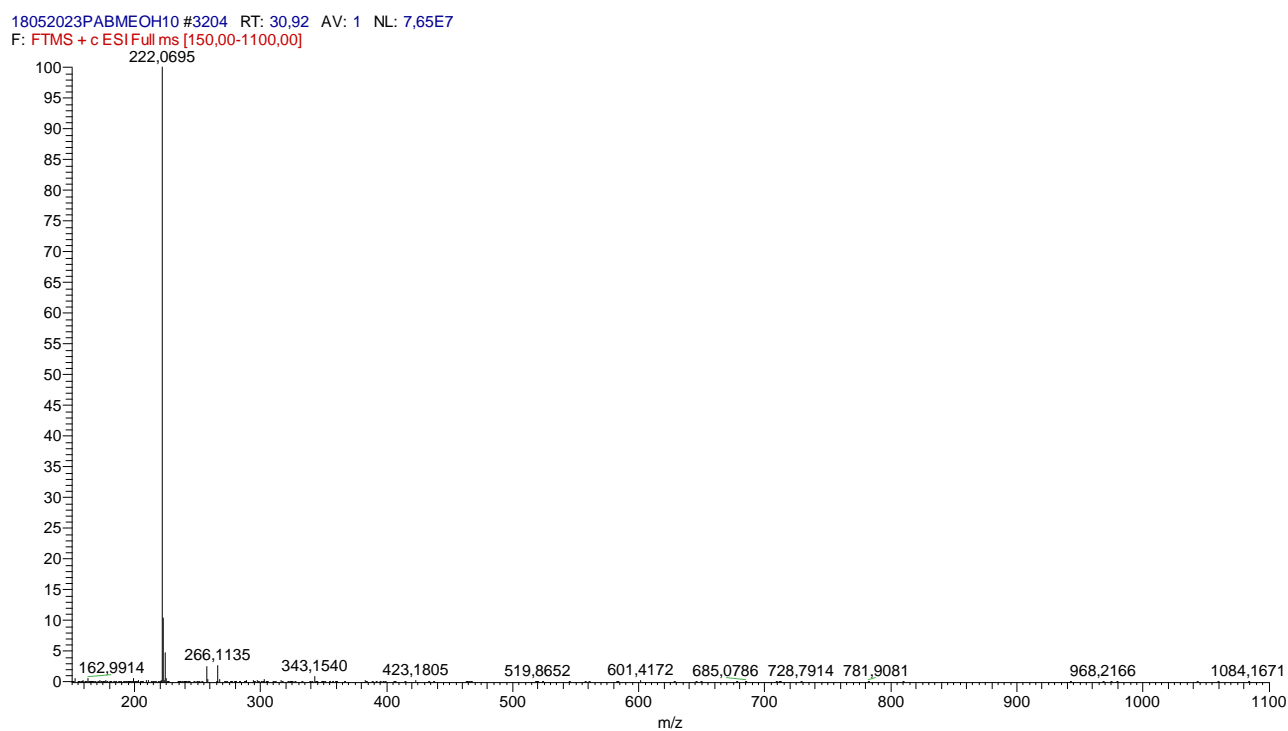
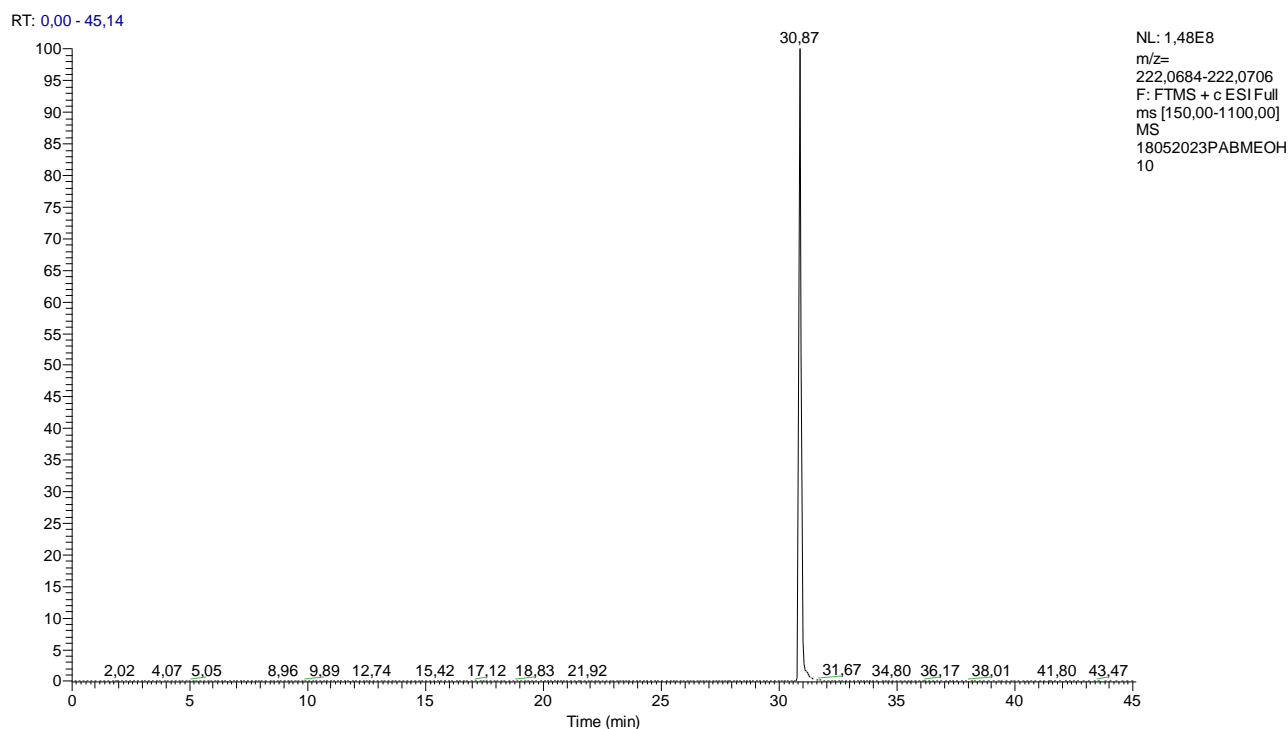
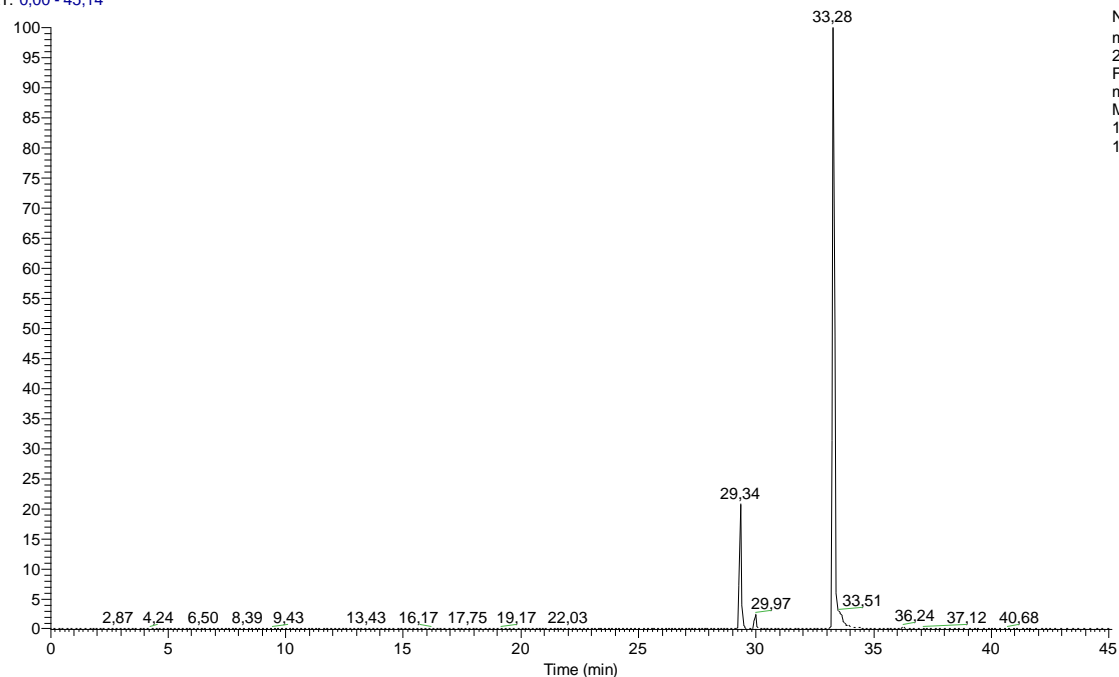


Figure S7. LC-HRMS analyses of **7** on an LTQ Orbitrap XL™ Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 222.0695, **(B)** relevant HRMS spectrum.

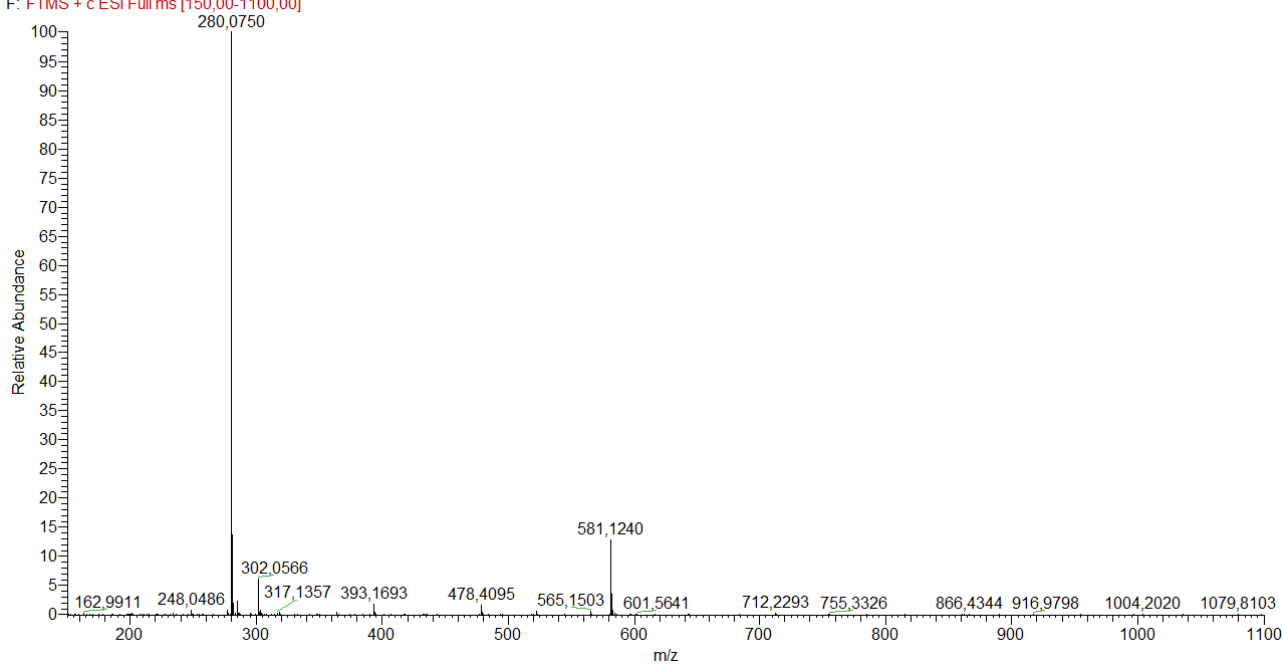
RT: 0,00 - 45,14



NL: 1,43E8
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F: FTMS + c ESI Full
ms [150,00-1100,00]
MS
18052023PABMEOH
10

18052023PABMEOH10 #3456 RT: 33,34 AV: 1 NL: 1,54E8

F: FTMS + c ESI Full ms [150,00-1100,00]



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T: FTMS + c ESI d Full ms2 280,13@cid25,00 [65,00-295,00]

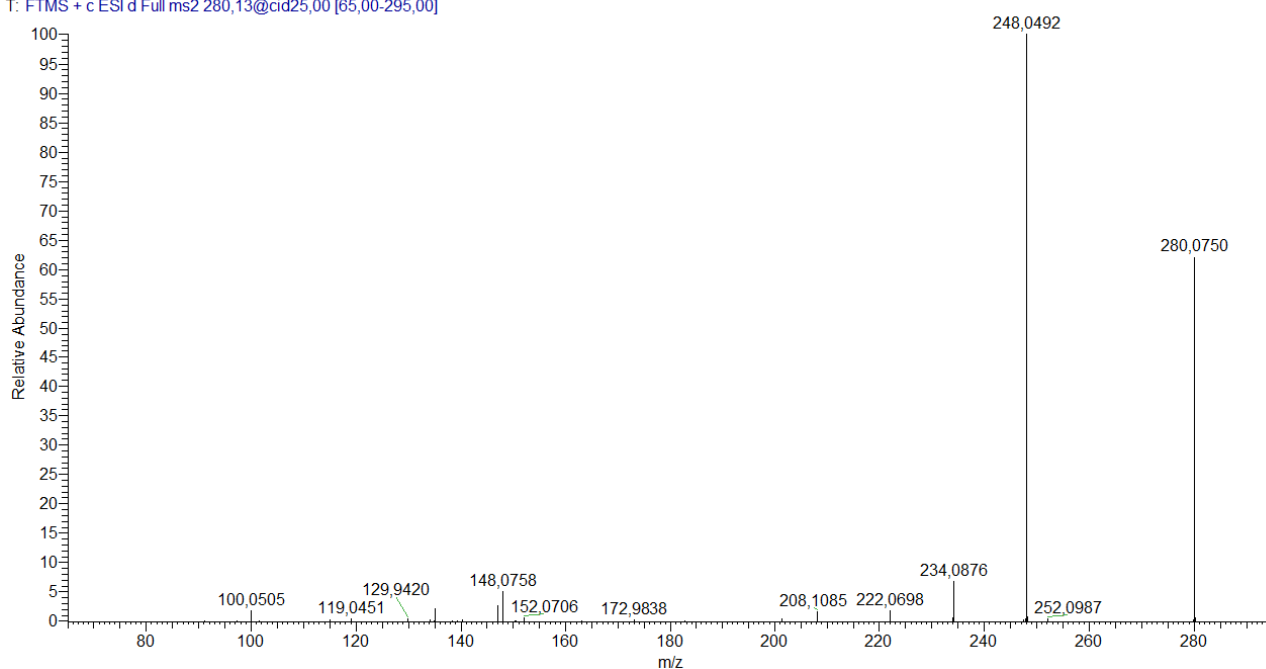


Figure S8. LC-HRMS analyses of **8** on an LTQ Orbitrap XLTM Hybrid FT Mass Spectrometer system: **(A)** Extracted ion Chromatogram (XIC) obtained by selecting the ion at m/z 280.0750, **(B)** relevant HRMS spectrum and **(C)** relevant HRMS² spectrum (Collision Induced Dissociation mode) obtained by using the ion at m/z 280.1 as precursor.

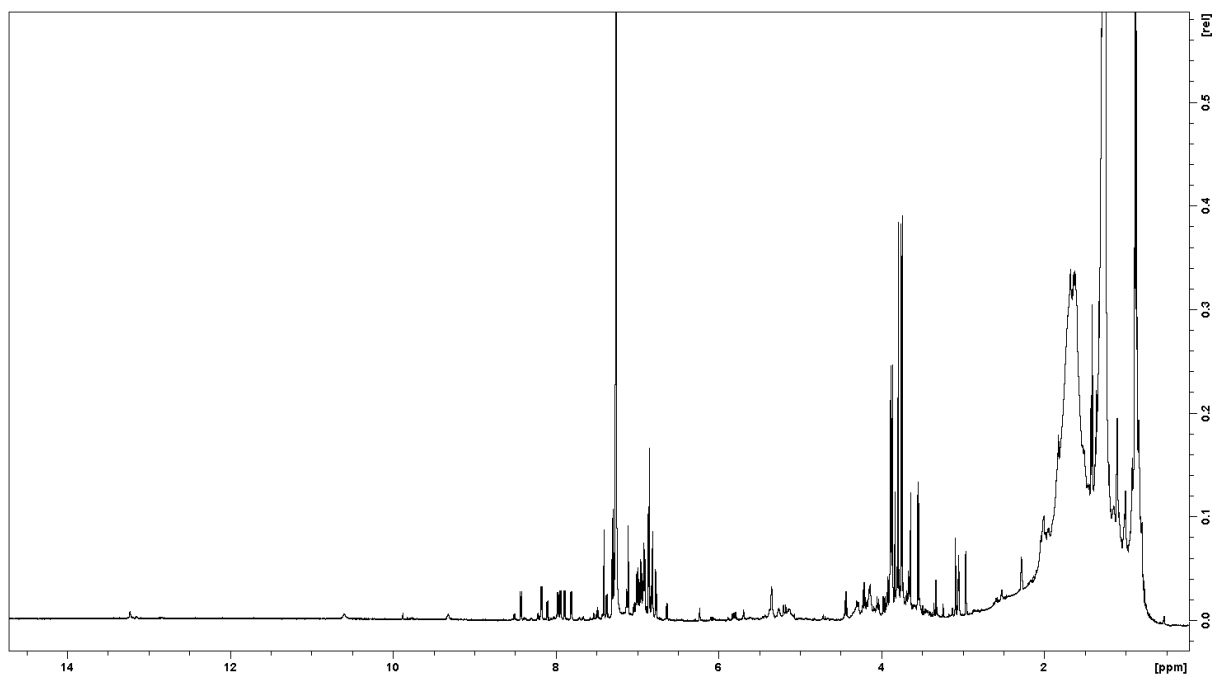


Figure S9. ^1H NMR spectrum (700 MHz) in CDCl_3 of PAB2.

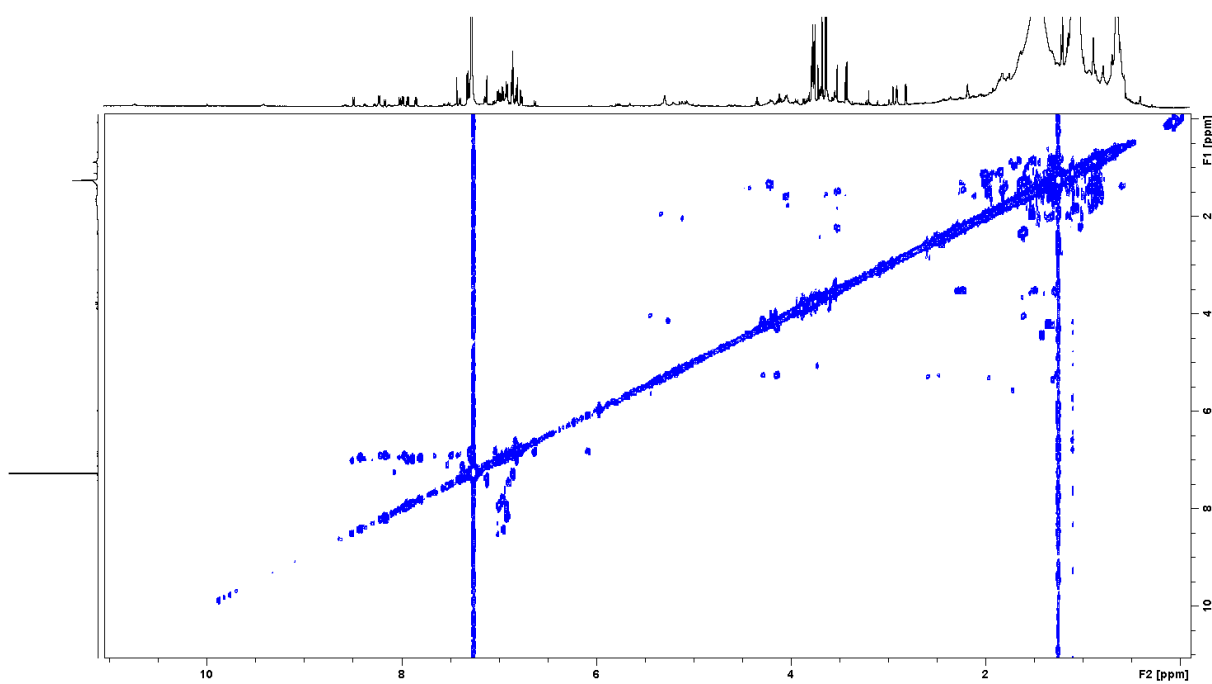


Figure S10. COSY spectrum in CDCl_3 of PAB2.

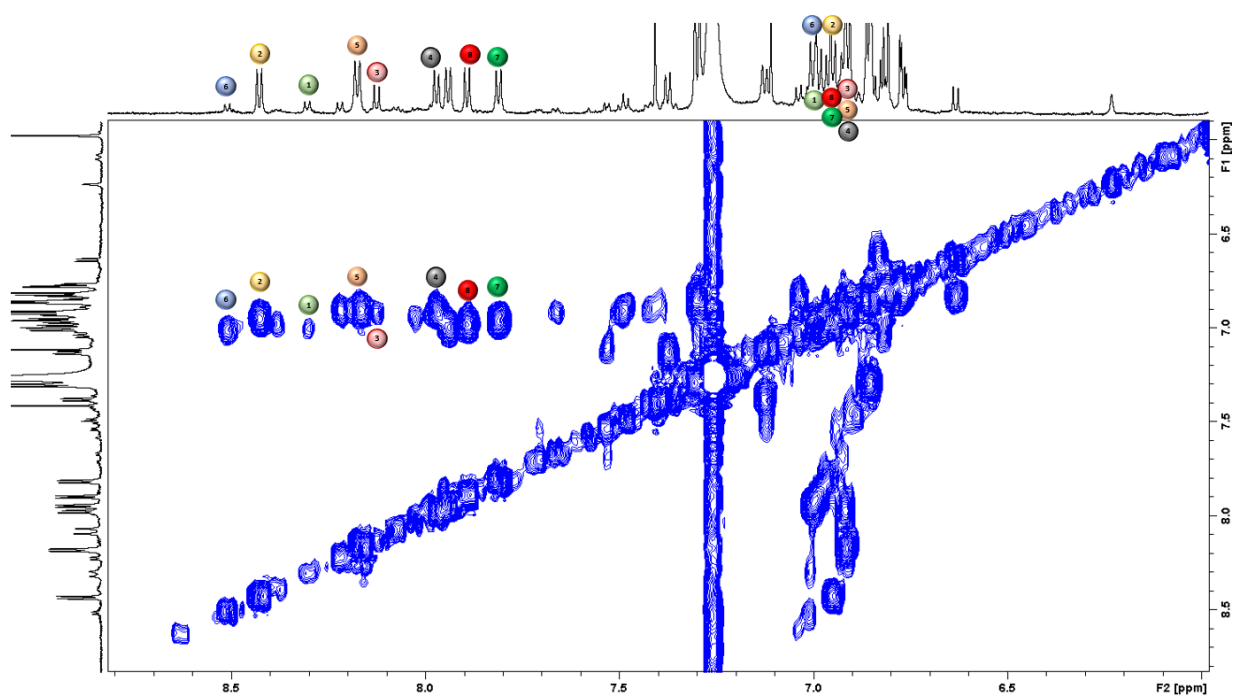


Figure S11. Downfield region enlargement of COSY spectrum in CDCl₃ of PAB2.

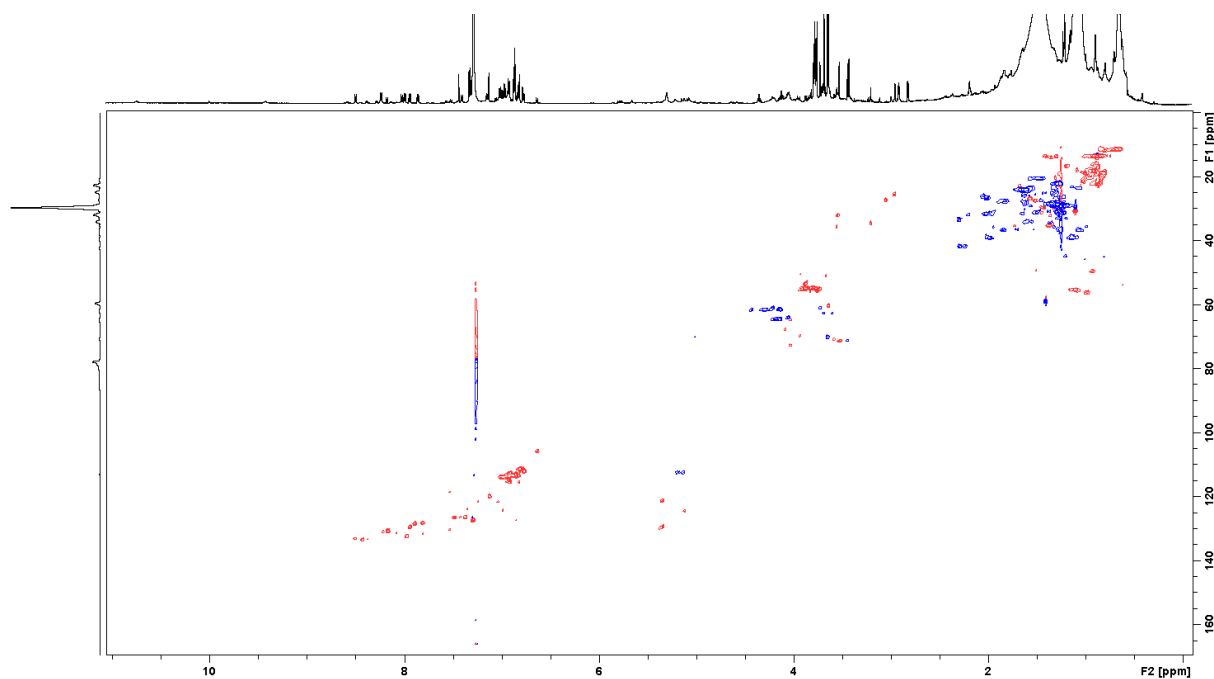


Figure S12. HSQC spectrum in CDCl₃ of PAB2.

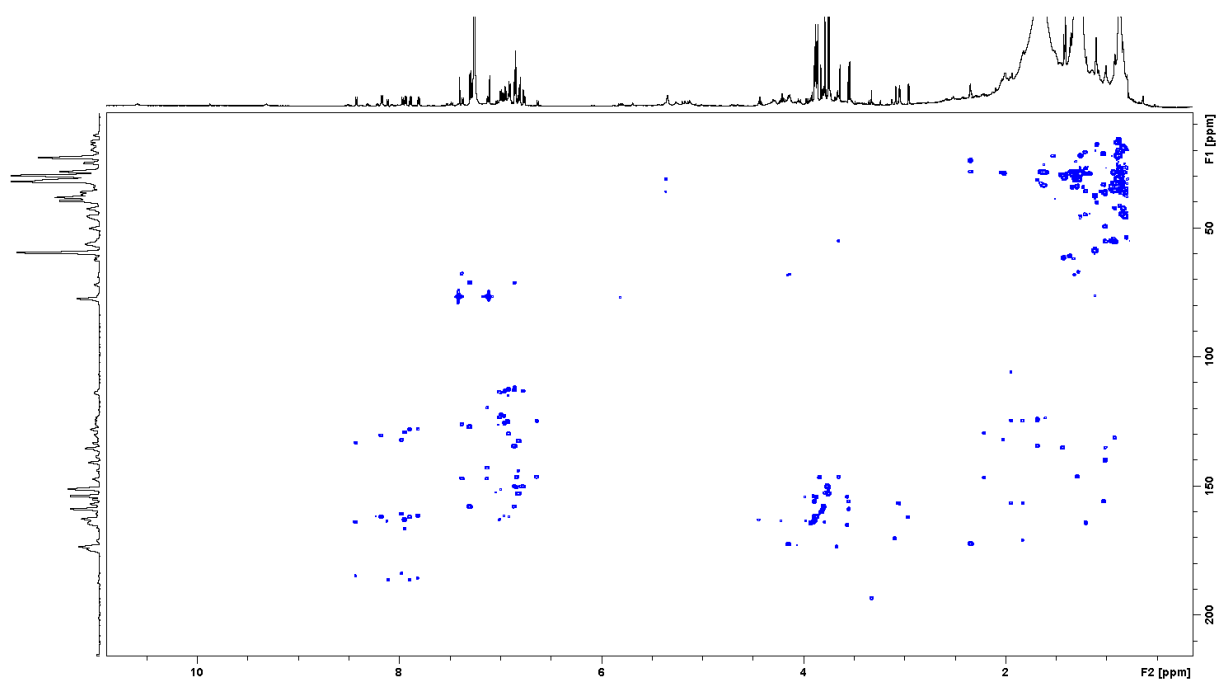


Figure S13. HMBC spectrum in CDCl_3 of PAB2.

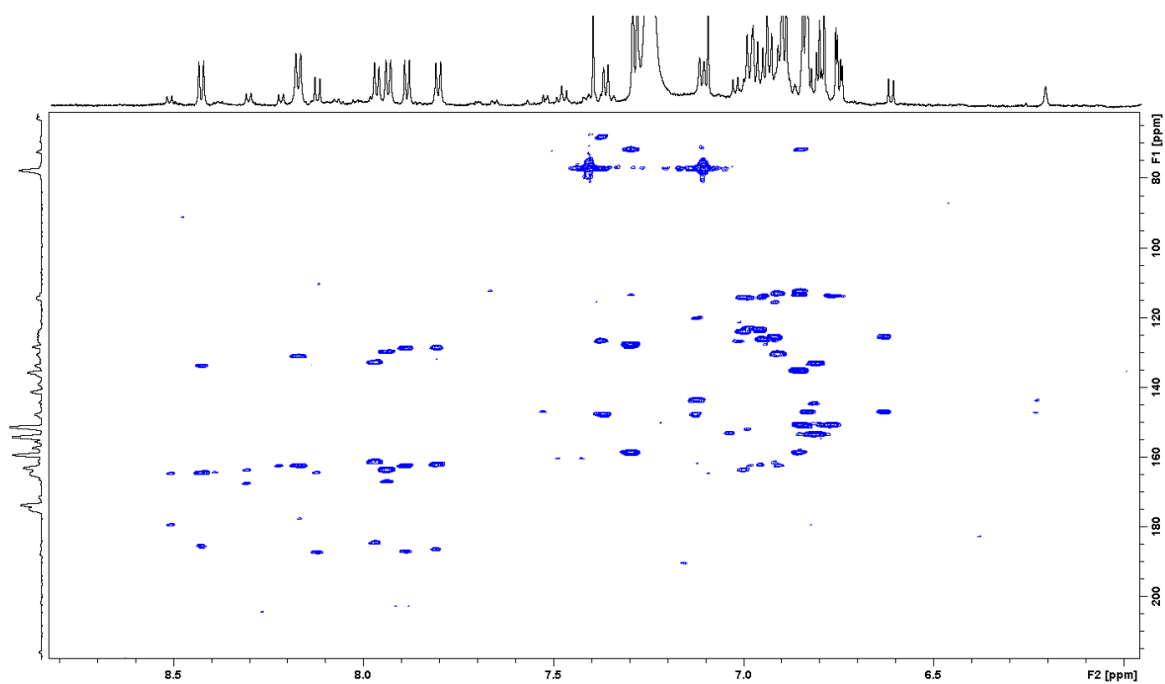


Figure S14. Downfield region enlargement of HMBC spectrum in CDCl_3 of PAB2.