

SUPPORTING INFORMATION

New Alkoxy Flavone Derivatives Targeting Caspases: Synthesis and Antitumor Activity Evaluation

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Table of Contents

NMR spectra	3
Figure S1. ¹ H and ¹³ C NMR of compound 6	3
Figure S2. ¹ H and ¹³ C NMR of compound 7	4
Figure S3. ¹ H and ¹³ C NMR of compound 13	5
Figure S4. ¹ H and ¹³ C NMR of compound 14	6
Figure S5. ¹ H and ¹³ C NMR of compound 17	7
Figure S6. ¹ H and ¹³ C NMR of compound 18	8
Figure S7. ¹ H and ¹³ C NMR of compound 19	9
Figure S8. ¹ H and ¹³ C NMR of compound 20	10
Figure S9. ¹ H and ¹³ C NMR of compound 21	11
Figure S10. ¹ H and ¹³ C NMR of compound 24	12
Figure S11. ¹ H and ¹³ C NMR of compound 27	13
HRMS spectra	14

Figure S12. HRMS of compound 6	14
Figure S13. HRMS of compound 7	15
Figure S14. HRMS of compound 13	16
Figure S15. HRMS of compound 14	17
Figure S16. HRMS of compound 17.....	18
Figure S17. HRMS of compound 18	19
Figure S18. HRMS of compound 19	20
Figure S19. HRMS of compound 20	21
Figure S20. HRMS of compound 21	22
Figure S21. HRMS of compound 24	23
Figure S22. HRMS of compound 27	24

NMR spectra

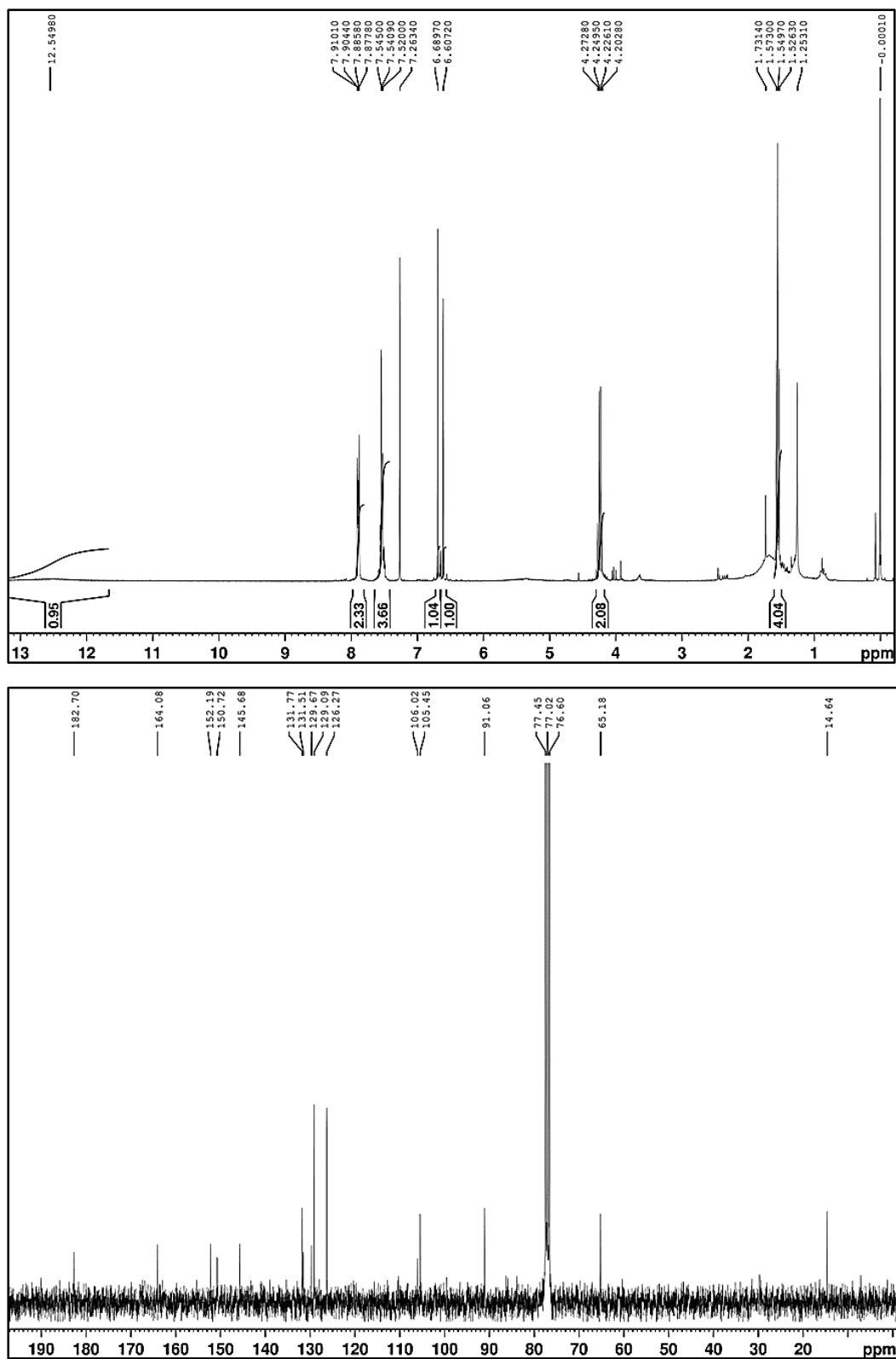


Figure S1. ^1H and ^{13}C NMR of compound 6.

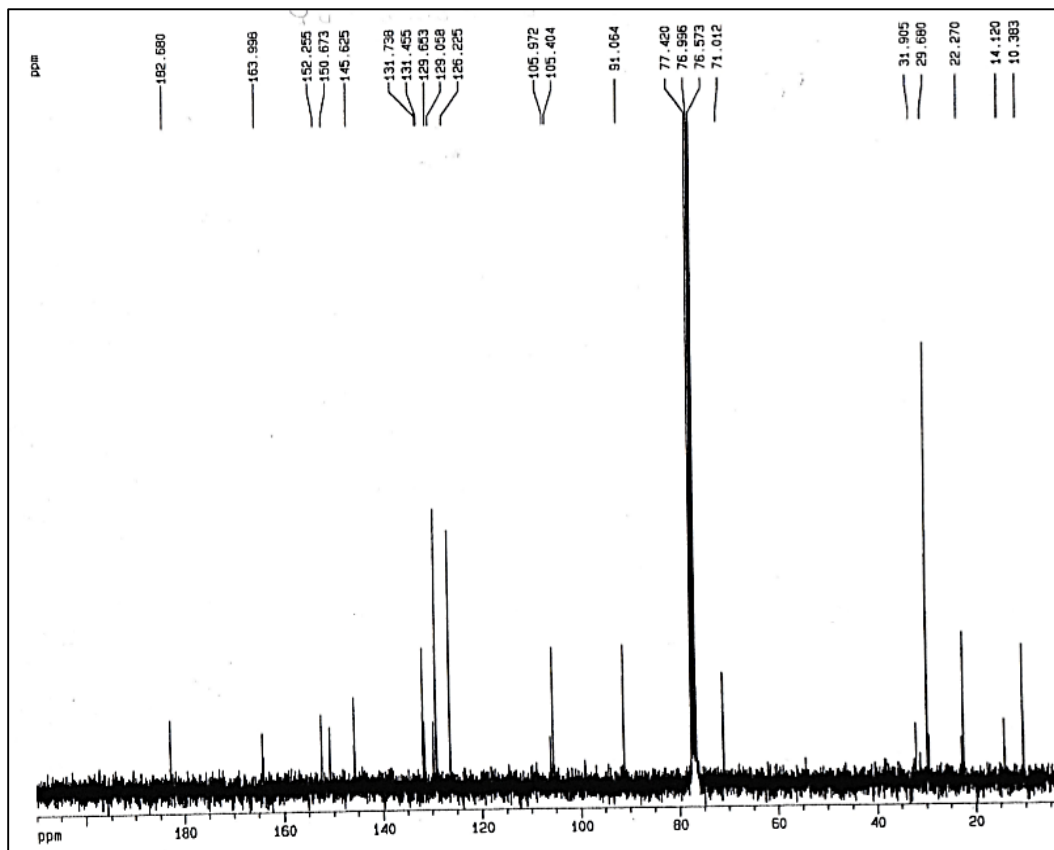
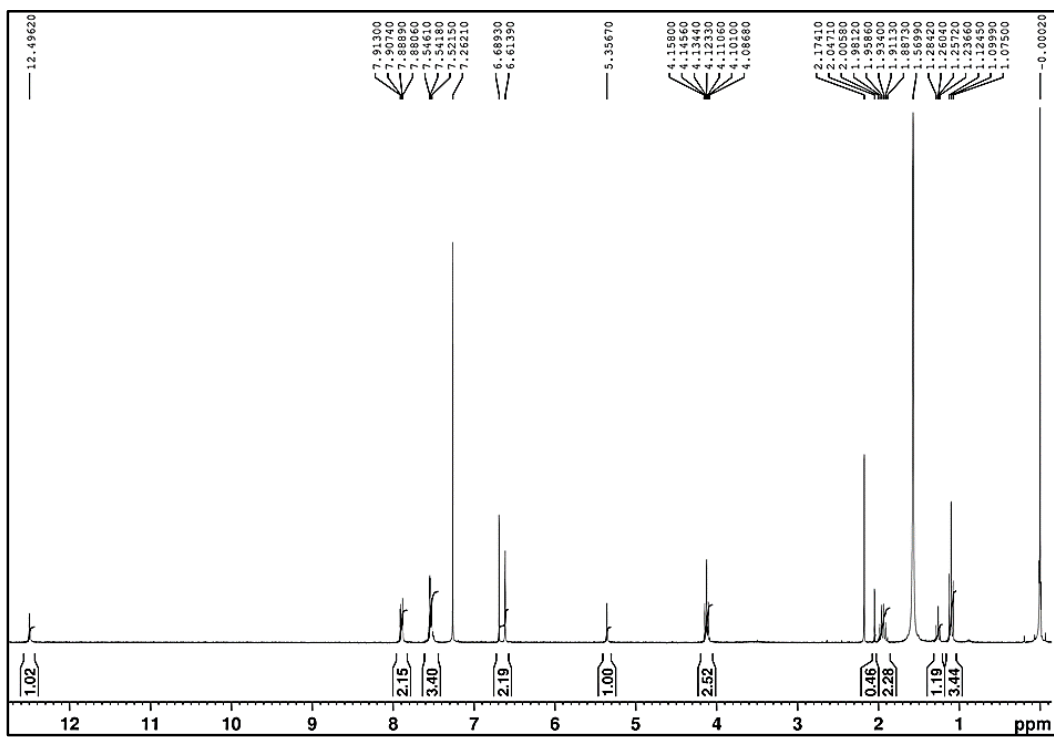


Figure S2. ¹H and ¹³C NMR of compound 7.

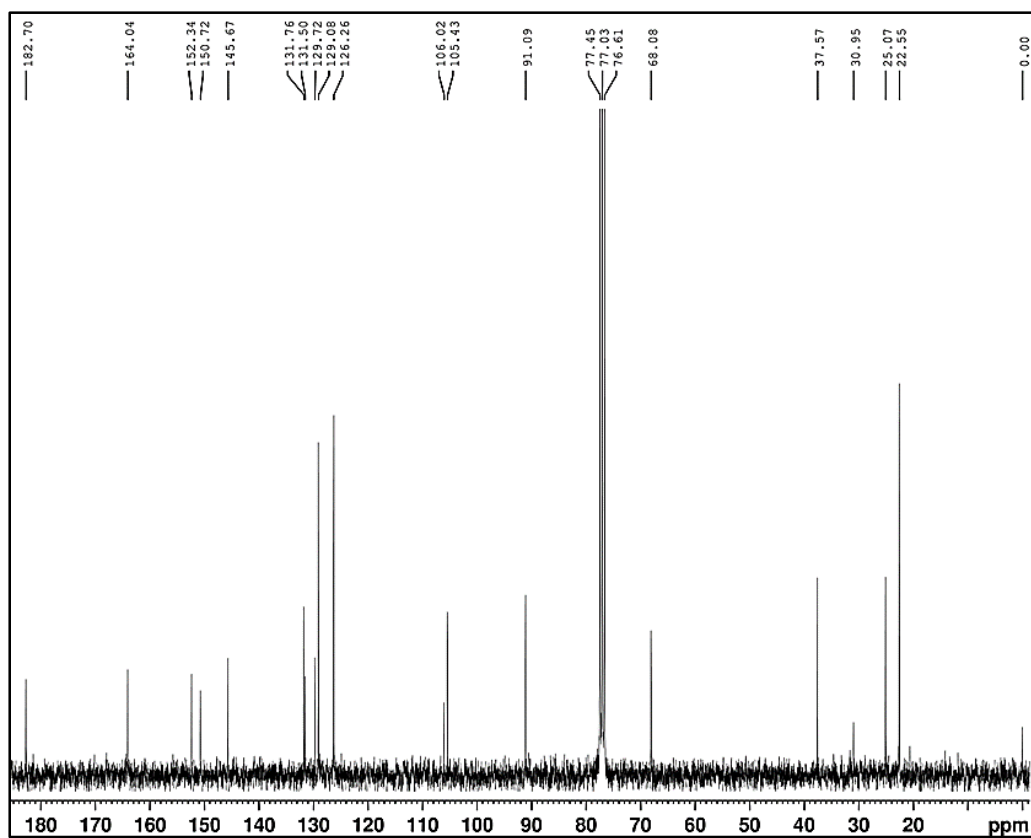
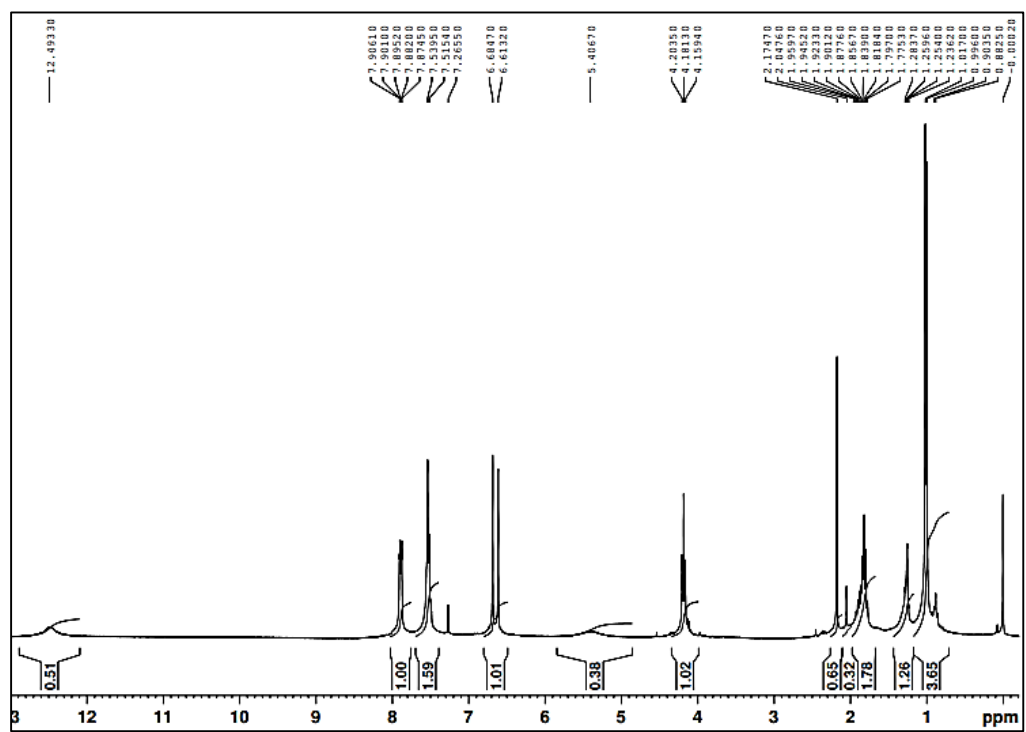


Figure S3. ¹H and ¹³C NMR of compound 13.

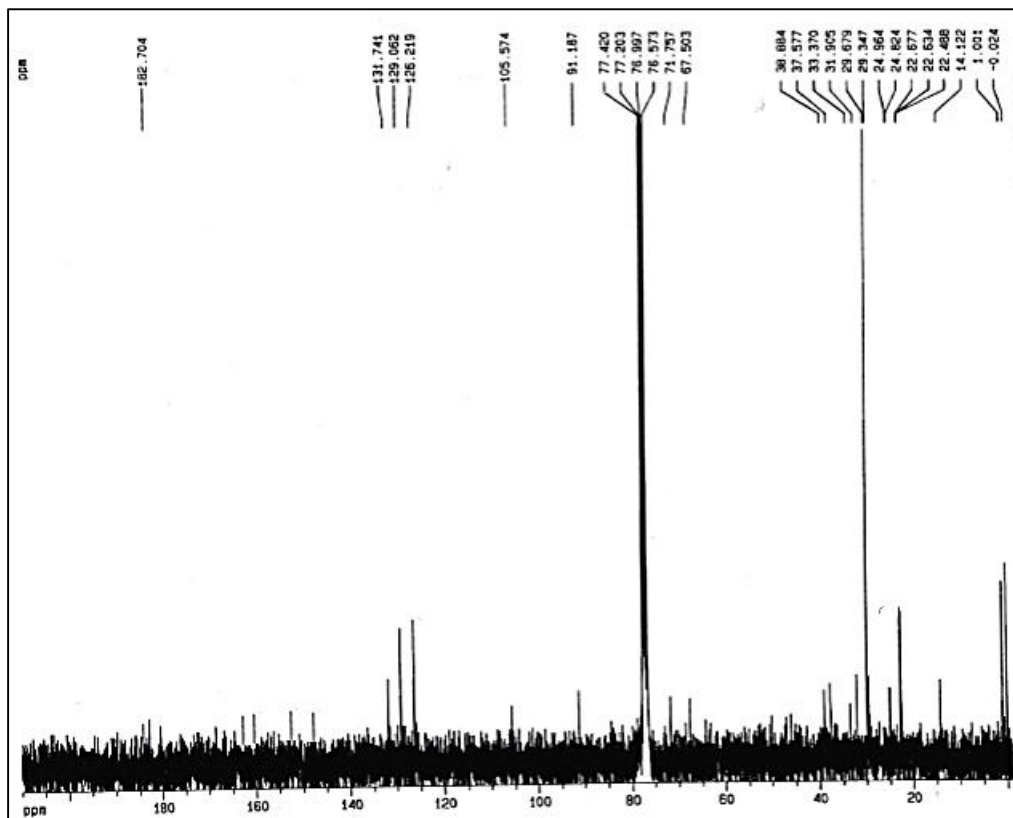
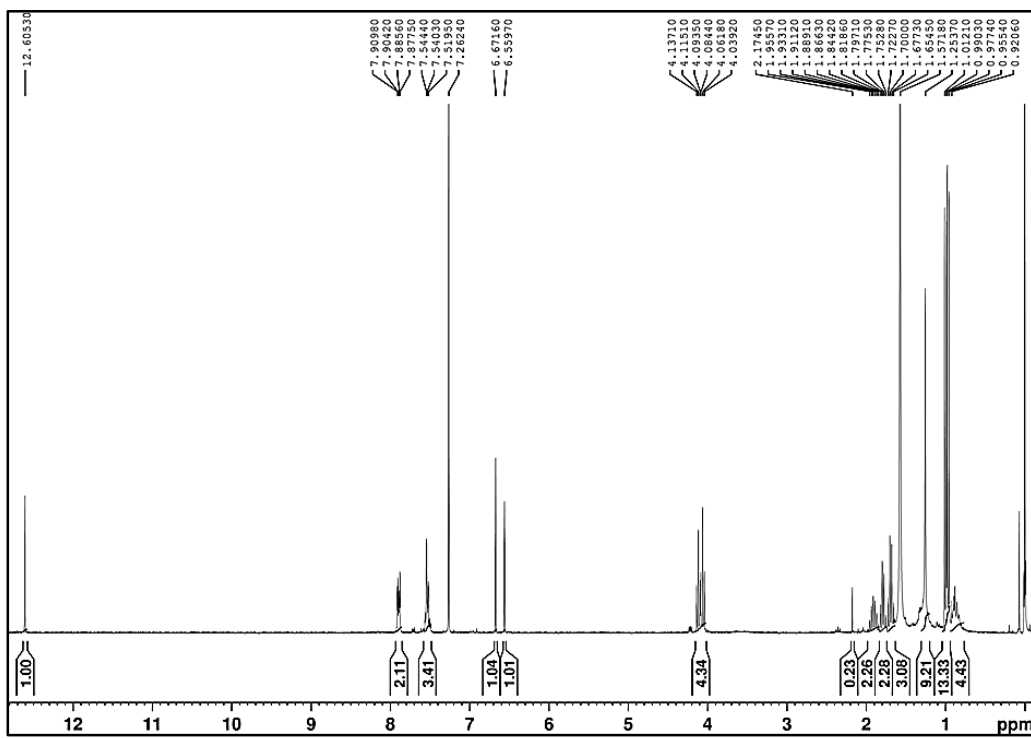


Figure S4. ^1H and ^{13}C NMR of compound 14.

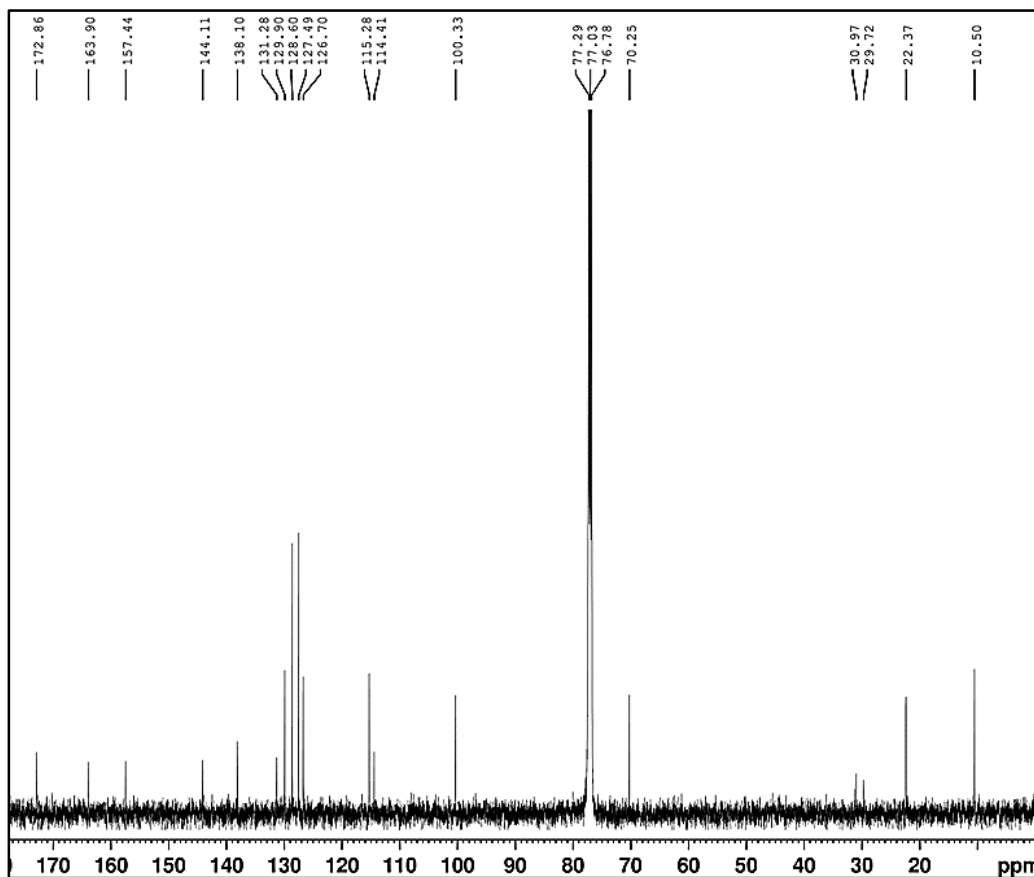
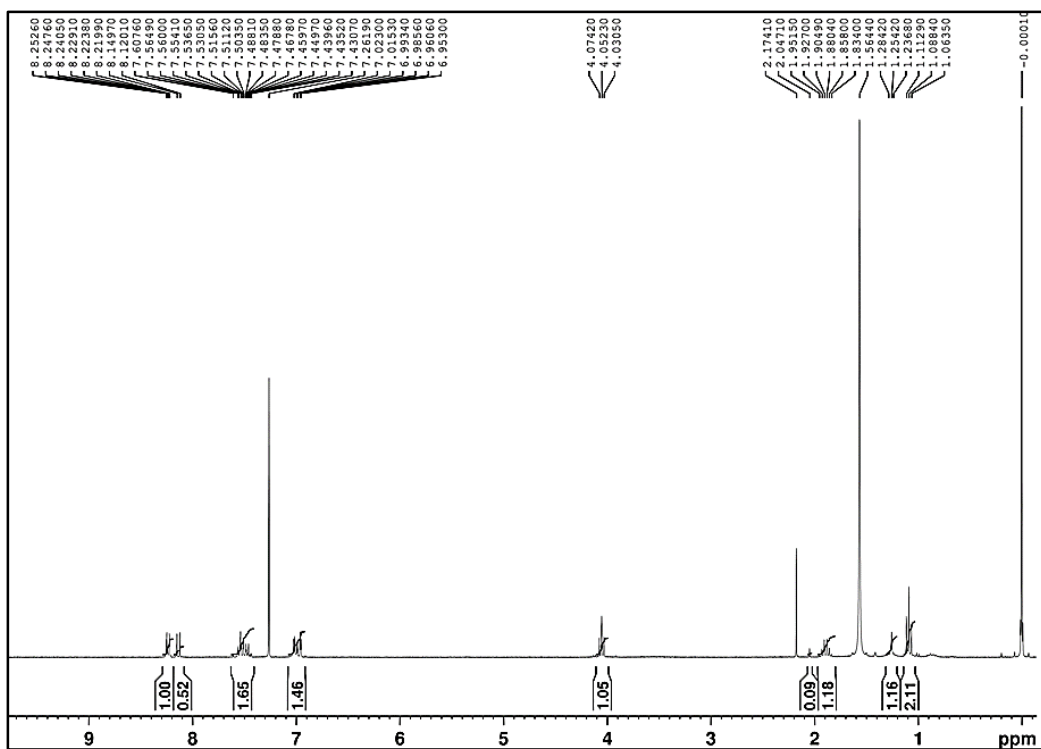


Figure S5. ¹H and ¹³C NMR of compound 17.

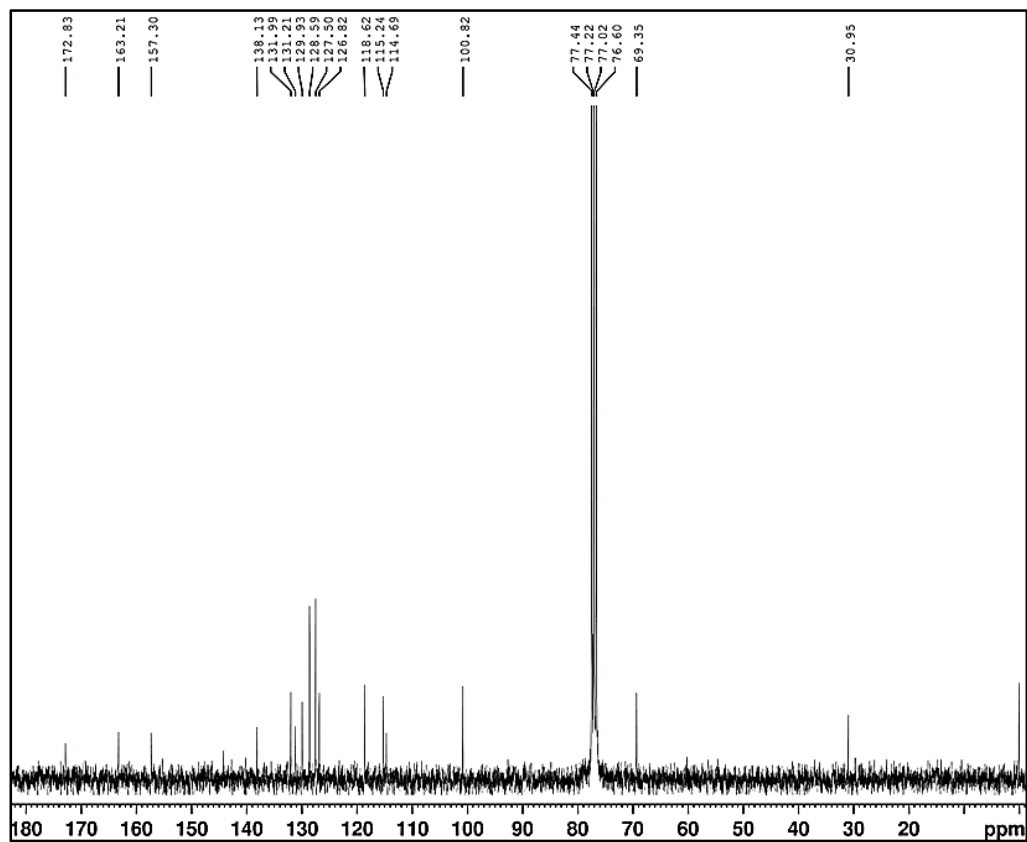
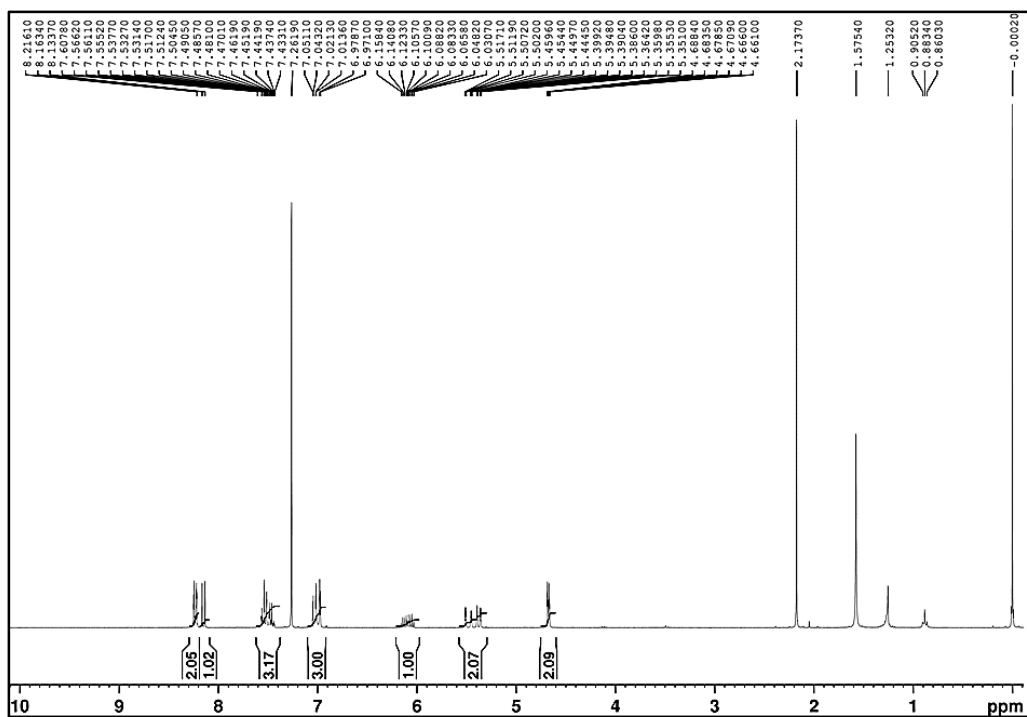


Figure S6. ^1H and ^{13}C NMR of compound 18.

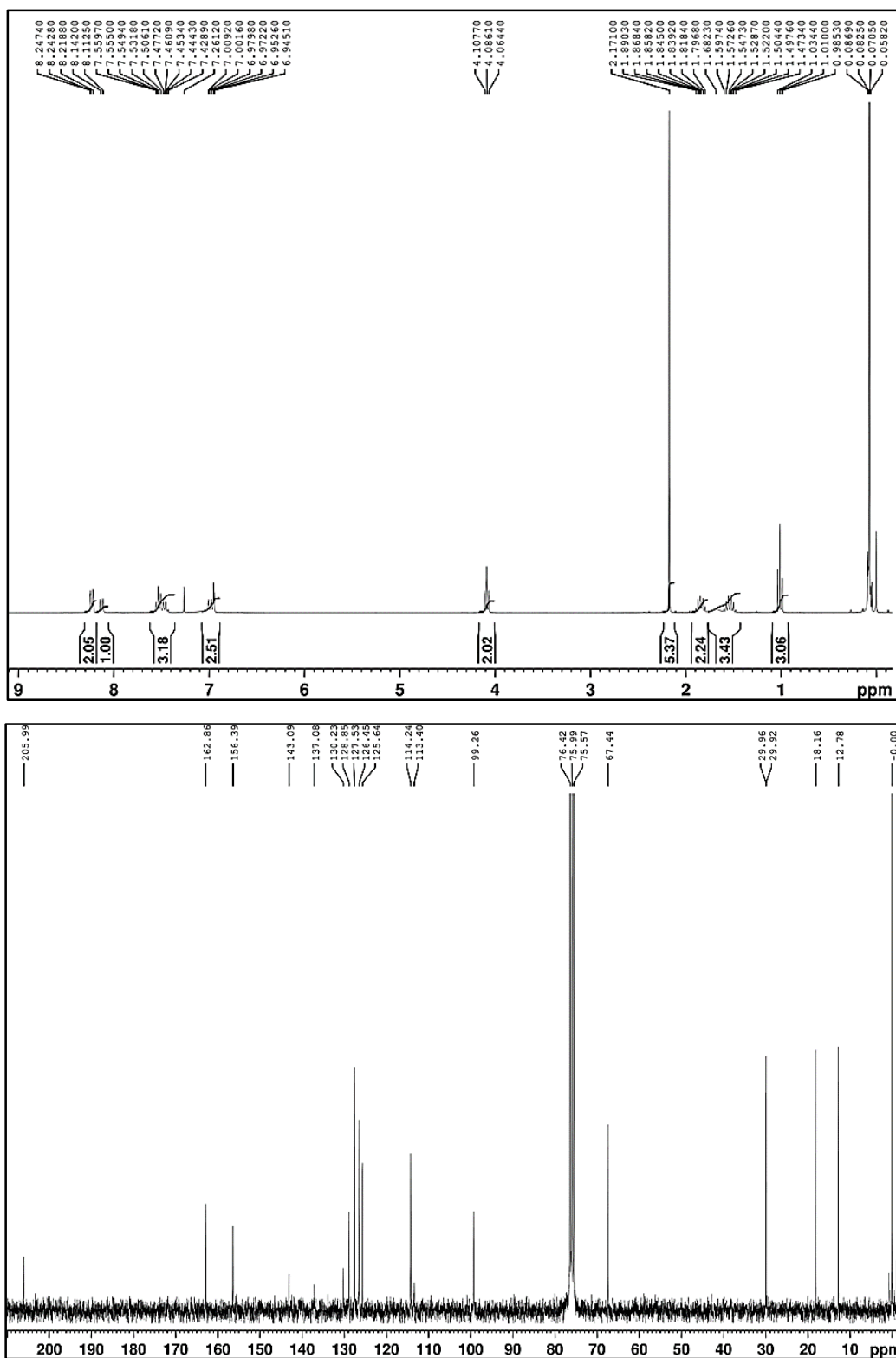


Figure S7. ^1H and ^{13}C NMR of compound 19.

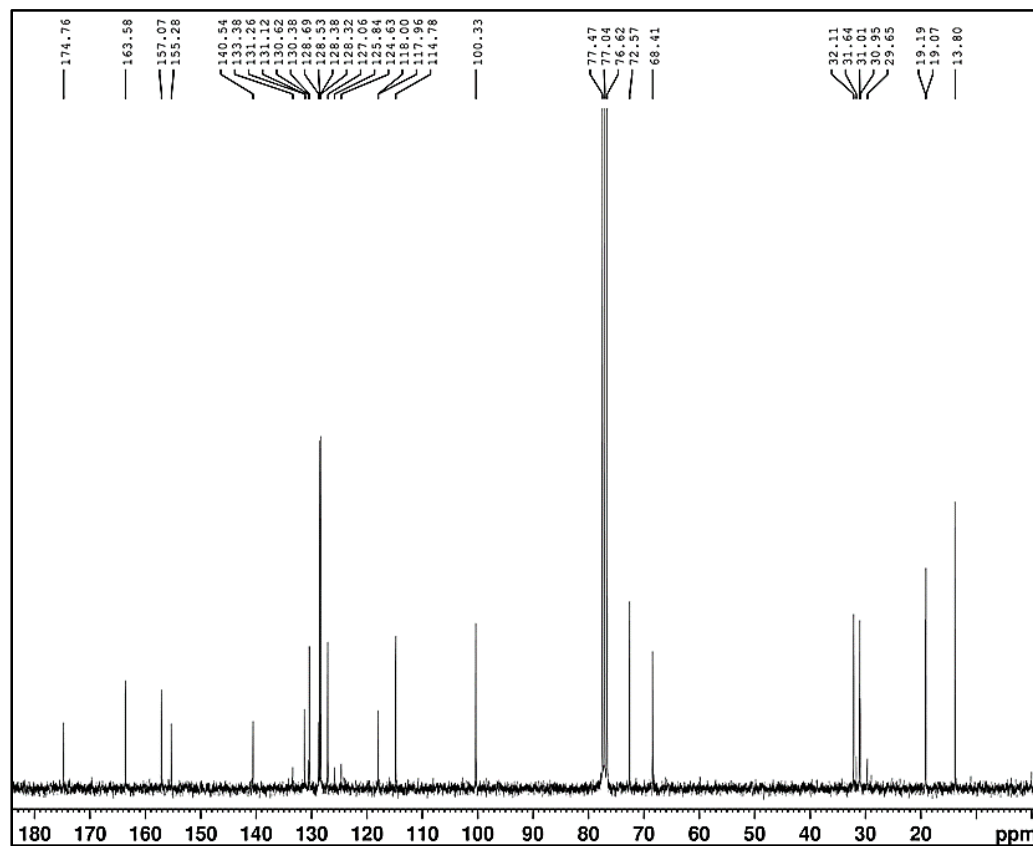
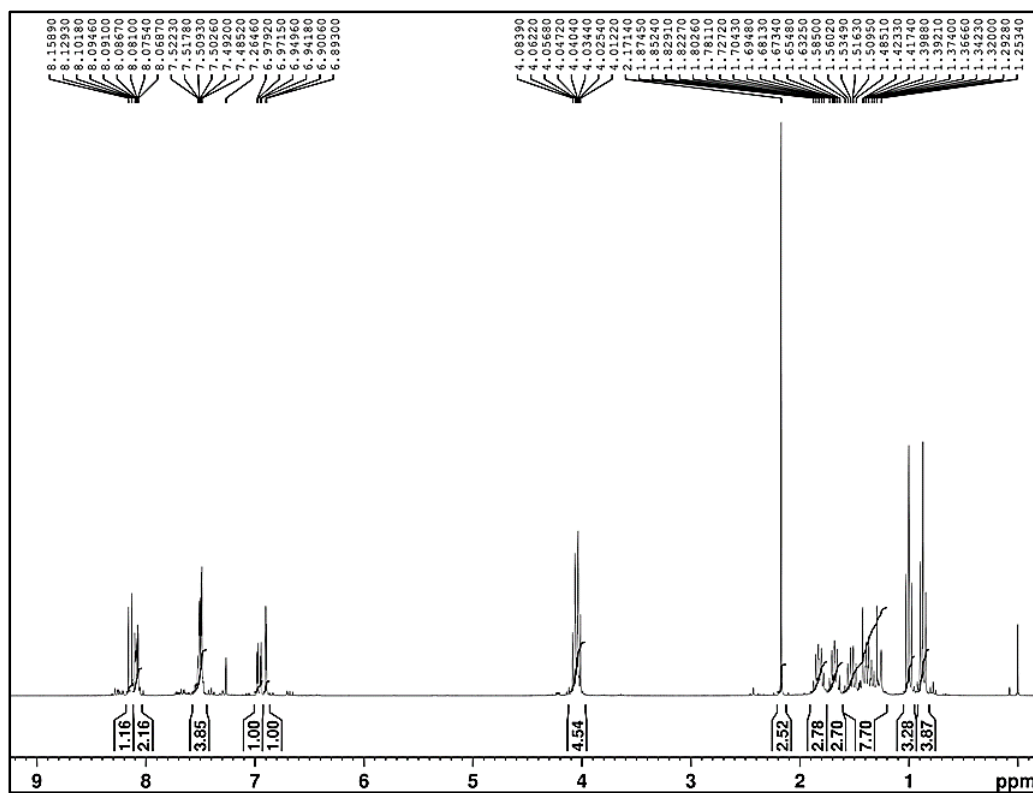


Figure S8. ¹H and ¹³C NMR of compound 20.

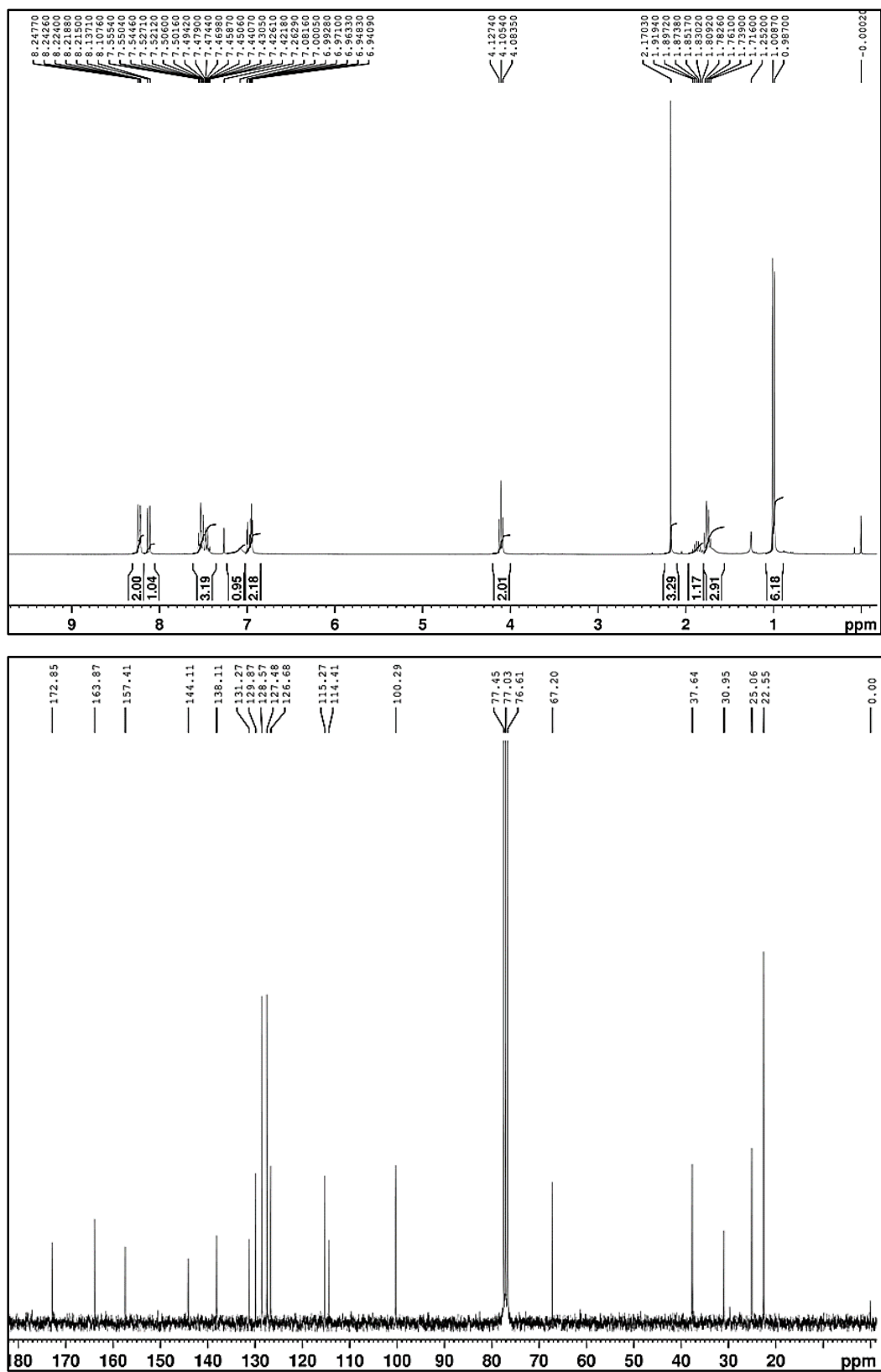


Figure S9. ¹H and ¹³C NMR of compound 21.

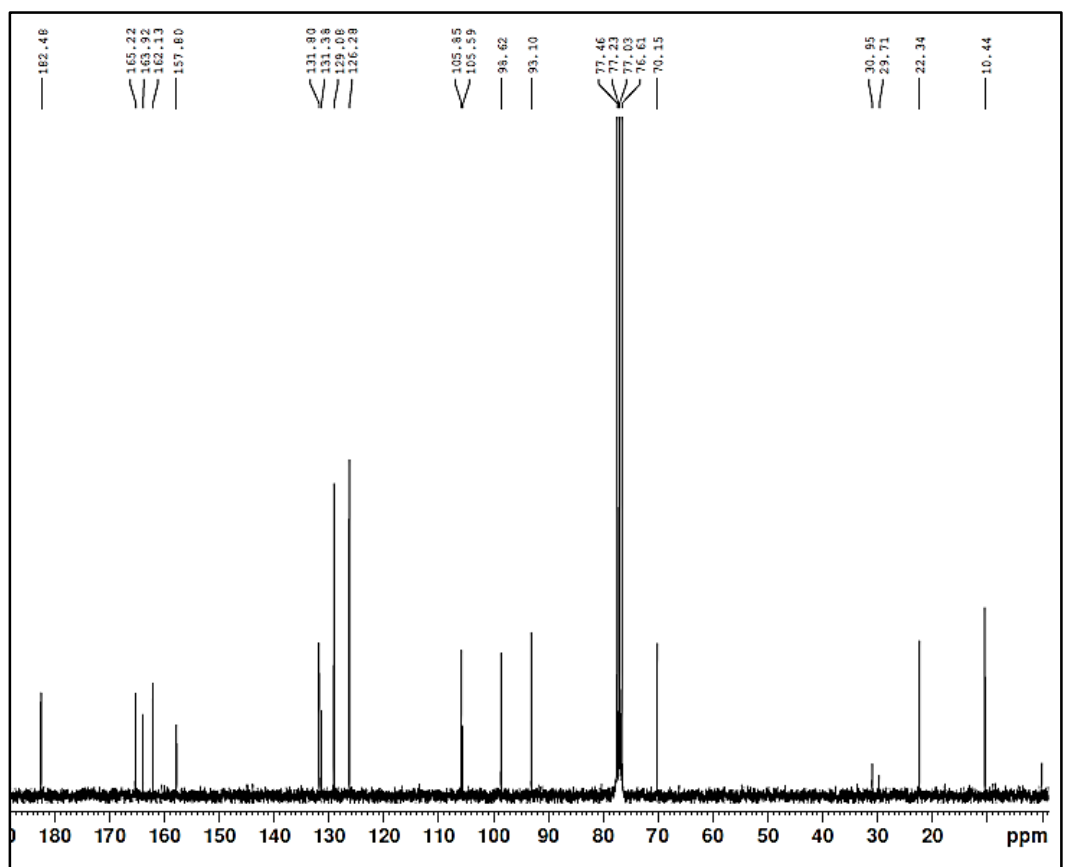
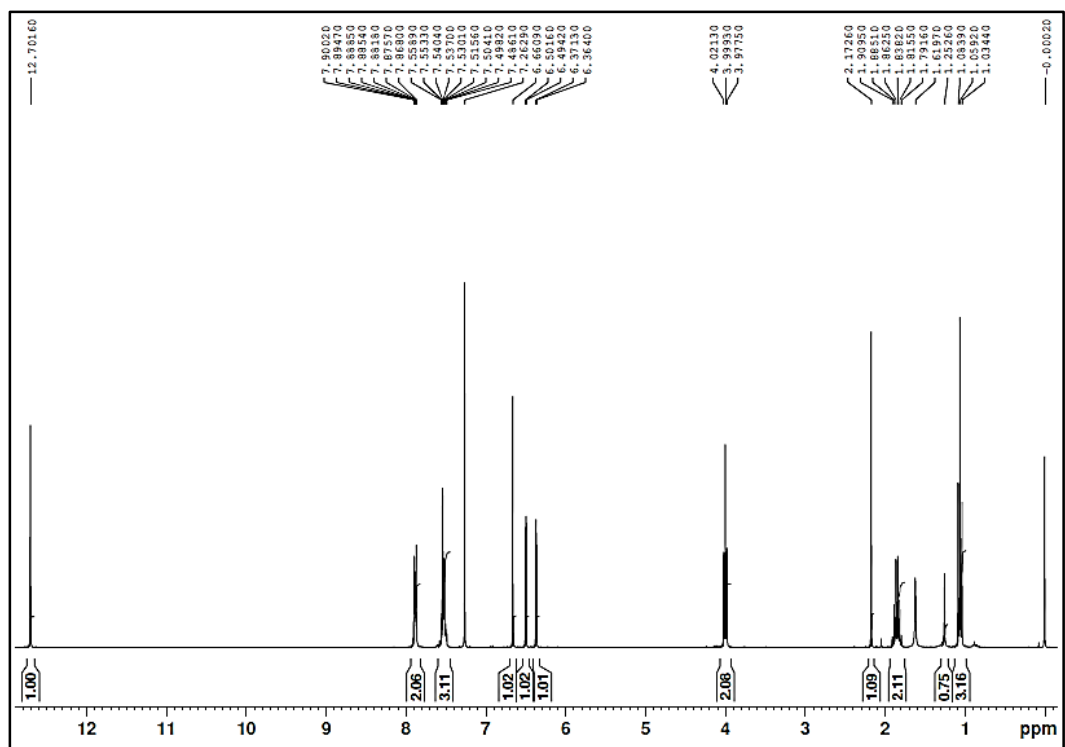


Figure S10. ¹H and ¹³C NMR of compound 24.

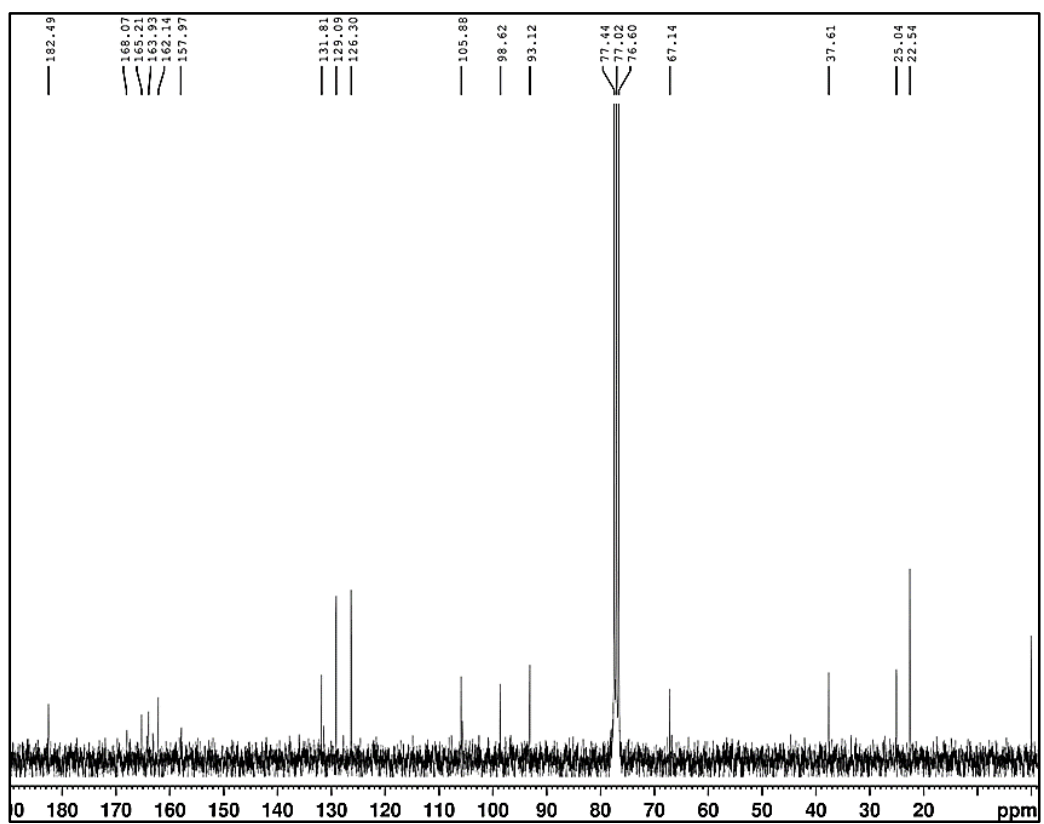
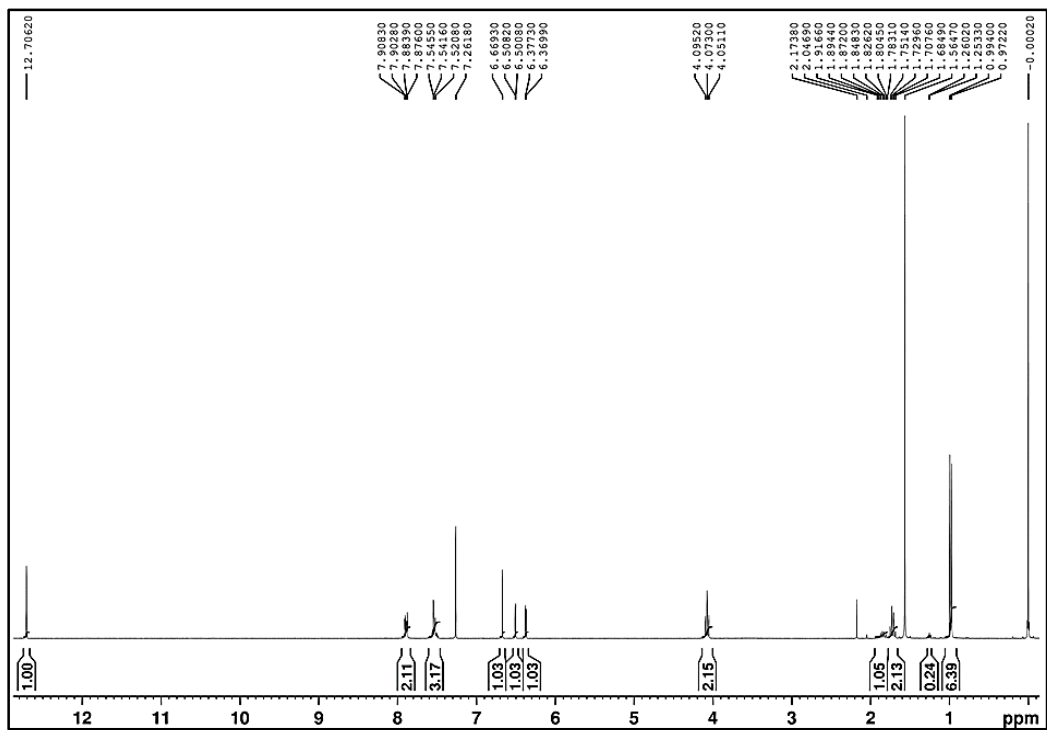
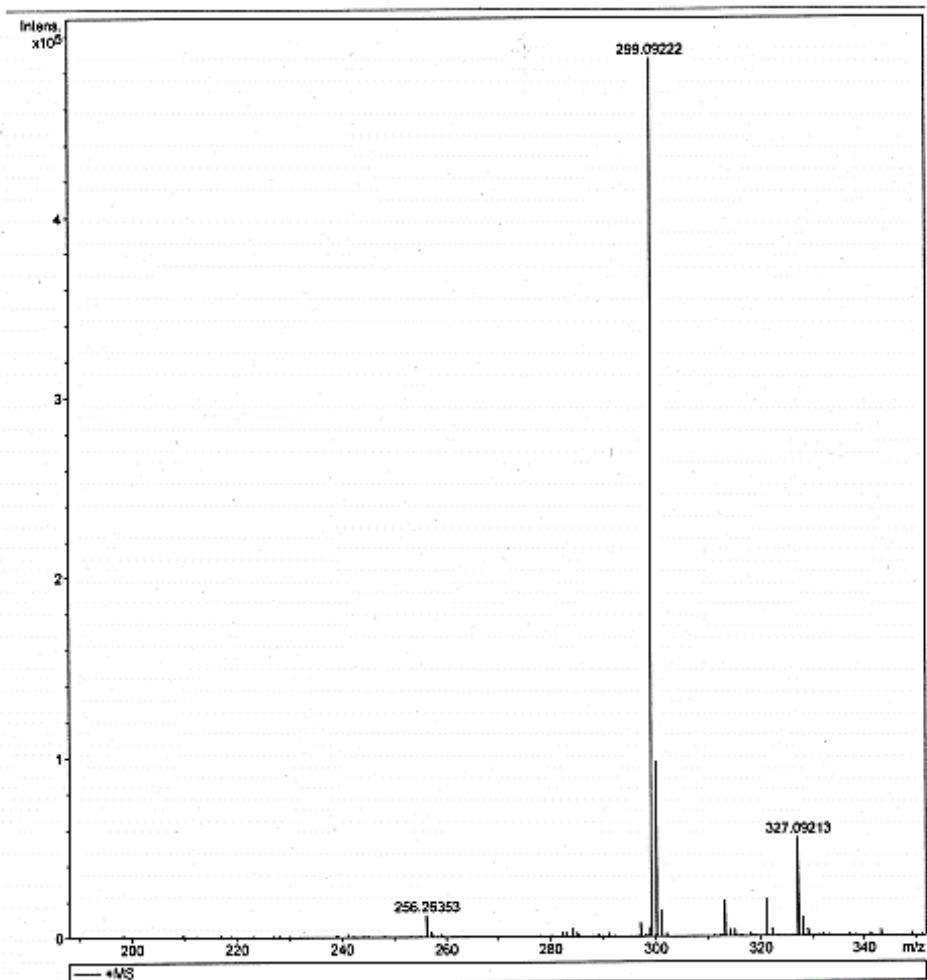


Figure S11. ^1H and ^{13}C NMR of compound 27.

HRMS spectra

Mass Spectrum List Report

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Sample Name BETIL 1 Instrument micrOTOF



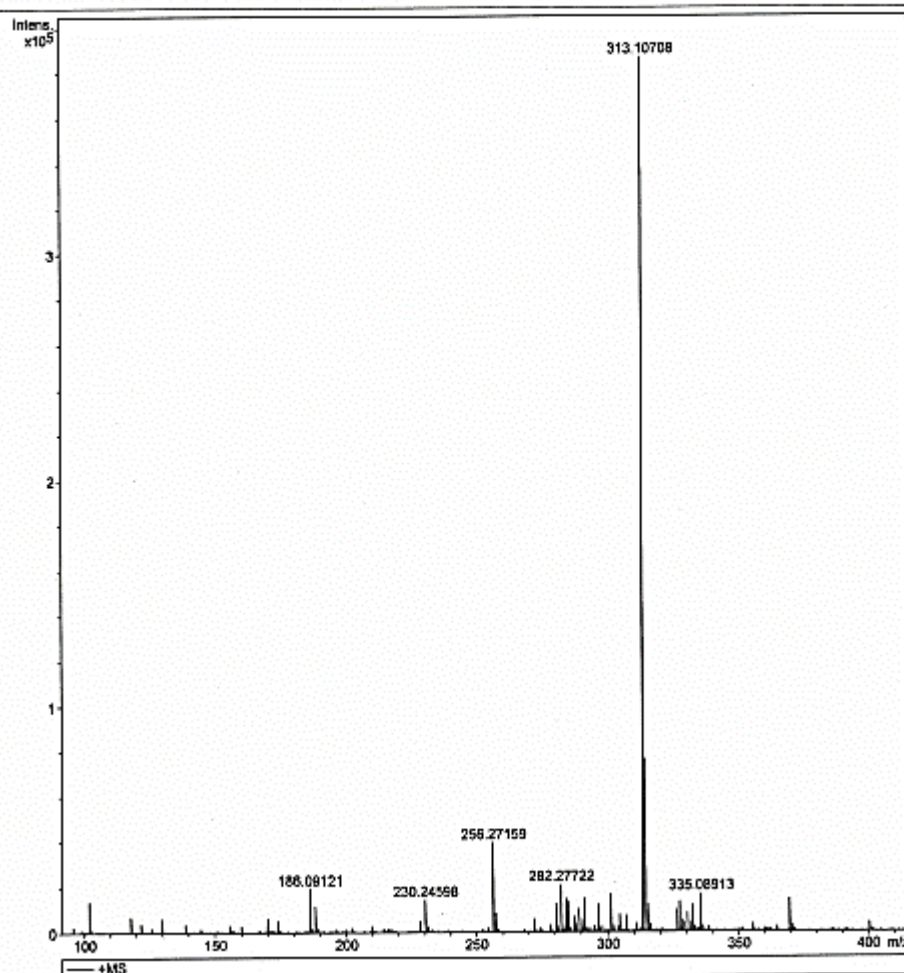
Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rb	e ⁻ Conf	N-Rule
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321.07421	1	C 17 H 14 Na O 5	100.00	321.07334	-0.9	-2.7	107.2	10.5	even	ok

Figure S12. HRMS of compound 6.

Mass Spectrum List Report

Analysis Info ESI -TOF
 Analysis Name JRHC1616444000001.d
 Sample Name BROP 1
 Acquisition Date 10/18/2016 12:10:52 PM
 Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

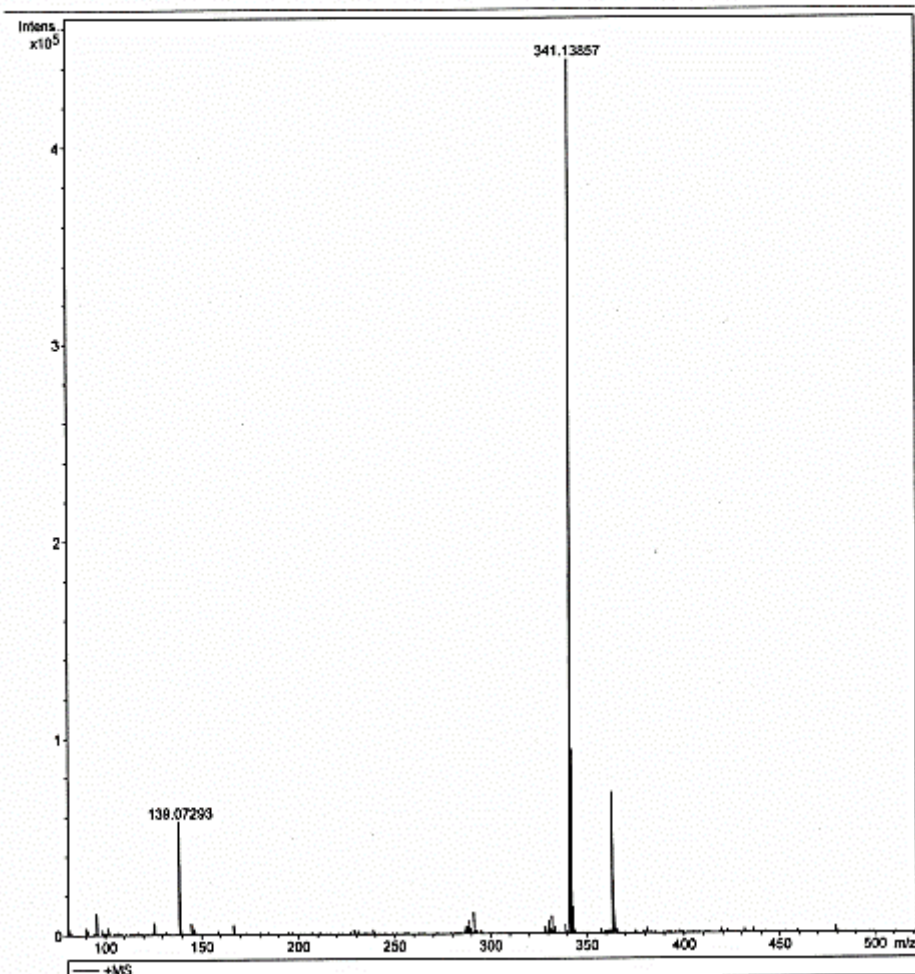
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rtb	e ⁻ Conf	N-Rule
313.10708	1	C ₁₈ H ₁₇ O ₅	100.00	313.10705	-0.0	-0.1	2.5	10.5	even	ok
335.08913	1	C ₁₈ H ₁₆ NaO ₅	100.00	335.08899	-0.1	-0.4	113.8	10.5	even	ok

Figure S13. HRMS of compound 7.

Mass Spectrum List Report

Analysis Info ESI -TOF
Analysis Name JRHC1616441000001.d
Sample Name BISO 1

Acquisition Date 10/18/2016 11:45:41 AM
Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err (mDa)	err (ppm)	mSigma	rb	e ⁻ Conf	N-Rule
341.13857	1	C ₂₀ H ₂₁ O ₅	100.00	341.13835	-0.2	-0.6	3.3	10.5	even	ok
363.12027	1	C ₂₀ H ₂₀ NaO ₅	100.00	363.12028	0.0	0.1	21.9	10.5	even	ok

Figure S14. HRMS of compound 13.

Mass Spectrum List Report

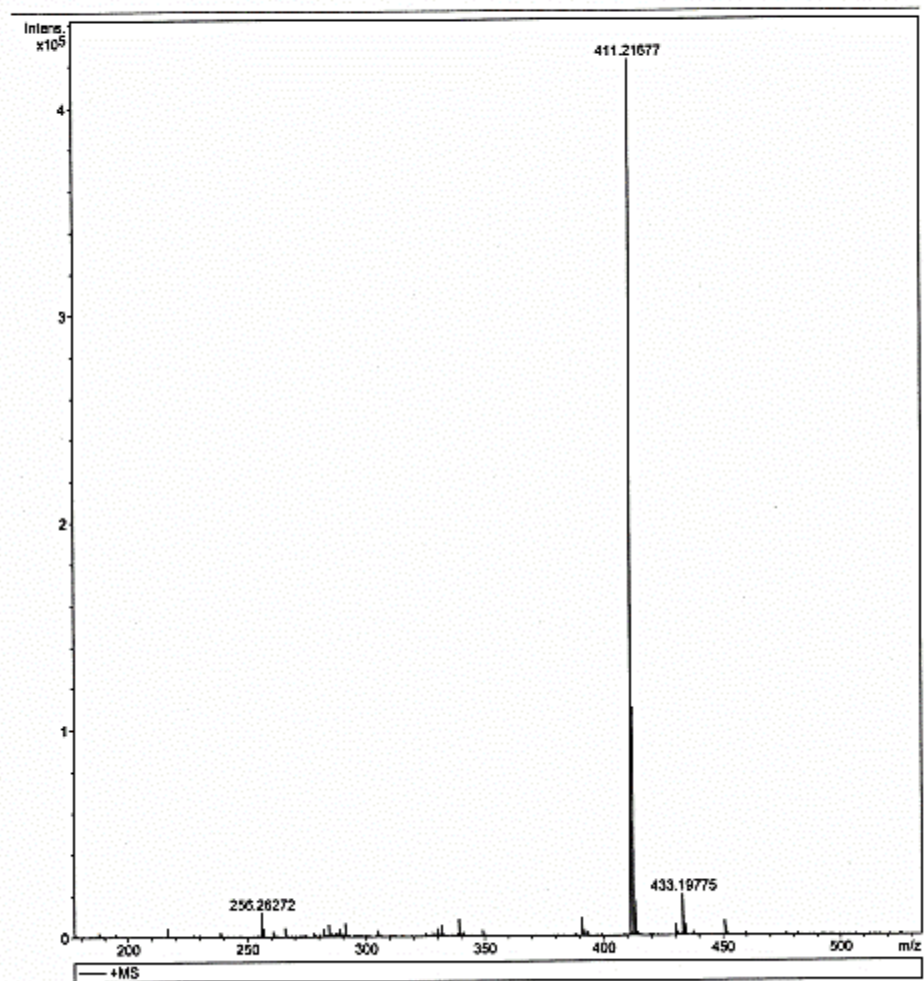
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Sample Name BISO 2

Acquisition Date 10/18/2016 11:53:31 AM

Instrument micrOTOF



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Page 1 of 2

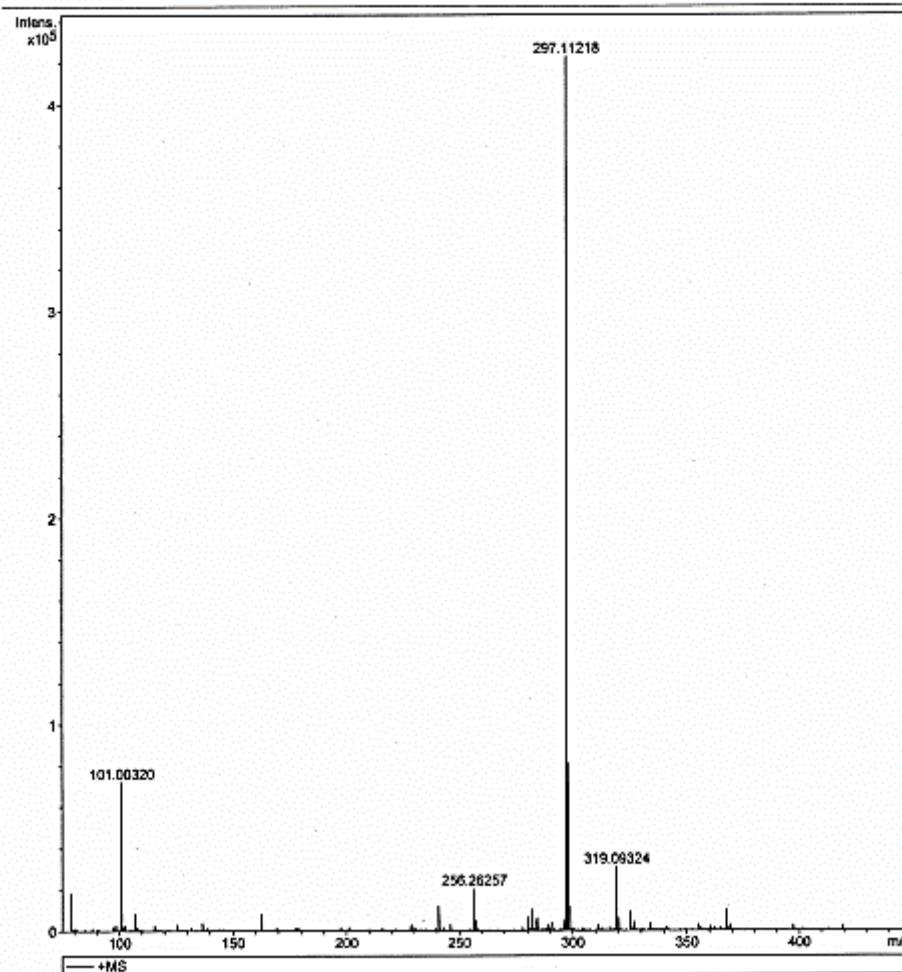
Mass Spectrum Molecular Formula Report

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411.21677	1	C ₂₅ H ₃₁ O ₅	100.00	411.21660	-0.2	-0.4	8.3	10.5	even	ok
433.19775	1	C ₂₅ H ₃₀ NaO ₅	100.00	433.19855	0.8	1.8	26.4	10.6	even	ok

Figure S15. HRMS of compound 14.

Mass Spectrum List Report

Analysis Info ESI-TOF
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Sample Name HRDP Instrument micrOTOF



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Page 1 of 2

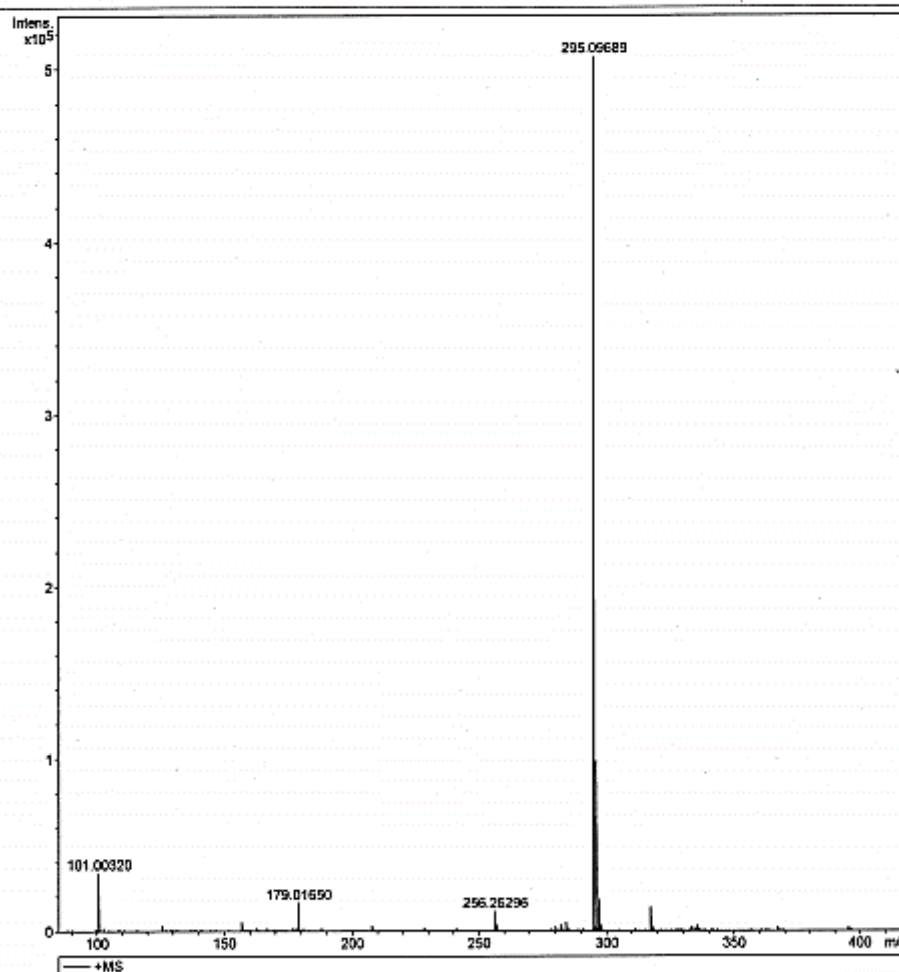
Mass Spectrum Molecular Formula Report

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297.11218	1	C ₁₈ H ₁₇ O ₄	100.00	297.11214	-0.0	-0.2	2.0	10.5	even	ok
319.09324	1	C ₁₈ H ₁₆ NaO ₄	100.00	319.09409	0.8	2.6	15.8	10.5	even	ok

Figure S16. HRMS of compound 17.

Mass Spectrum List Report

Analysis Info ESI -TOF
Analysis Name JRHC16164411000001.d Acquisition Date 10/18/2016 1:17:57 PM
Sample Name HALI Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

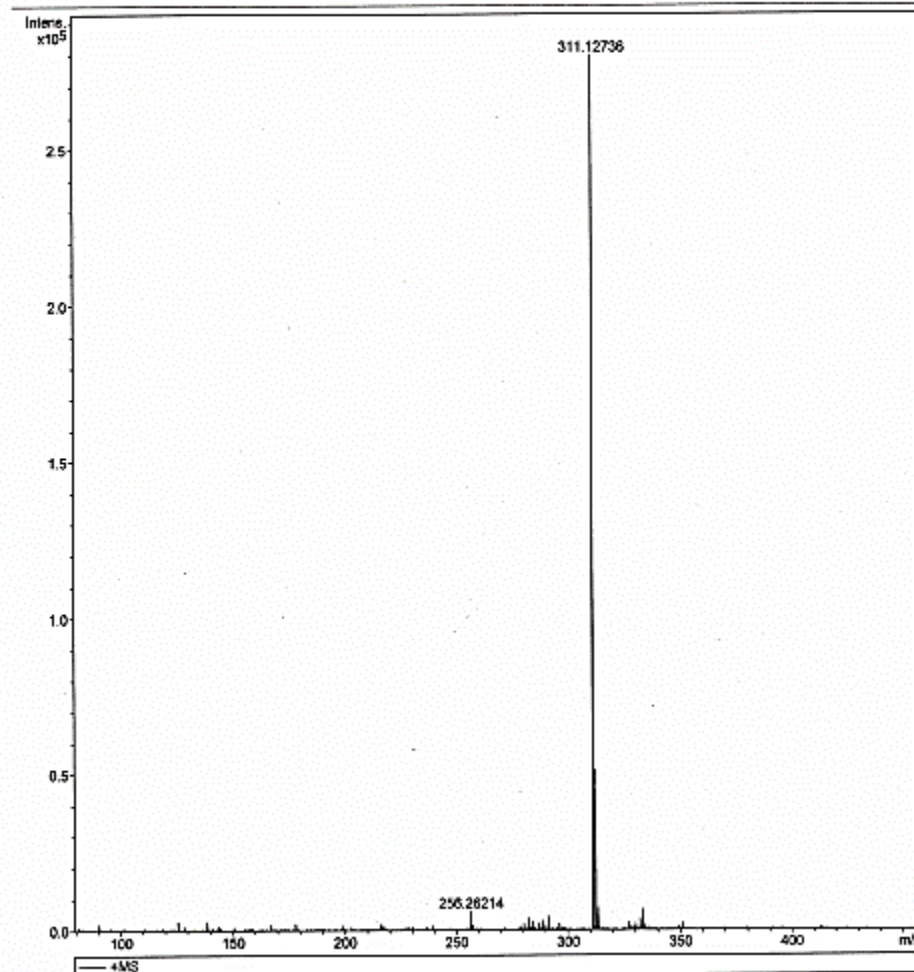
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295.09689	1	C 18 H 15 O 4	100.00	295.09649	-0.4	-1.4	5.8	11.5	even	ok
317.07857	1	C 18 H 14 Na O 4	100.00	317.07843	-0.2	-0.8	113.4	11.5	even	ok

Figure S17. HRMS of compound 18.

Mass Spectrum List Report

Analysis Info ESI-TOF
Analysis Name JRHC1616448000001.d
Sample Name HUTIL 1

Acquisition Date 10/18/2016 12:44:36 PM
Instrument micrOTOF



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Page 1 of 2

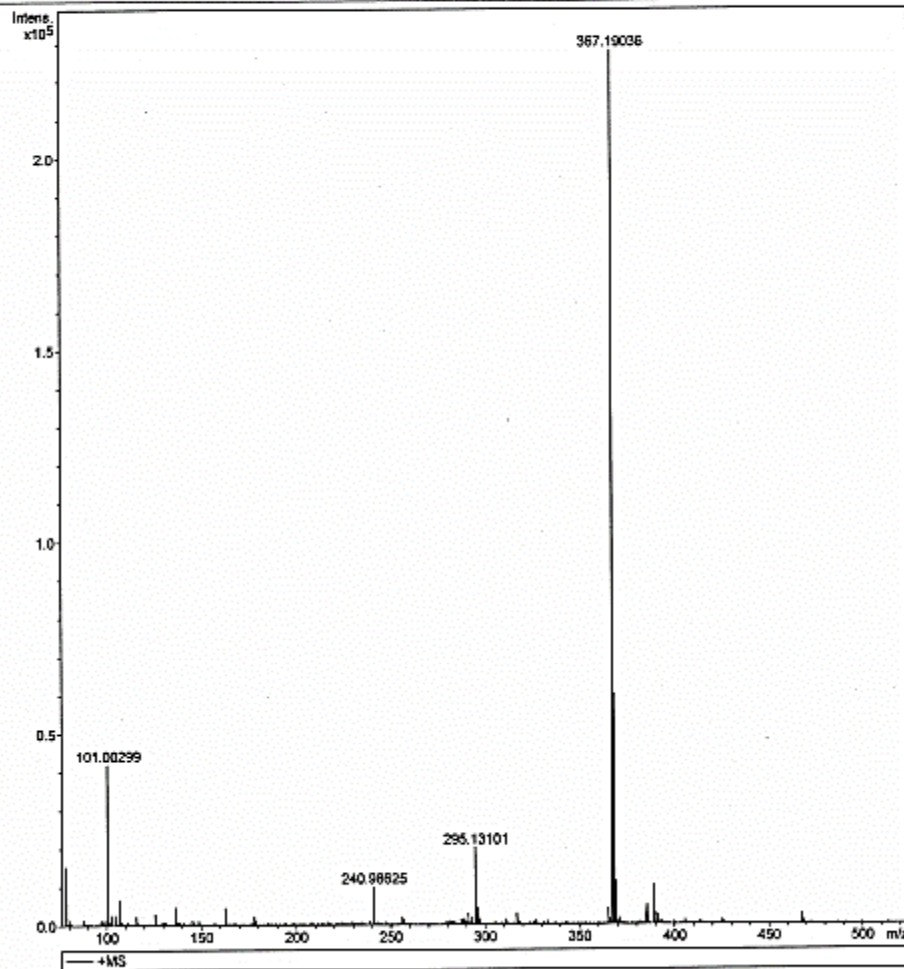
Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
311.12736	1	C ₁₉ H ₁₉ O ₄	100.00	311.12779	0.4	1.4	13.0	10.5	even	ok
333.10593	1	C ₁₉ H ₁₈ NaO ₄	100.00	333.10973	-0.2	-0.6	119.8	10.5	even	ok

Figure S18. HRMS of compound 19.

Mass Spectrum List Report

Analysis Info ESI -TOF
Analysis Name JRHC161644900001.d Acquisition Date 10/18/2016 12:52:20 PM
Sample Name HUTIL 2 Instrument microTOF



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Page 1 of 2

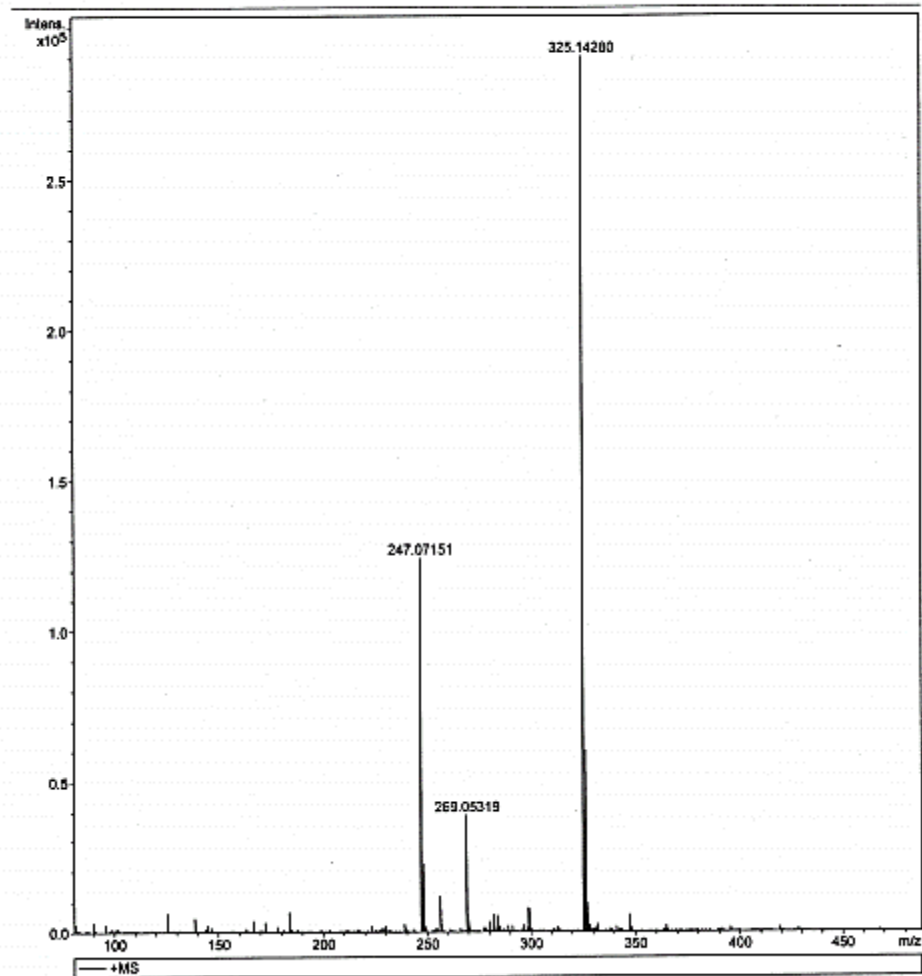
Mass Spectrum Molecular Formula Report

Mass. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
367.19036	1	C ₂₃ H ₂₇ O ₄	100.00	367.19039	0.0	0.1	11.3	10.5	even	ok
369.17123	1	C ₂₃ H ₂₆ NaO ₄	100.00	369.17233	1.1	2.8	28.8	10.5	even	ok

Figure S19. HRMS of compound 20.

Mass Spectrum List Report

Analysis Info ESI-TOF
Analysis Name JRHC1616447000001.d Acquisition Date 10/18/2018 12:37:54 PM
Sample Name HISO Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

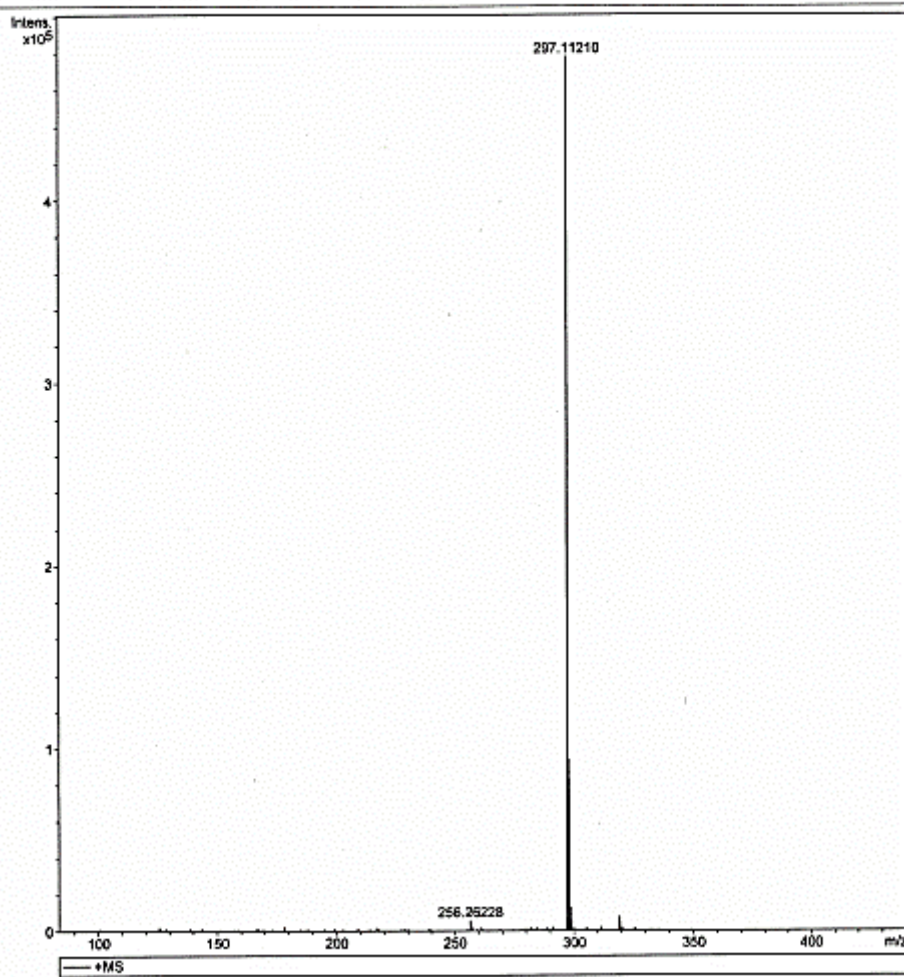
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325.14280	1	C ₂₀ H ₂₁ O ₄	100.00	325.14344	0.6	2.0	5.1	10.5	even	ok

Figure S20. HRMS of compound 21.

Mass Spectrum List Report

Analysis Info ESI -TOF
Analysis Name JRHC16164416000001.d
Sample Name CROP

Acquisition Date 10/18/2016 1:49:55 PM
Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rcb	e ⁻ Conf	N-Rule
297.11210	1	C ₁₈ H ₁₇ O ₄	100.00	297.11214	0.0	0.1	0.6	10.5	even	ok

Figure S21. HRMS of compound 24.

Mass Spectrum List Report

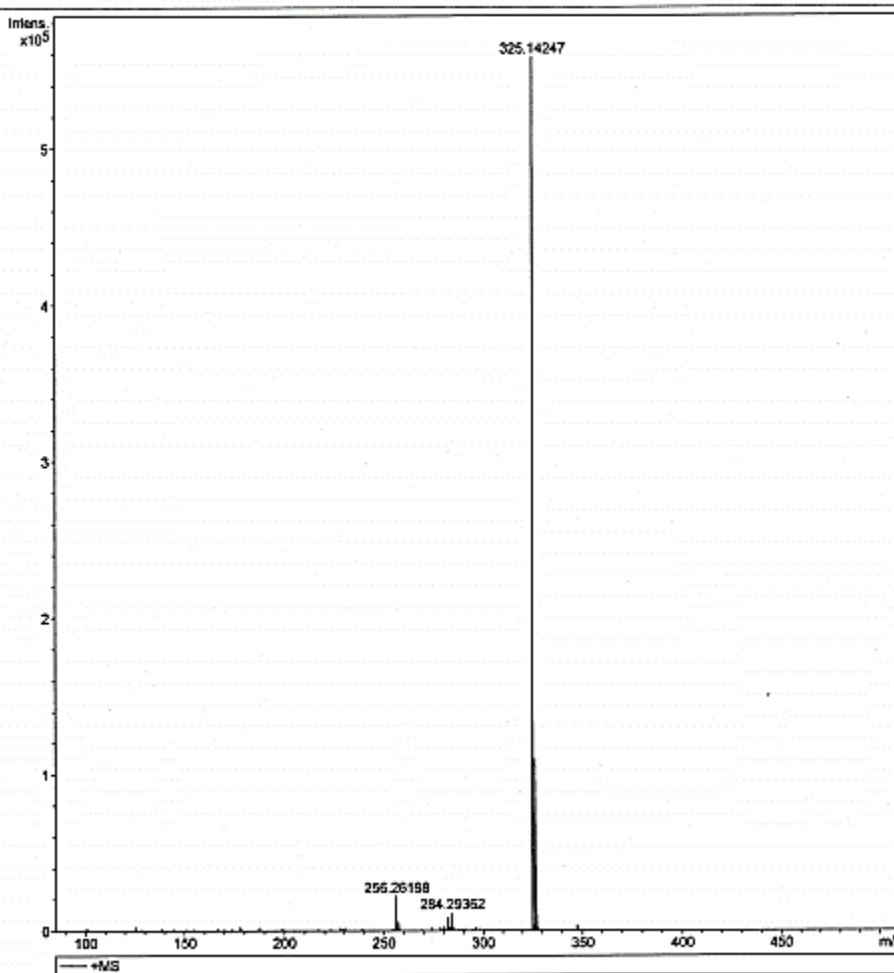
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Acquisition Date 10/18/2016 1:37:37 PM

Sample Name CISO

Instrument micrOTOF



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Page 1 of 2

Mass Spectrum Molecular Formula Report

Mass. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdt	e ⁻ Conf	N-Rule
325.14247	1	C ₂₀ H ₂₁ O ₄	100.00	325.14344	1.0	3.0	11.2	10.5	even	ok

Figure S22. HRMS of compound 27.