Supporting Information Available

Chaetosemins A-E, New Chromones Isolated from an Ascomycete *Chaetomium seminudum* and Their Biological Activities

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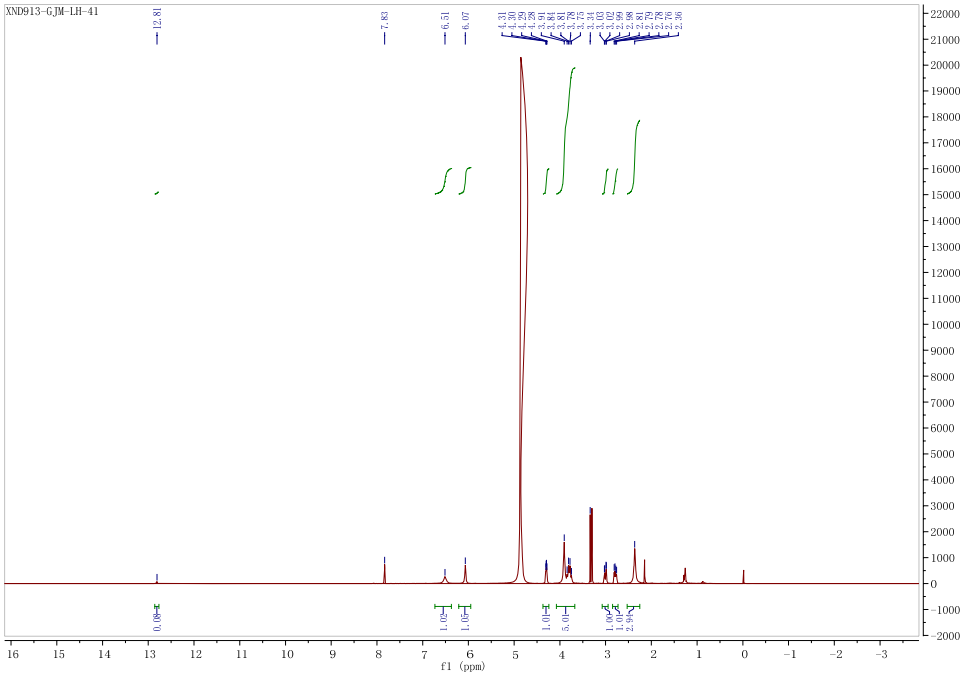

Figure S1. ^{1}H spectra of chaetosemin A in CD3OD

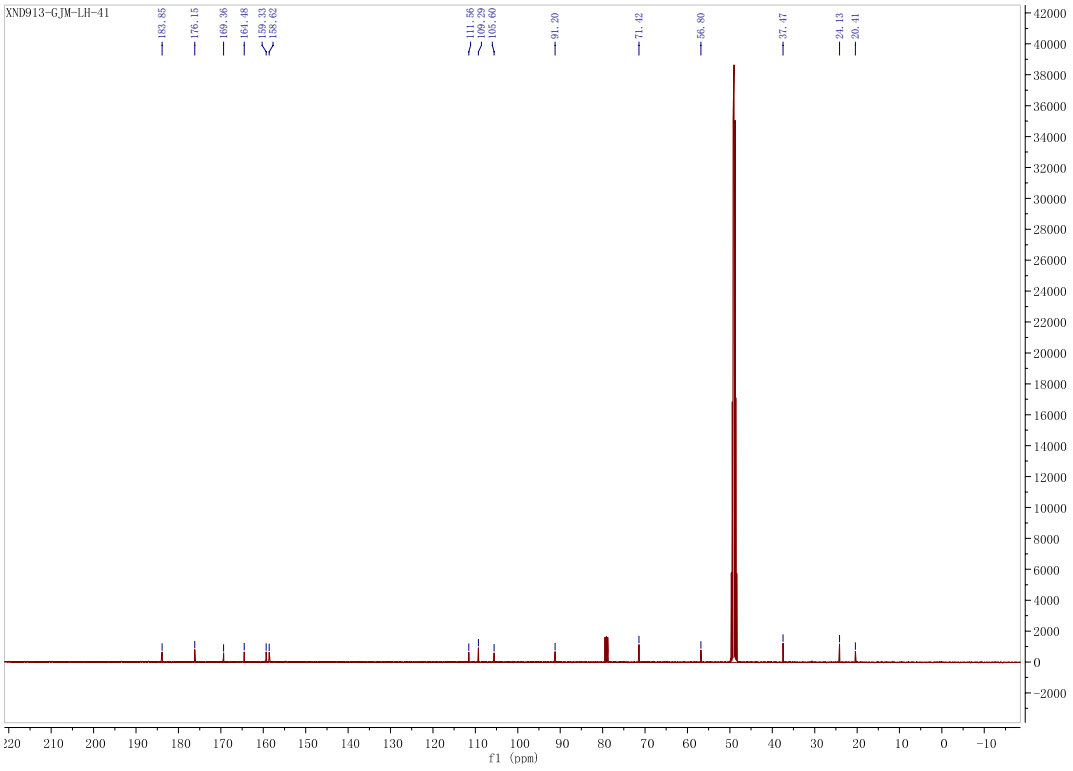

Figure S2. ^{13}C spectra of chaetosemin A in CD3OD

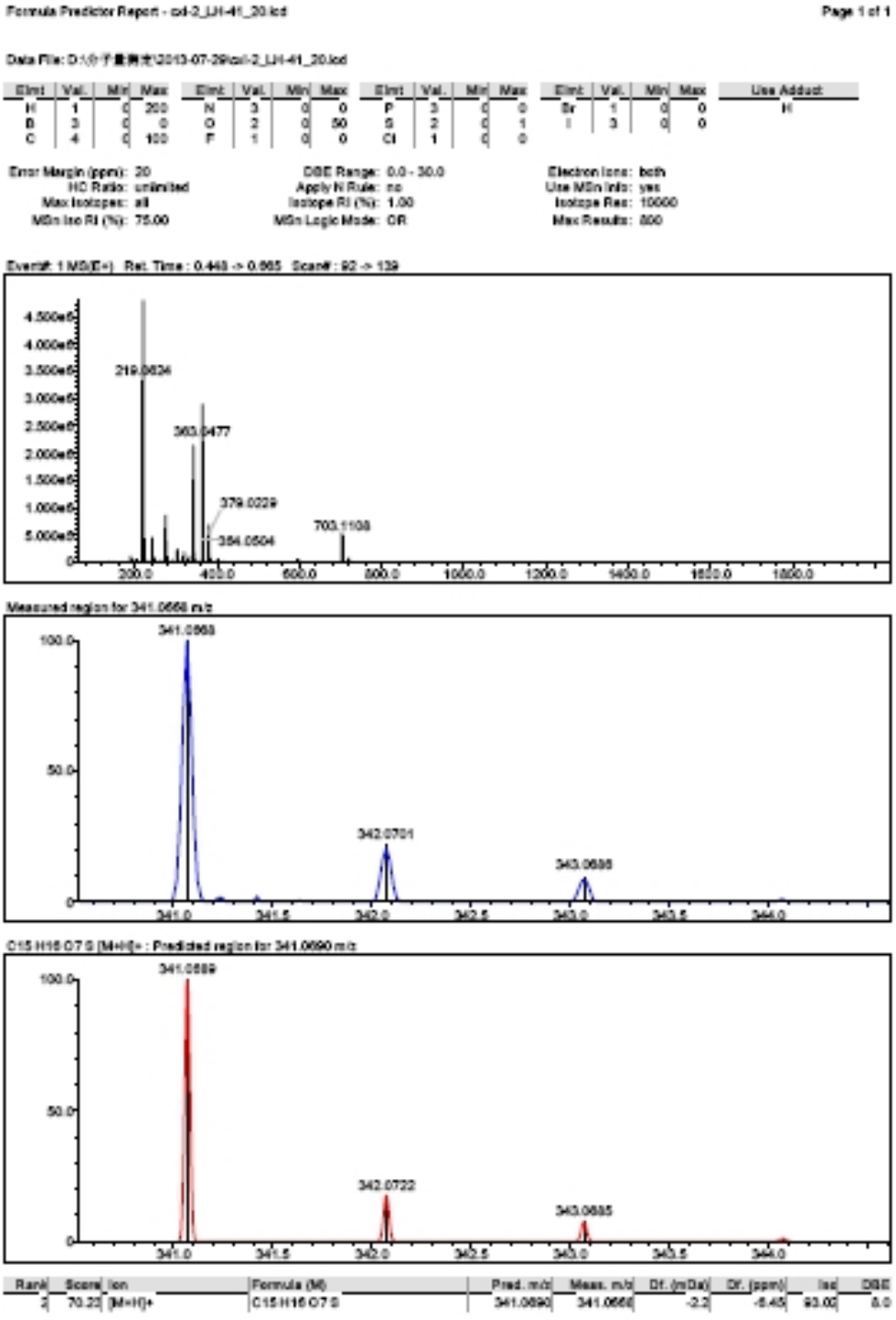

Figure S3. HRESIMS spectra of chaetosemin A

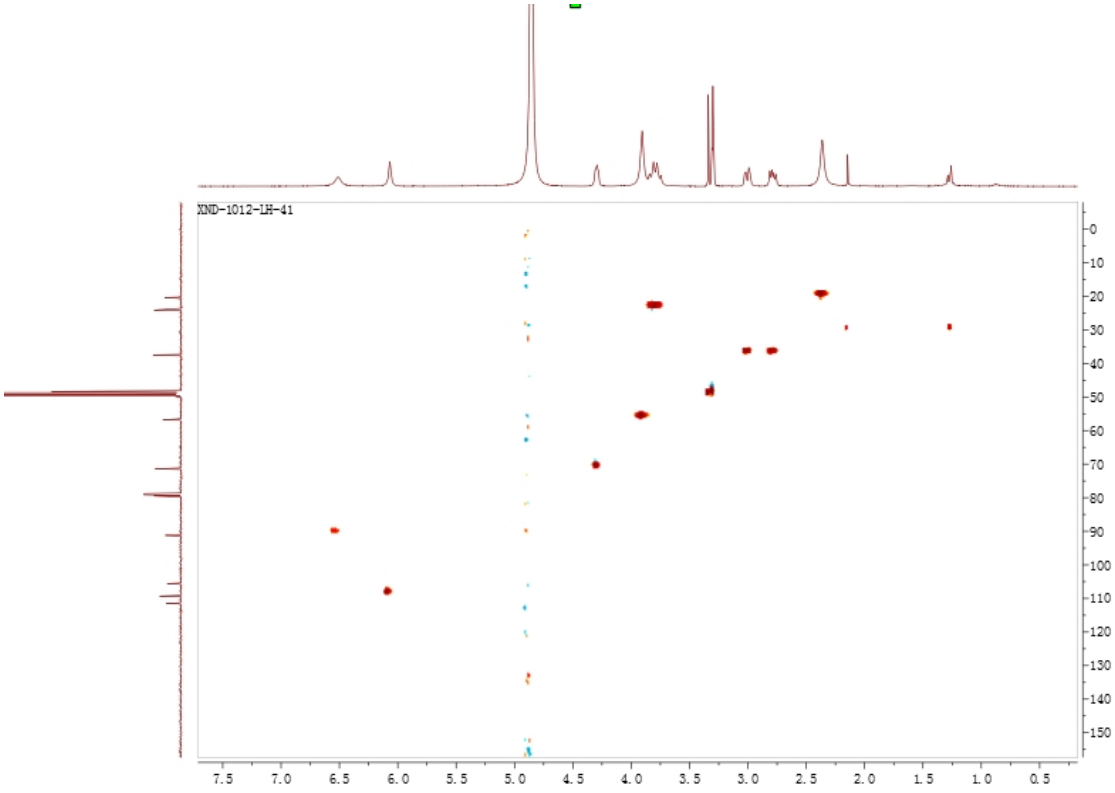

Figure S4. HSQC spectra of chaetosemin A

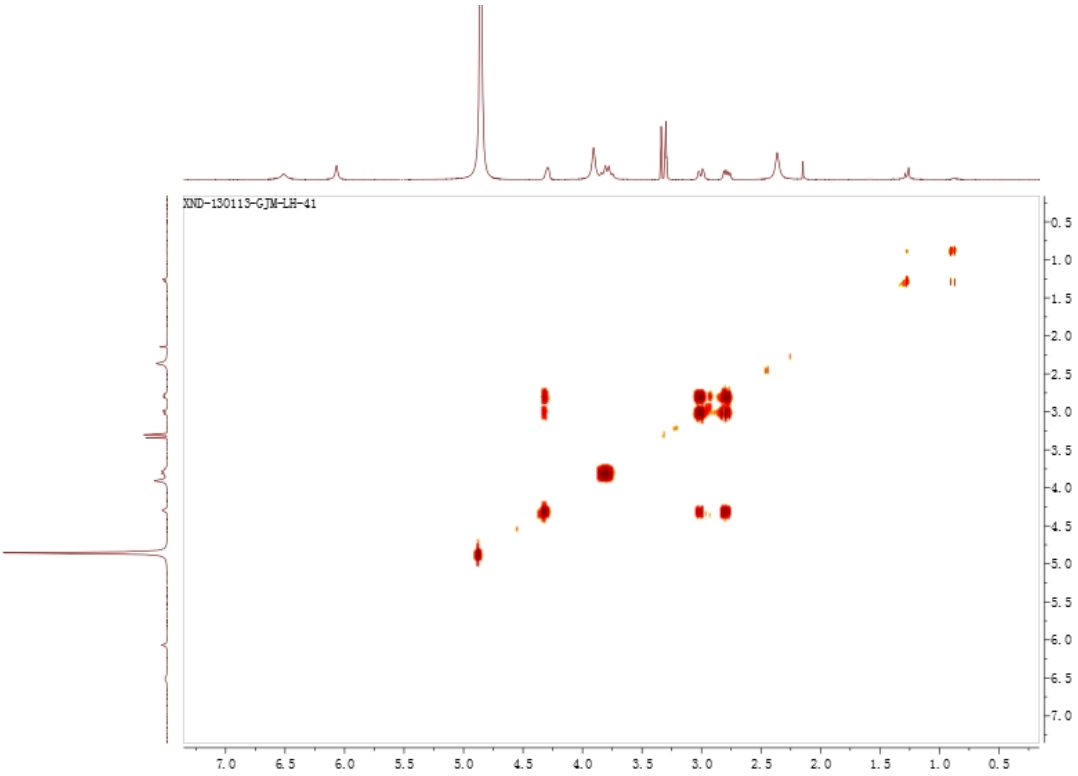

Figure S5. COSY spectra of chaetosemin A

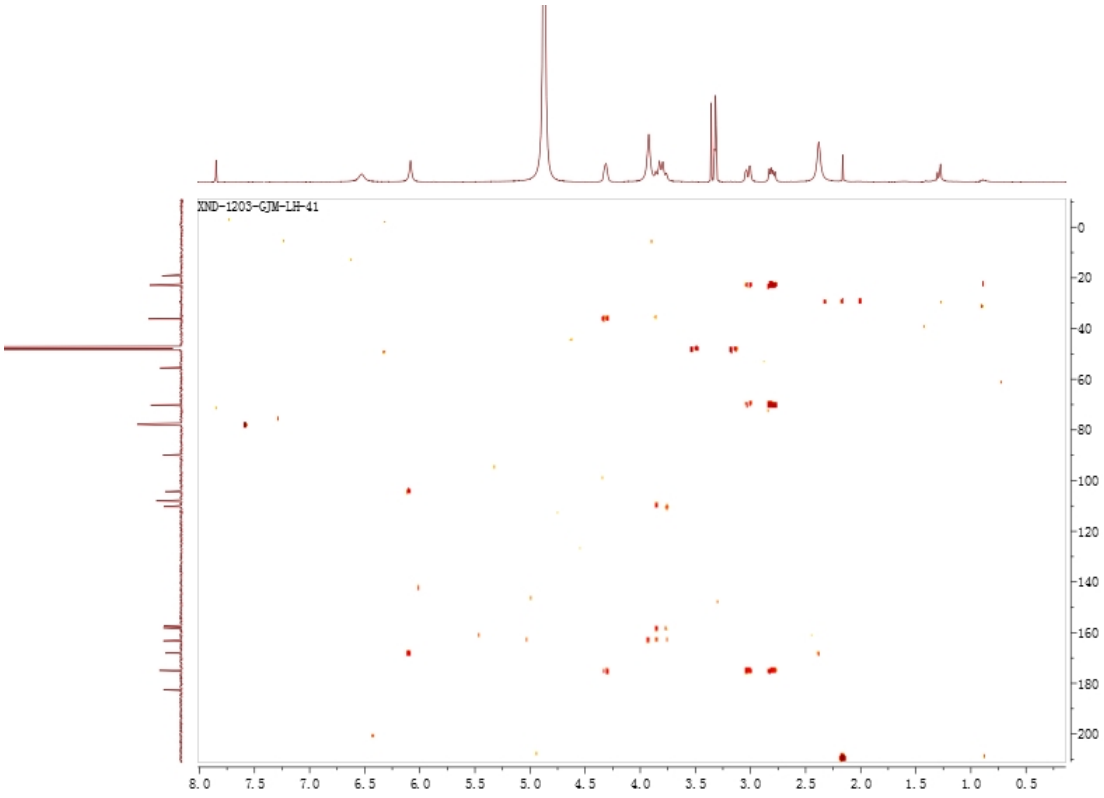

Figure S6. HMBC spectra of chaetosemin A

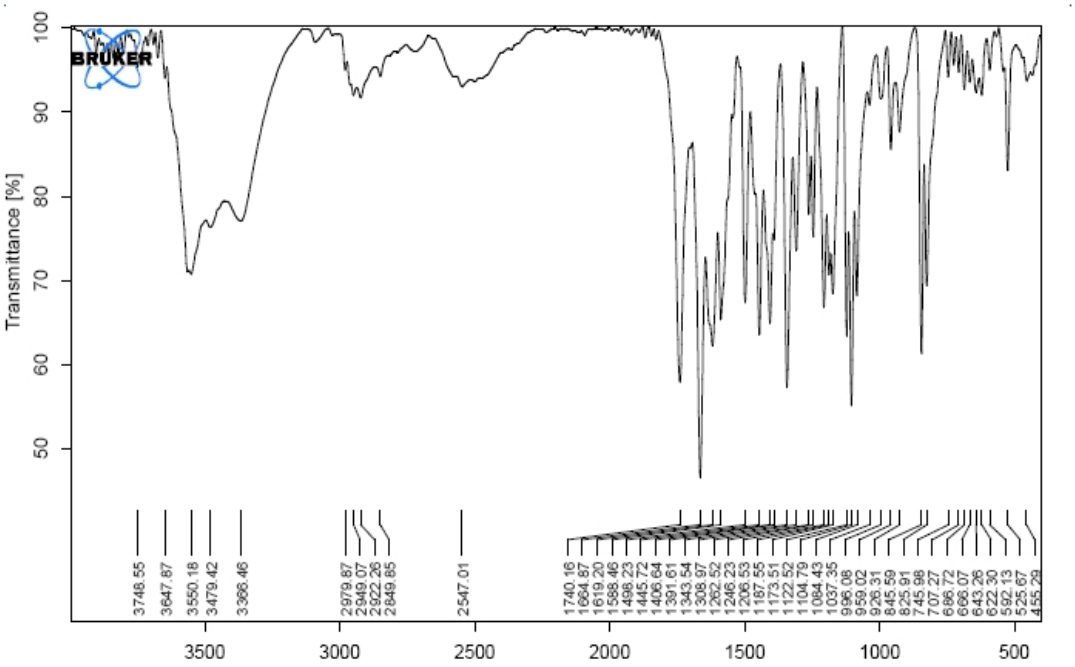

Figure S7. IR spectra of chaetosemin A

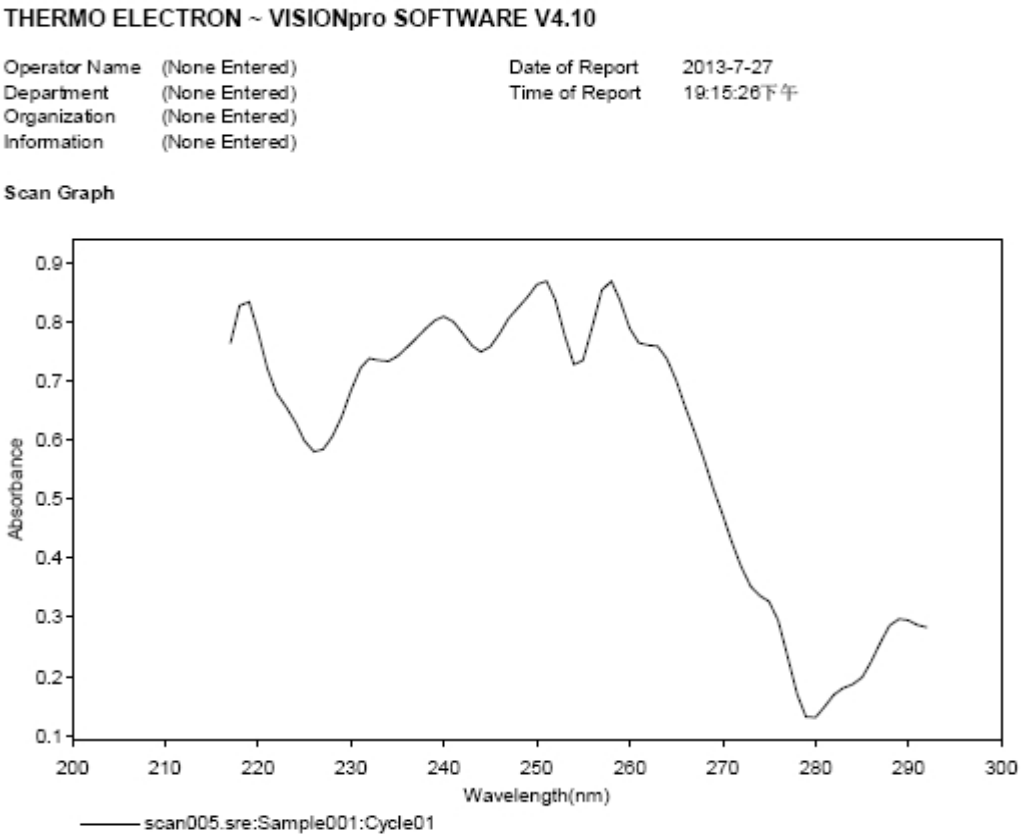

Figure S8. UV spectra of chaetosemin A

Table S1. Crystal data and structure refinement for chaetosemin A

Empirical formula	$C_{15}H_{16}O_7S \cdot H_2O$
Formula weight	358.35
Temperature (K)	298(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	
a (Å)	4.5675(5)
b (Å)	7.6532(8)
c (Å)	45.491(3)
α (°)	90
β (°)	90
γ (°)	90
Volume ($Å^3$)	1590.18(26)
Z	4
Calculated density (mg/m^3)	1.497
Absorption coefficient (mm^{-1})	0.245
F(0 0 0)	752
Crystal size (mm)	0.42 × 0.30 × 0.28
θ Range (°)	2.808-22.65
Limiting indices	
h	-5-5
k	-8-9
l	-53-39
Reflections collected	7980
Independent reflections	2790[R_{int} = 0.0434, R_{sigma} = 0.0530]
Data/restraints/parameters	2790/0/219
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0525, wR_2 = 0.1052
Final R indexes [all data]	R_1 = 0.0680, wR_2 = 0.1110
Largest diff. peak/hole / e $Å^{-3}$	0.210/-0.213

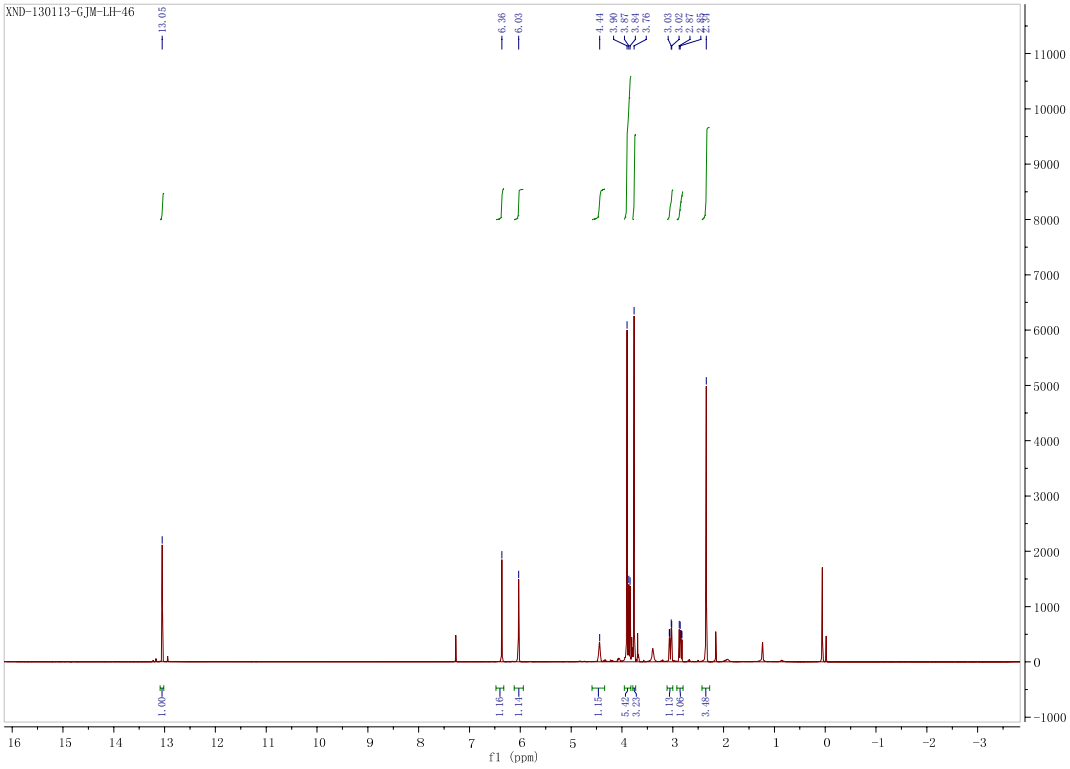

Figure S9. ^{1}H spectra of chaetoseminBin $CDCl_3$

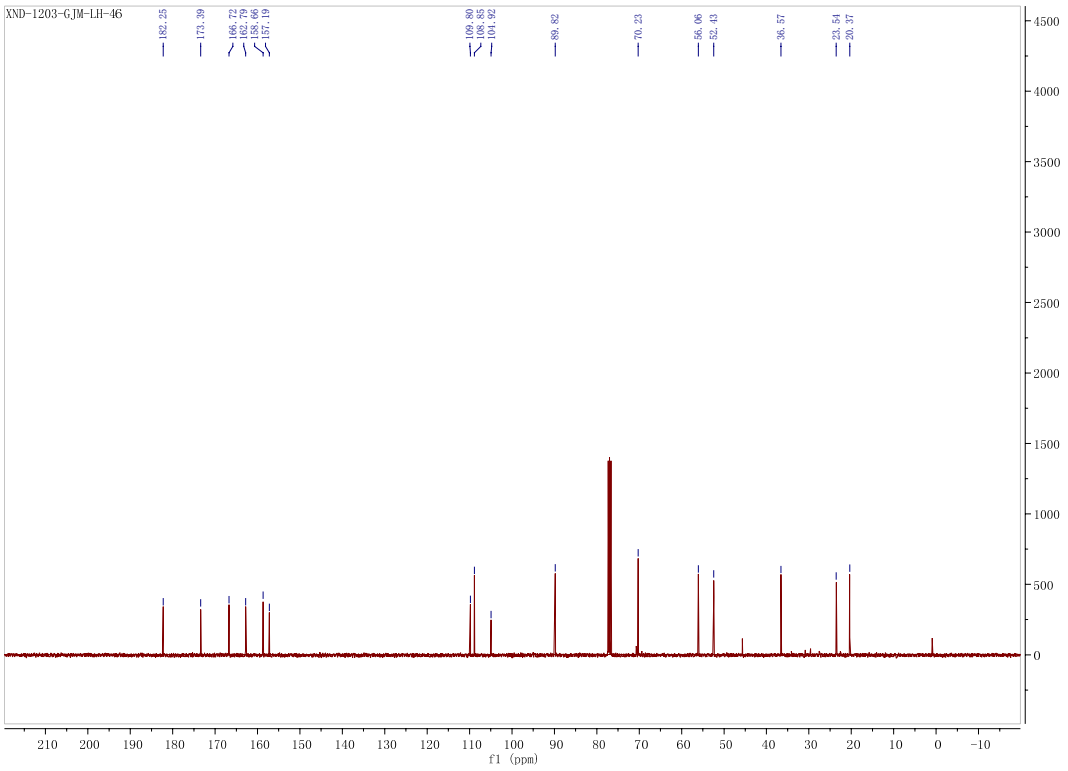

Figure S10. ^{13}C spectra of chaetoseminBin $CDCl_3$

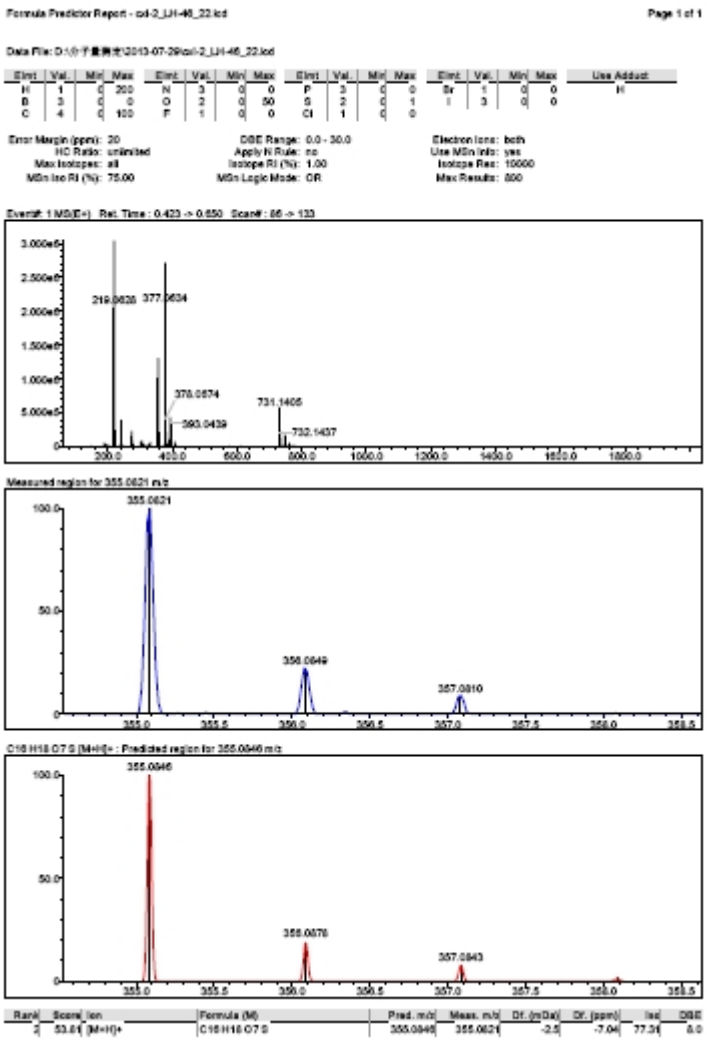

Figure S11.HRESIMS spectra of chaetoseminB

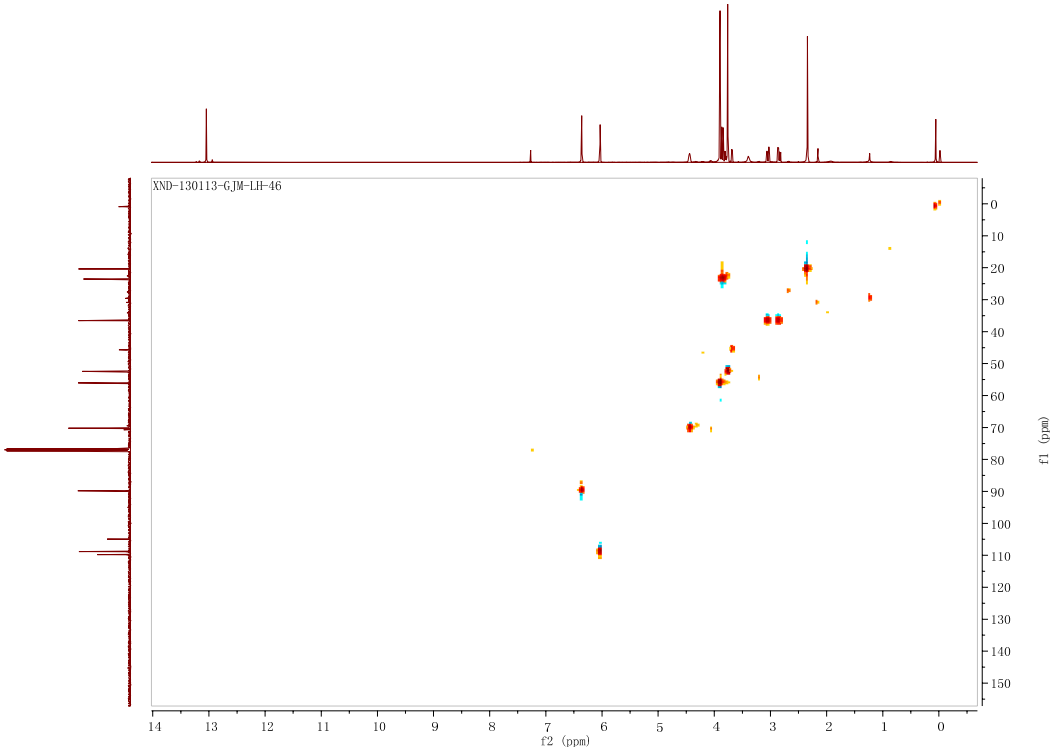

Figure S12. HSQC spectra of chaetoseminB

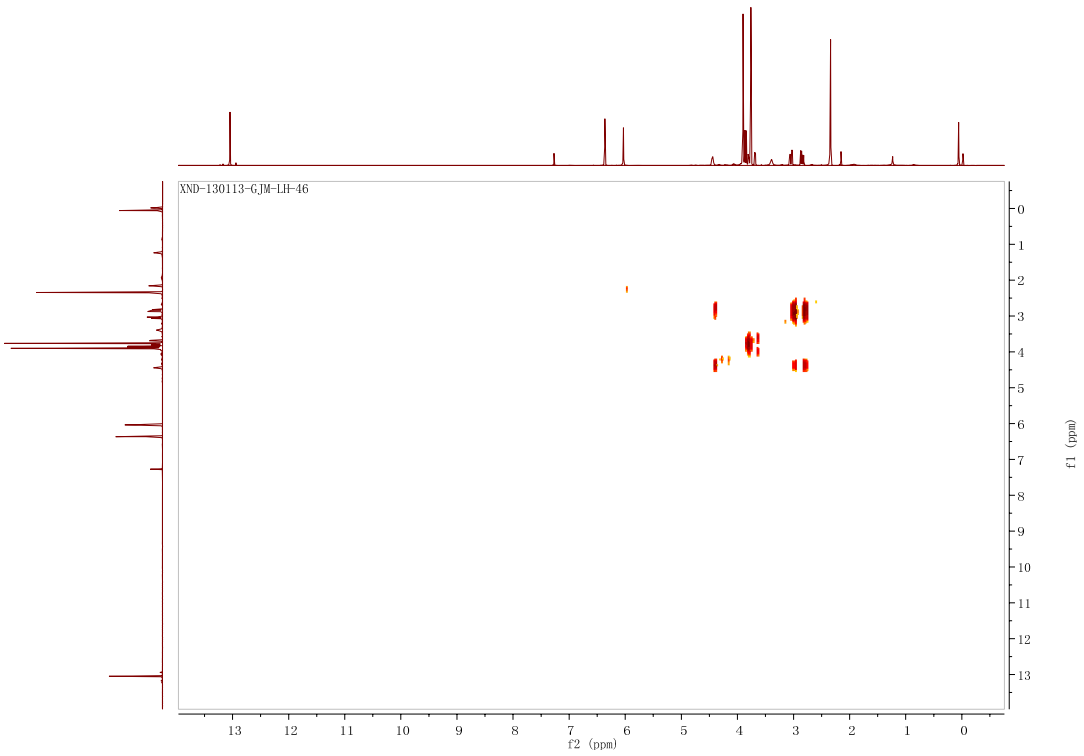

Figure S13. COSY spectra of chaetoseminB

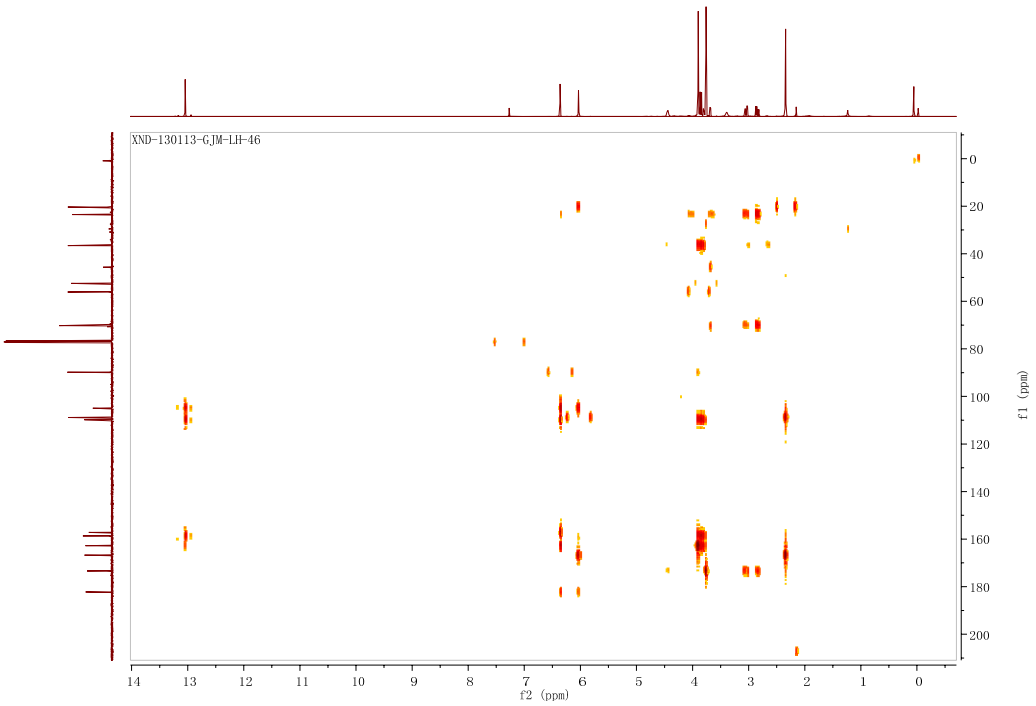

Figure S14. HMBC spectra of chaetoseminB

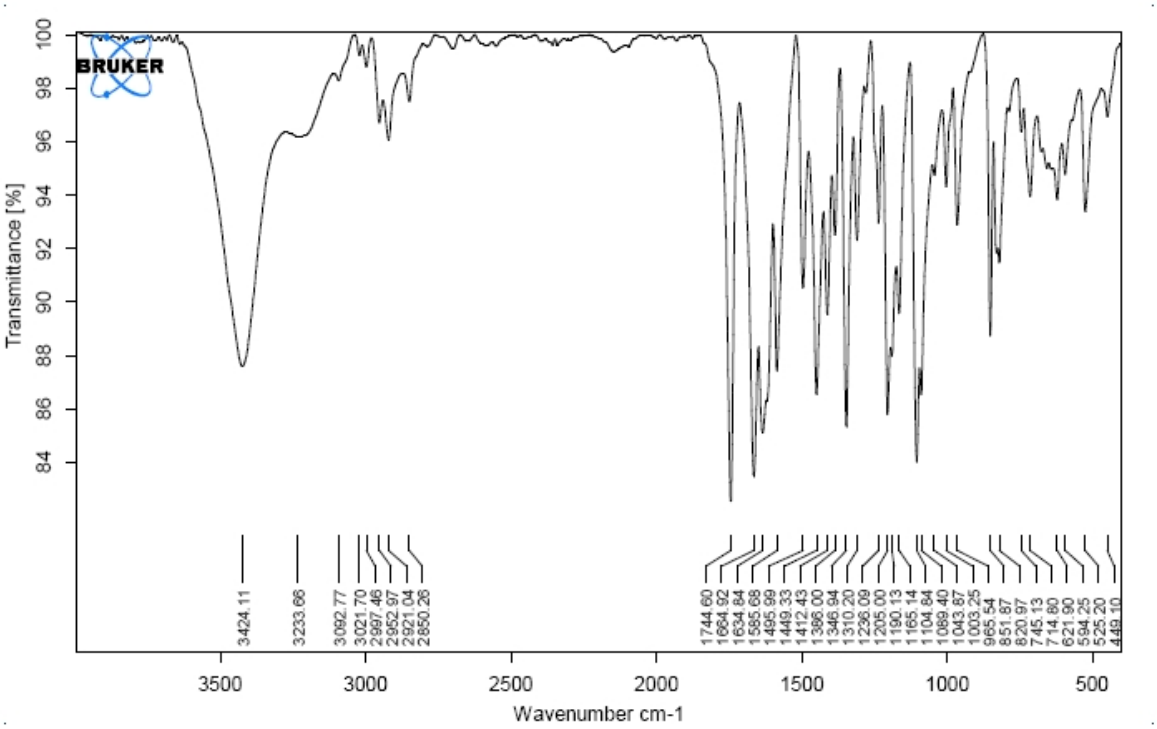

Figure S15. IR spectra of chaetoseminB

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Department	(None Entered)	Time of Report	19:36:08下午
Organization	(None Entered)		
Information	(None Entered)		

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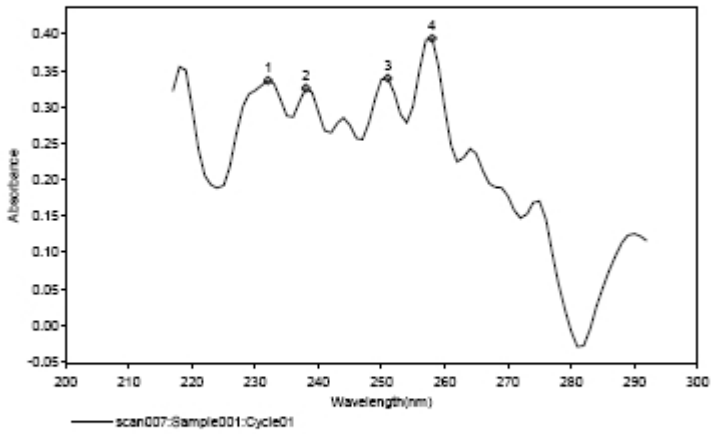

Results Table - scan007, Sample001, Cycle01

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238.00	.326	Start Wavelength 200.00 nm
251.00	.339	Stop Wavelength 300.00 nm
258.00	.394	Sort By Wavelength
Sensitivity	Auto	

Figure S16. UV spectra of chaetoseminB

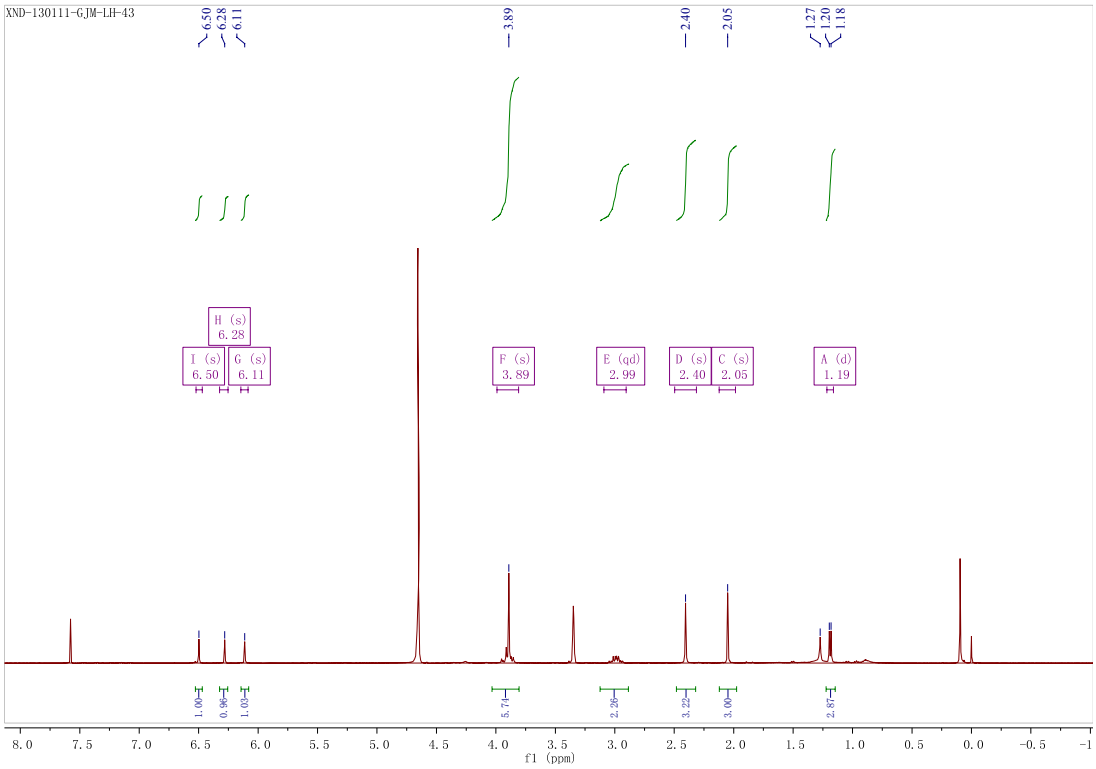

Figure S17. ^{1}H spectra of chaetoseminCin MeOD

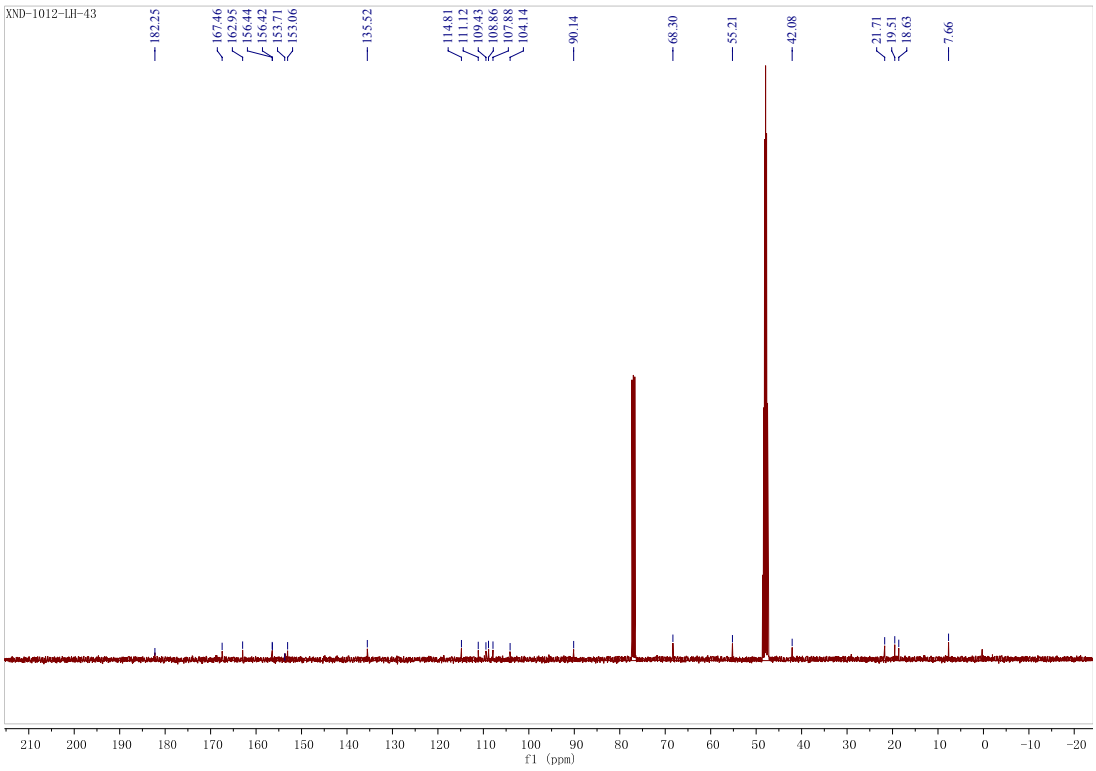

Figure S18. ^{13}C spectra of chaetoseminCin MeOD

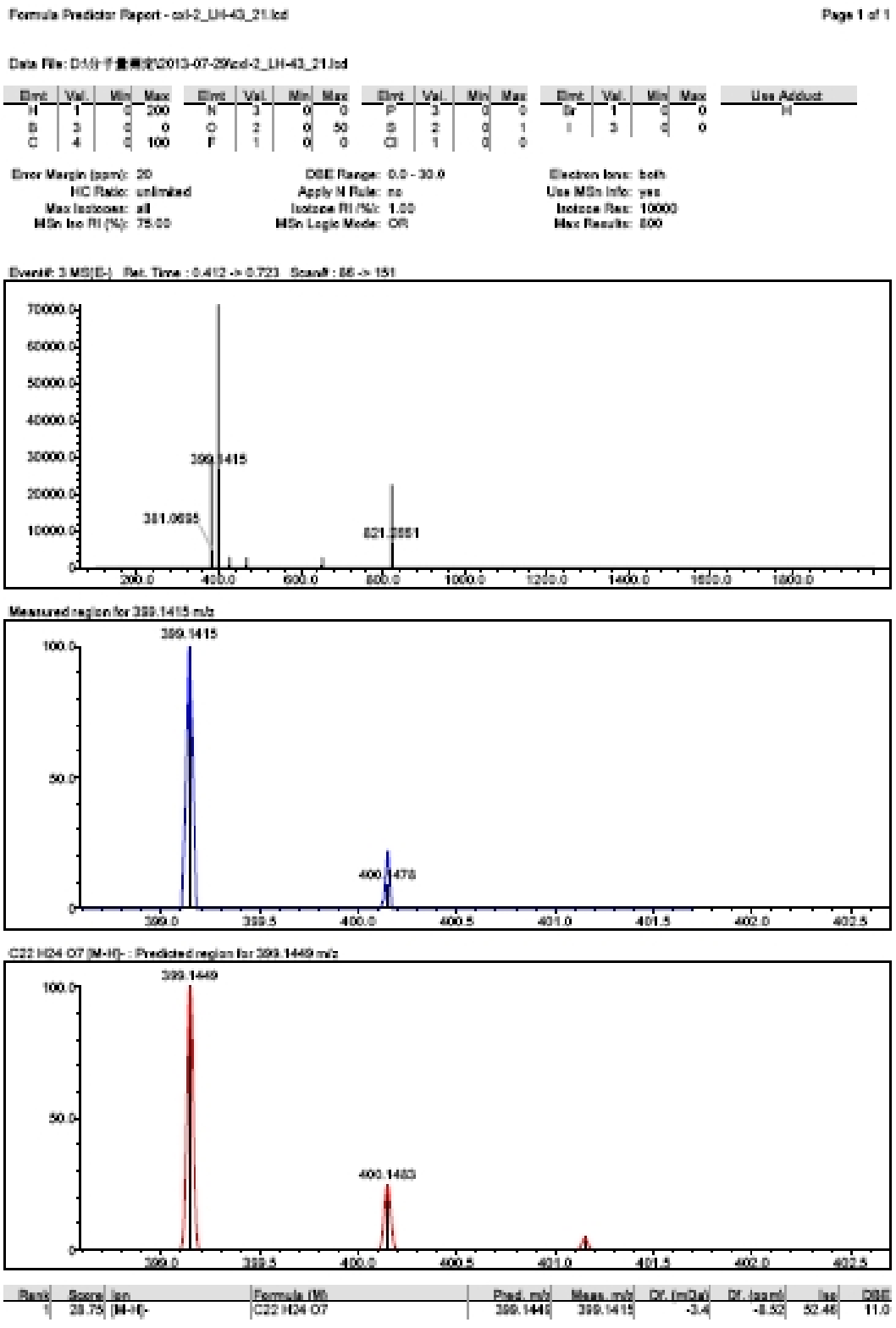

Figure S19.HRESIMS spectra of chaetoseminC

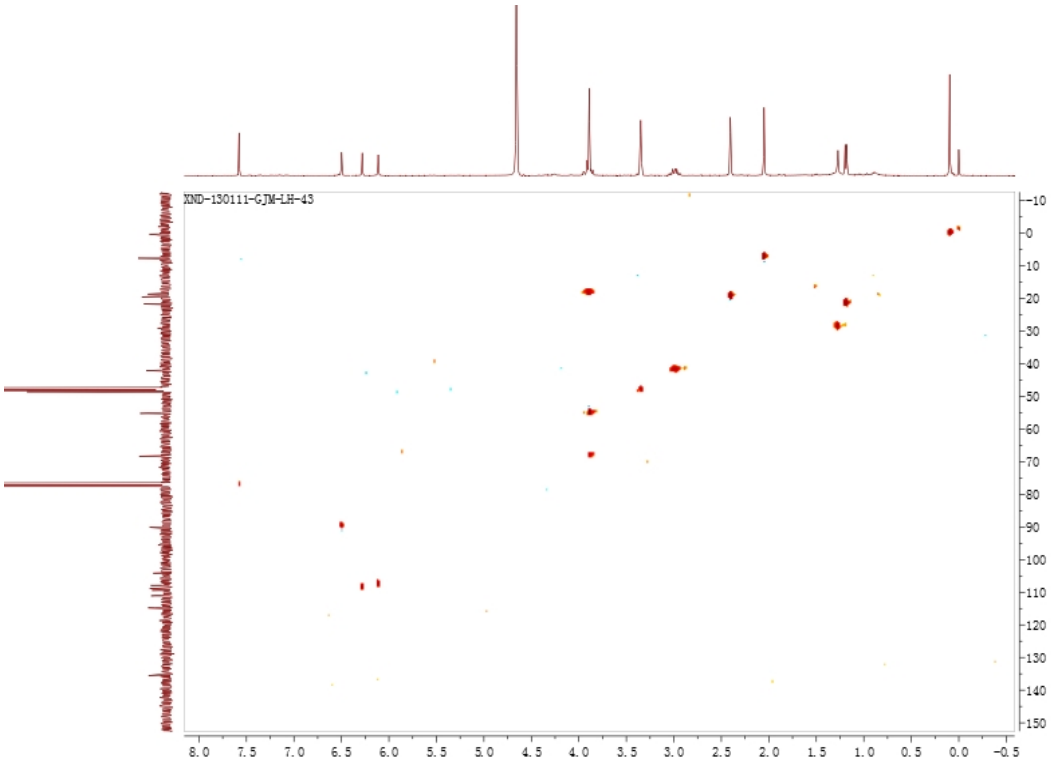

Figure S20. HSQC spectra of chaetoseminC

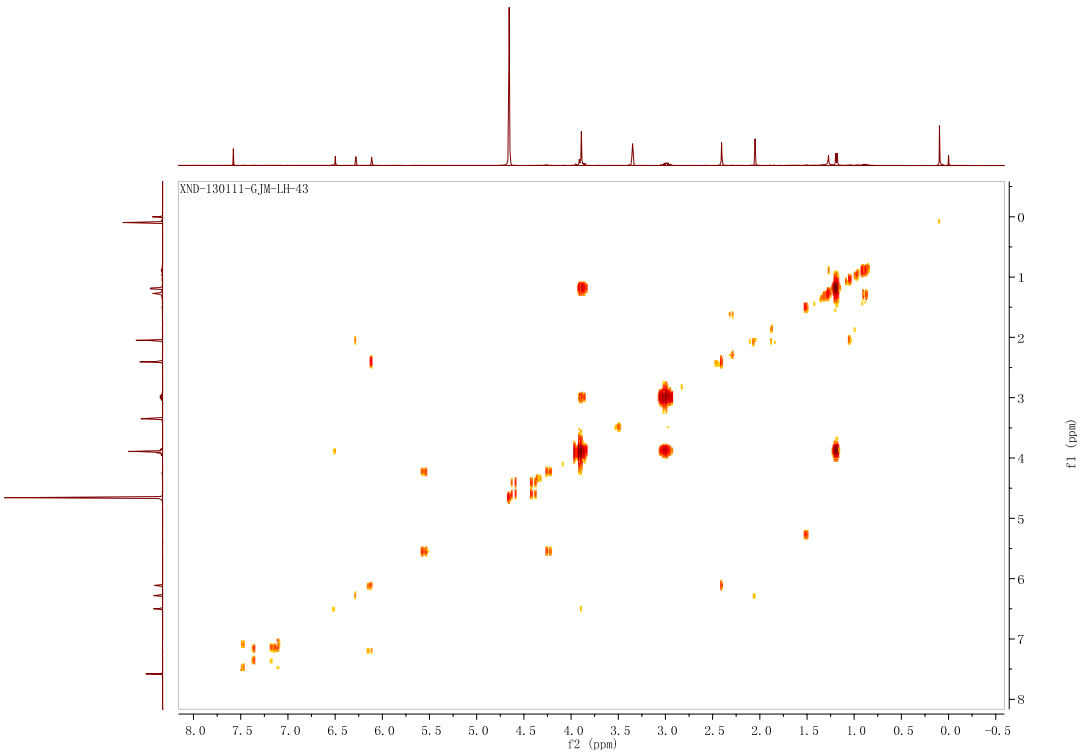

Figure S21. COSY spectra of chaetoseminC

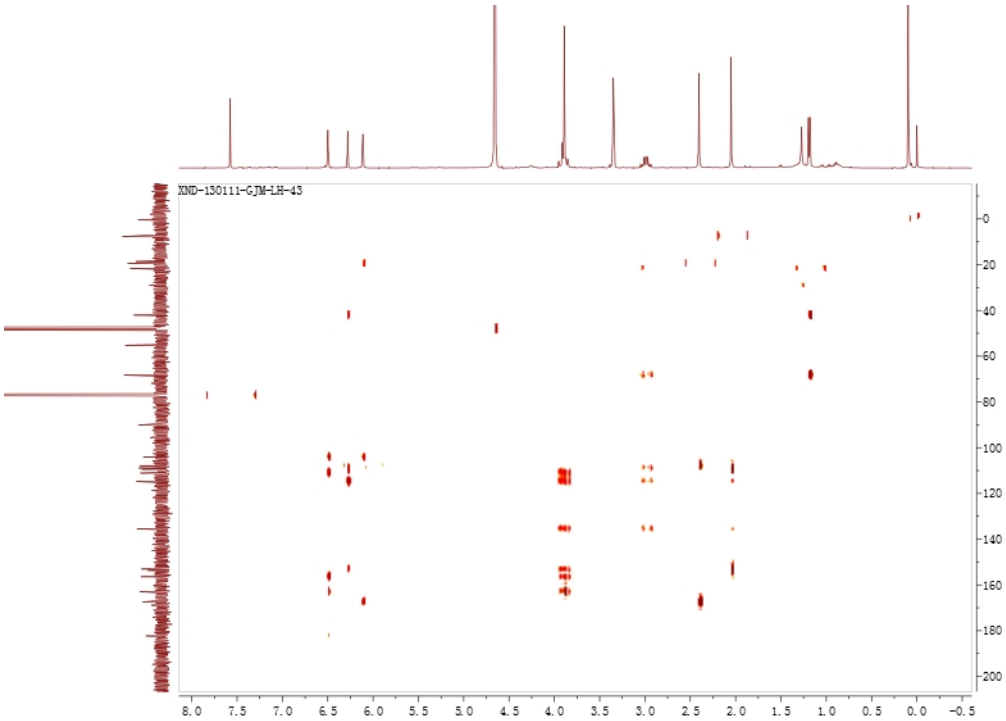

Figure S22. HMBC spectra of chaetoseminC

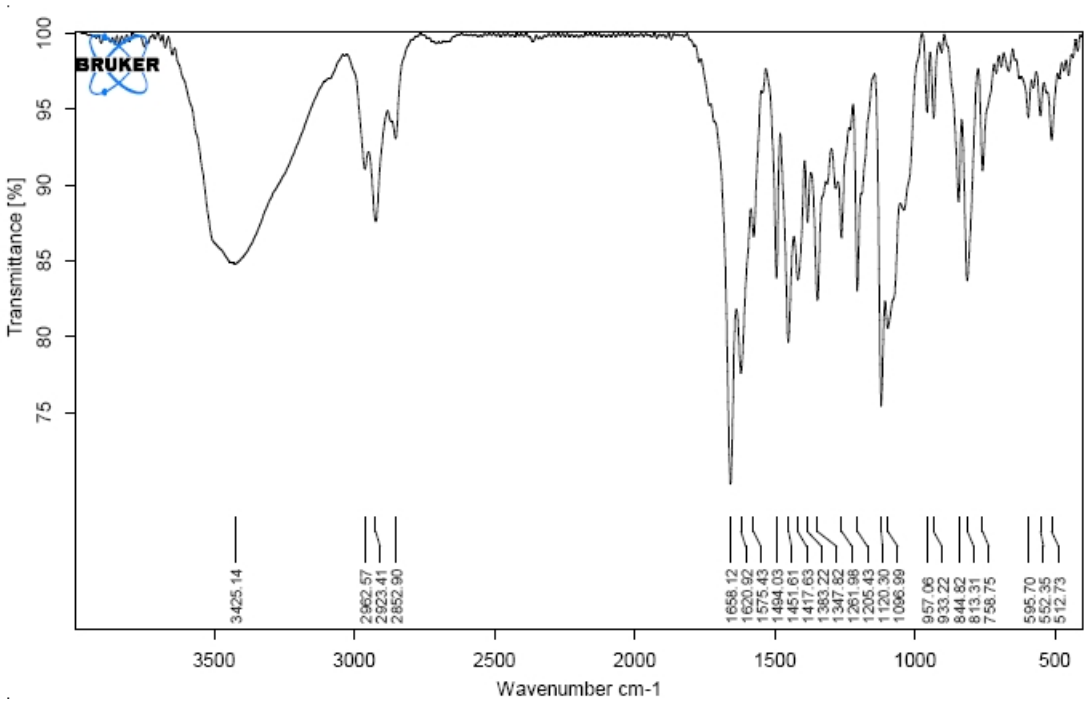

Figure S23. IR spectra of chaetoseminC

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Department	(None Entered)	Time of Report	19:26:04下午
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Information	(None Entered)		

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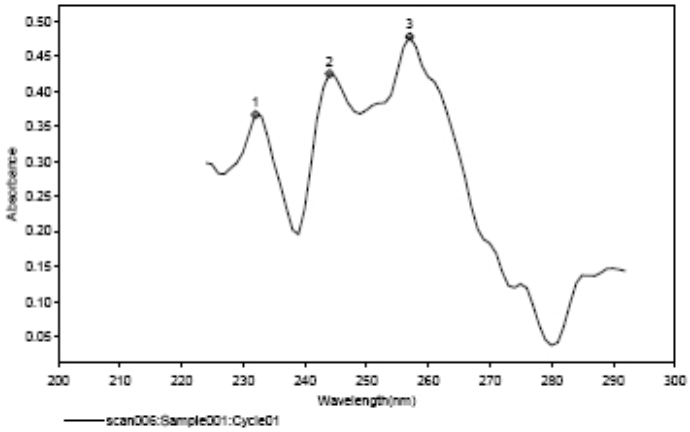

Results Table - scan006.sre, Sample001, Cycle01

nm	A	Peak Pick Method
232.00	.367	Find 8 Peaks Above -3.0000 A
244.00	.426	Start Wavelength 200.00 nm
257.00	.479	Stop Wavelength 300.00 nm
		Sort By Wavelength
Sensitivity	Auto	

Figure S24. UV spectra of chaetoseminC

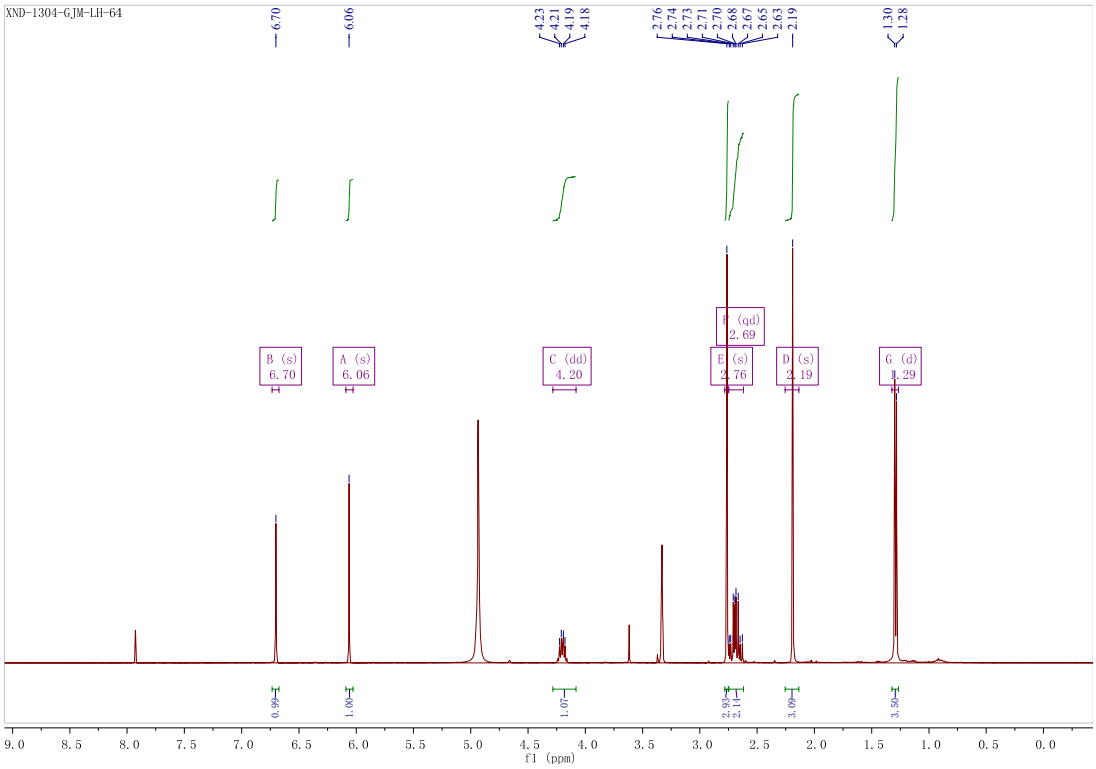

Figure S25. ^{1}H spectra of chaetoseminDin MeOD

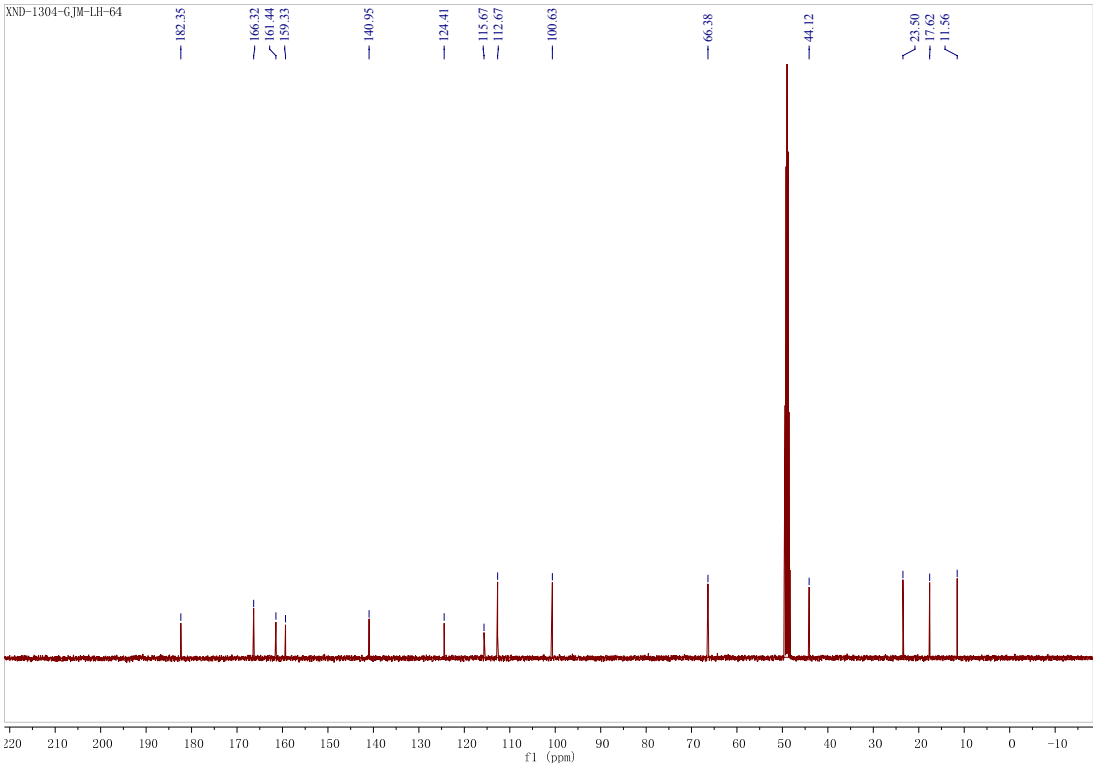

Figure S26. ^{13}C spectra of chaetoseminDin MeOD

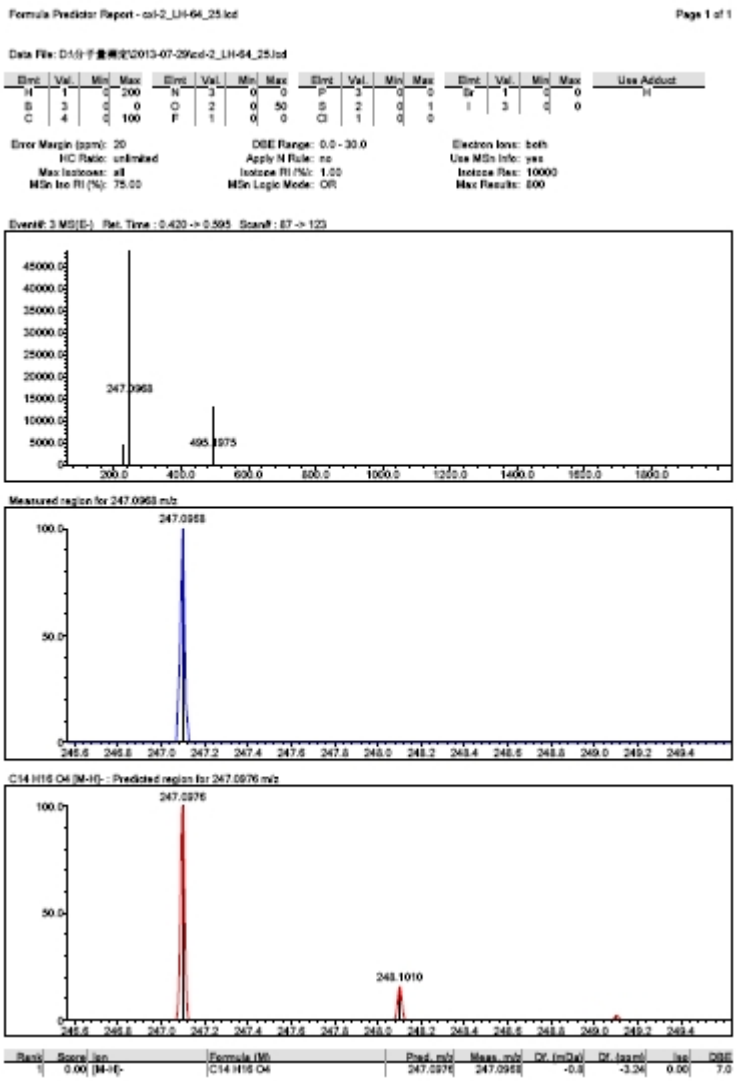

Figure S27.HRESIMS spectra of chaetoseminD

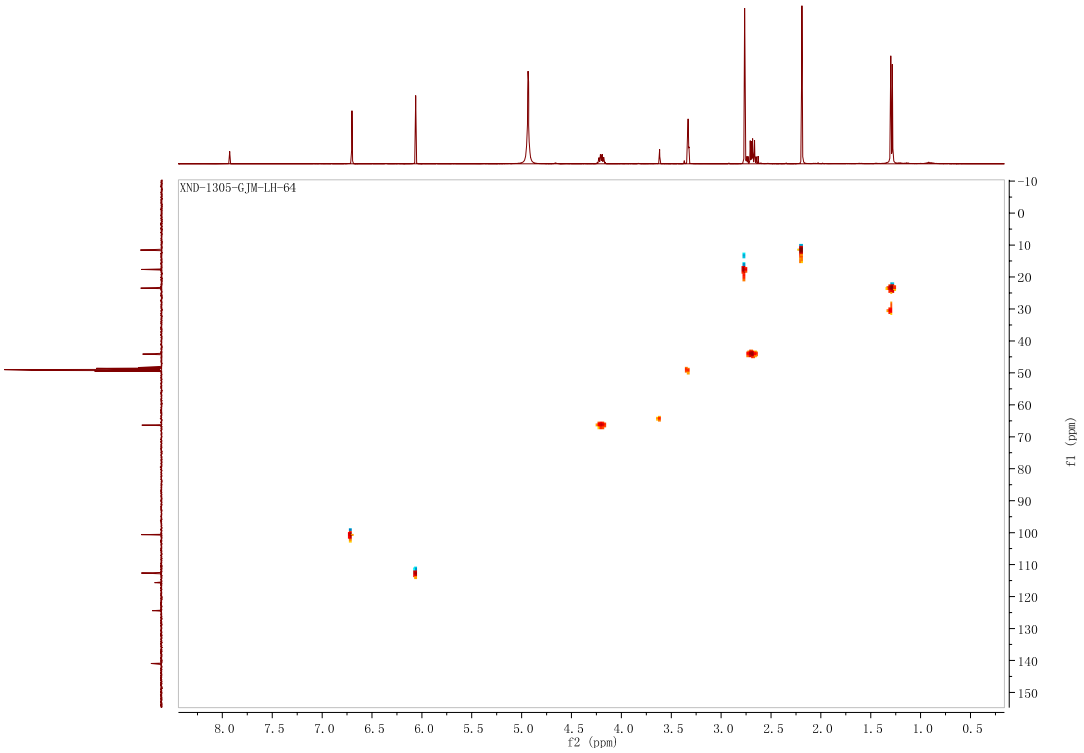

Figure S28. HSQC spectra of chaetoseminD

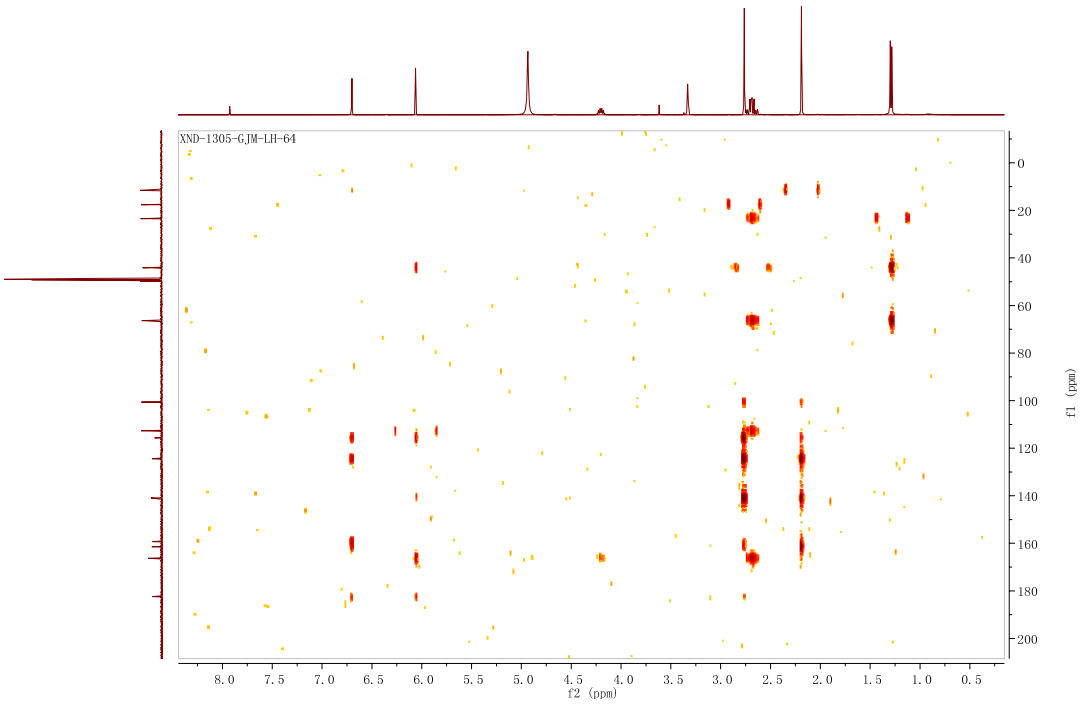

Figure S29. HMBC spectra of chaetoseminD

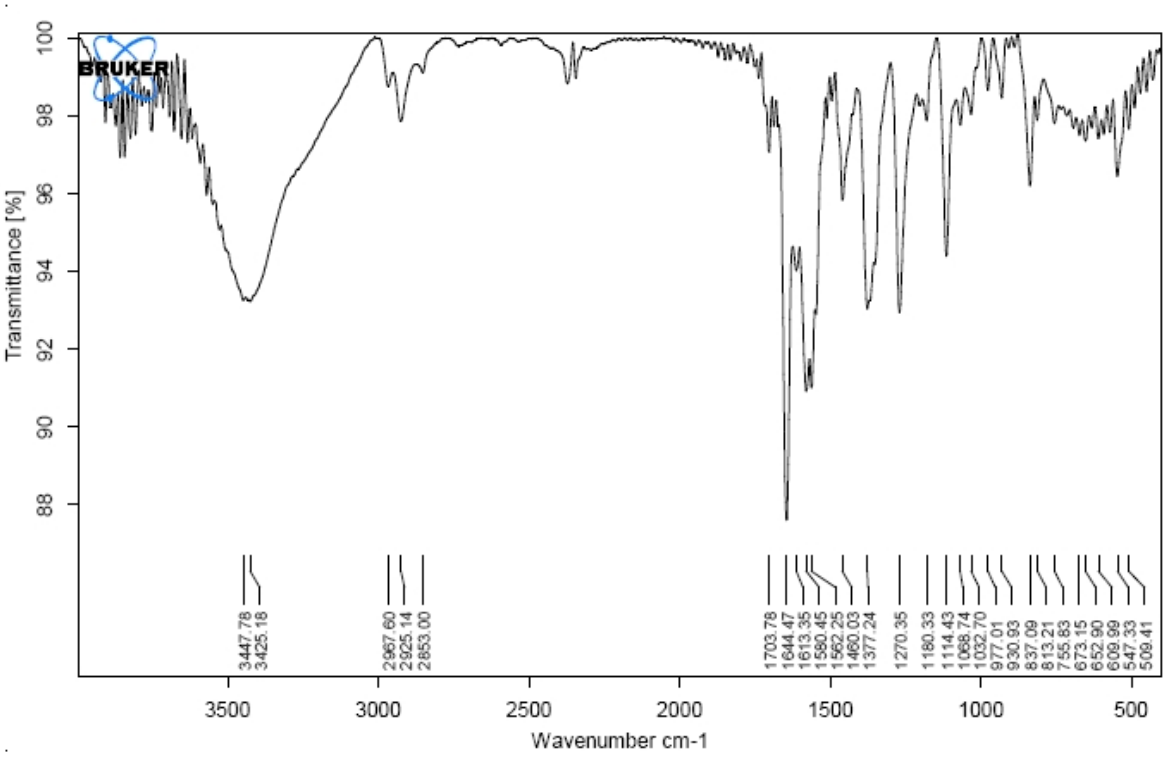

Figure S30. IR spectra of chaetoseminD

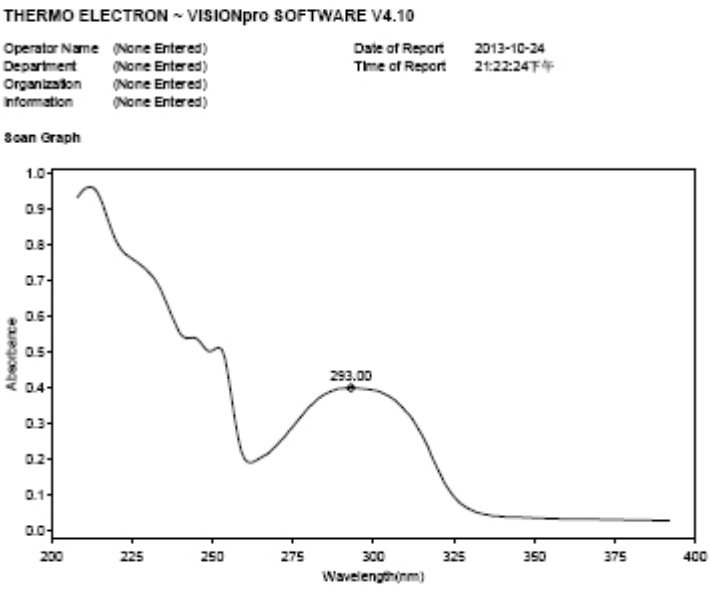

Figure S31. UV spectra of chaetoseminD

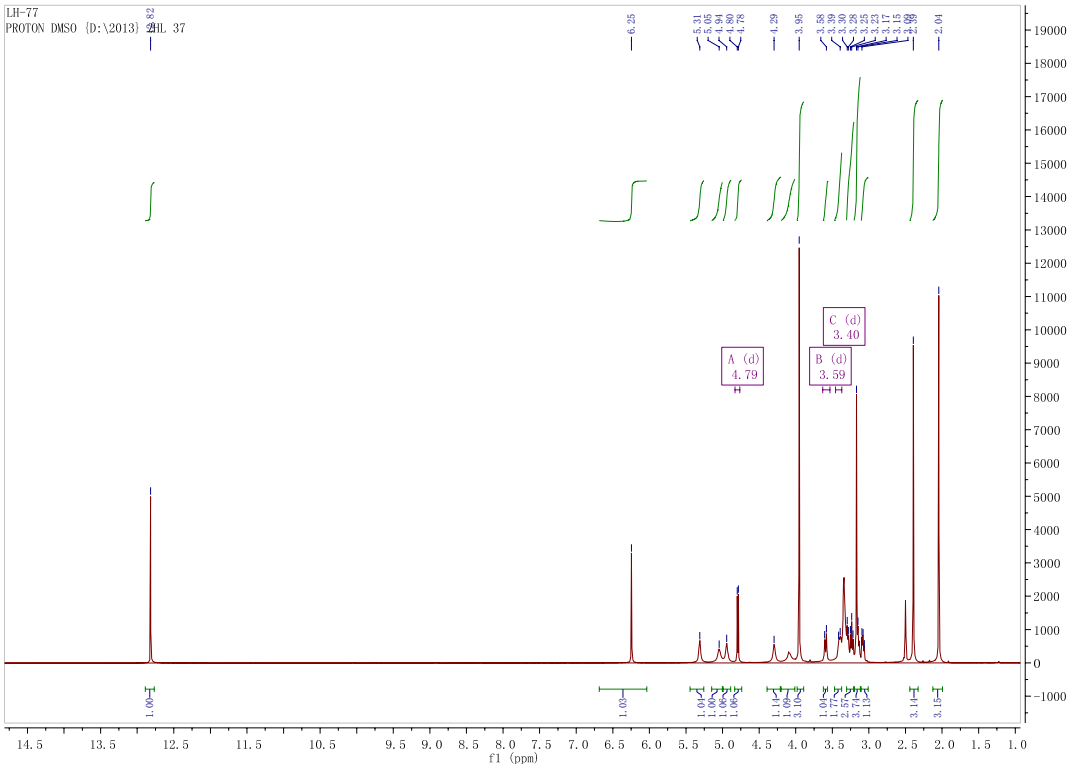

Figure S32. ^{1}H spectra of chaetoseminEin DMSO

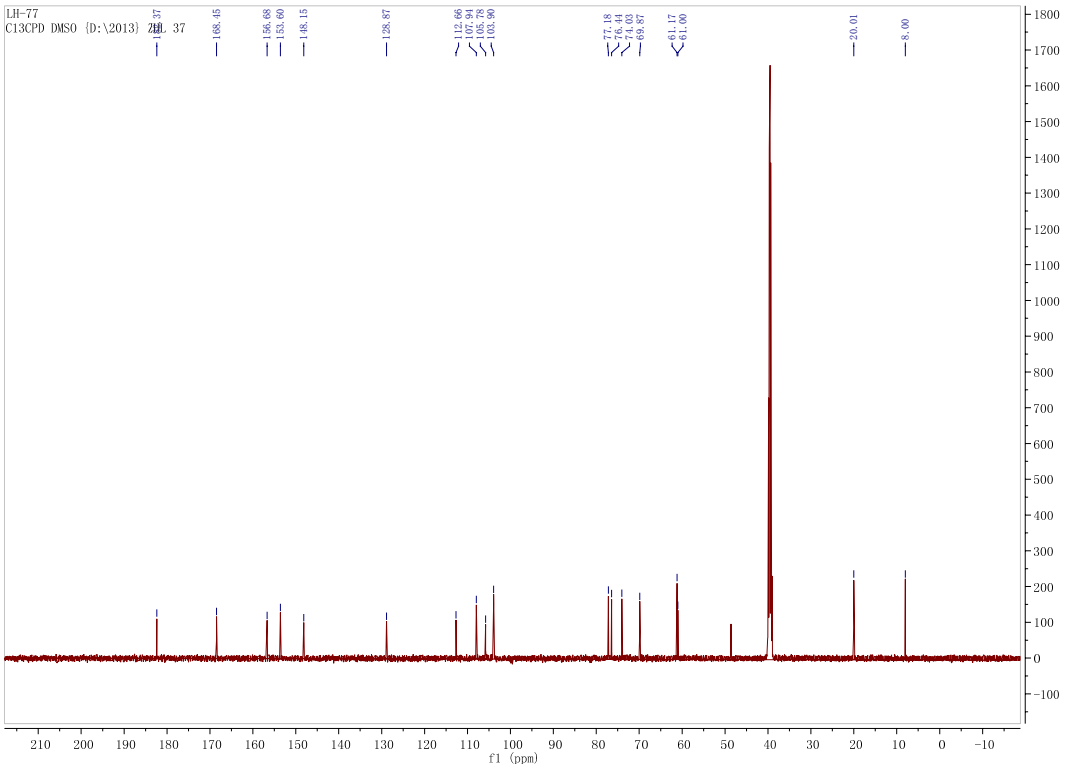

Figure S33. ^{13}C spectra of chaetoseminEin DMSO

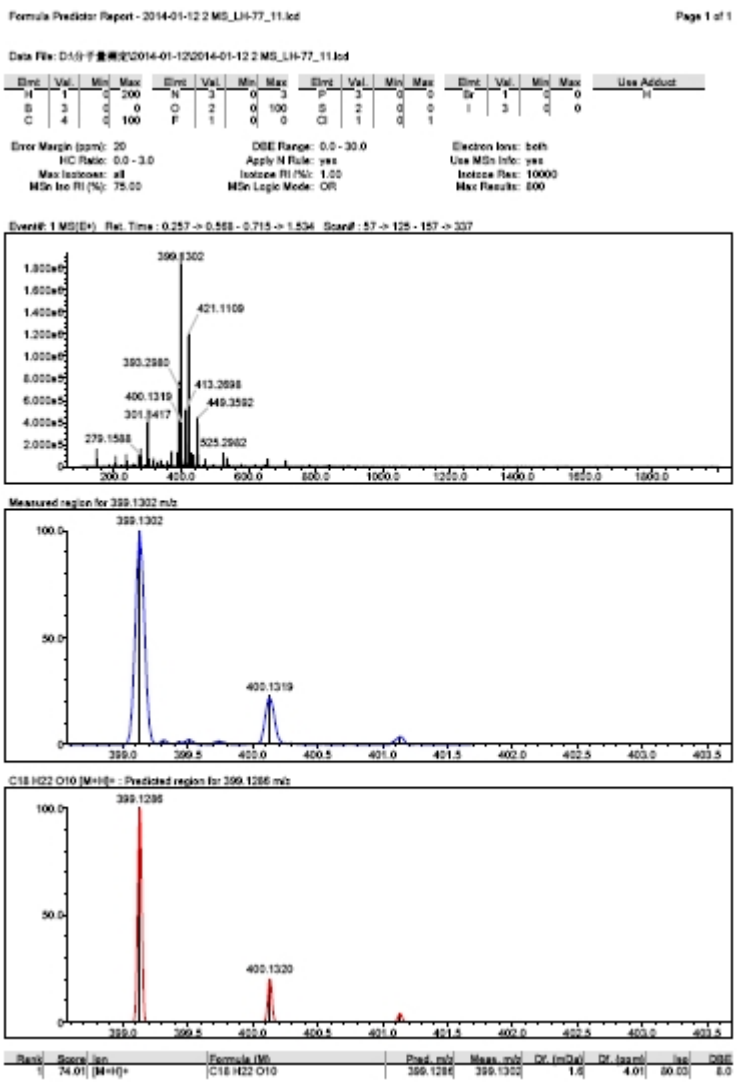

Figure S34.HRESIMS spectra of chaetoseminE

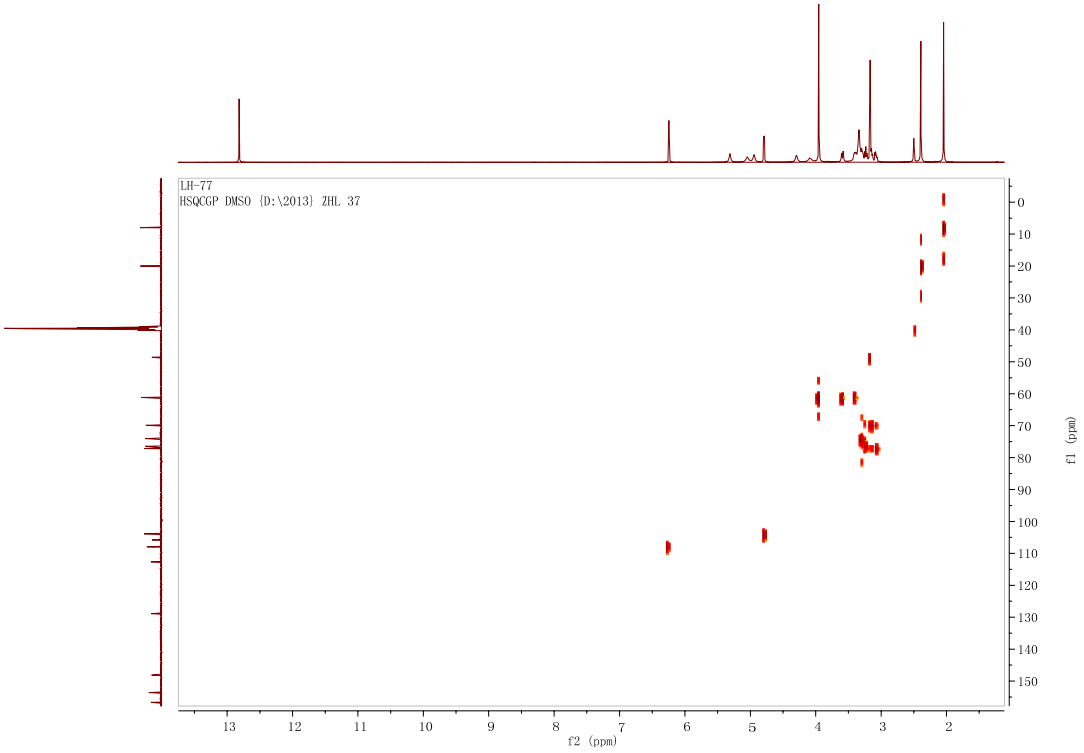

Figure S35. HSQC spectra of chaetoseminE

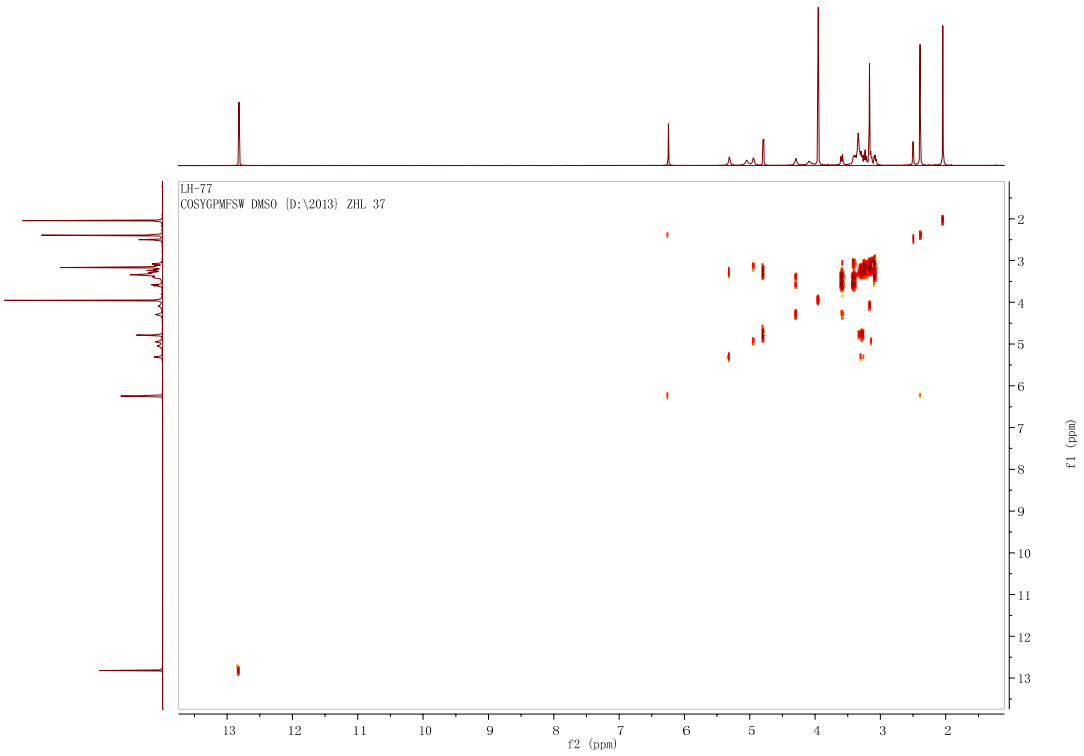

Figure S36. COSY spectra of chaetoseminE

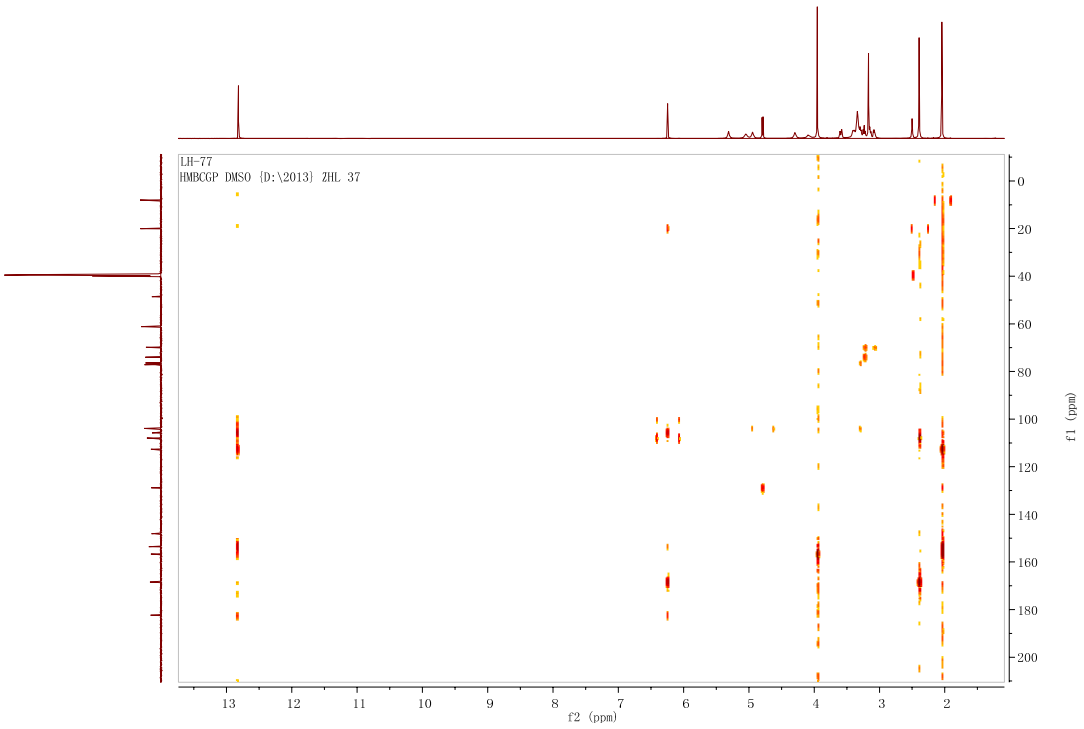

Figure S37. HMBC spectra of chaetoseminE

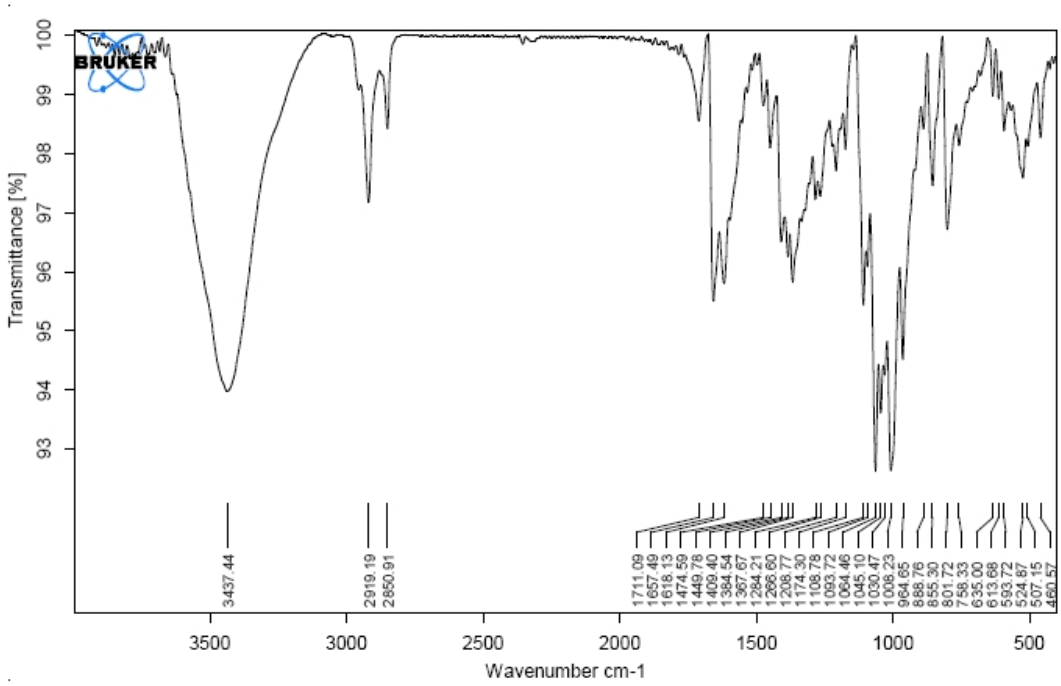

Figure S38. IR spectra of chaetoseminE

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Department	(None Entered)	Time of Report	21:47:24下午
Organization	(None Entered)		
Information	(None Entered)		

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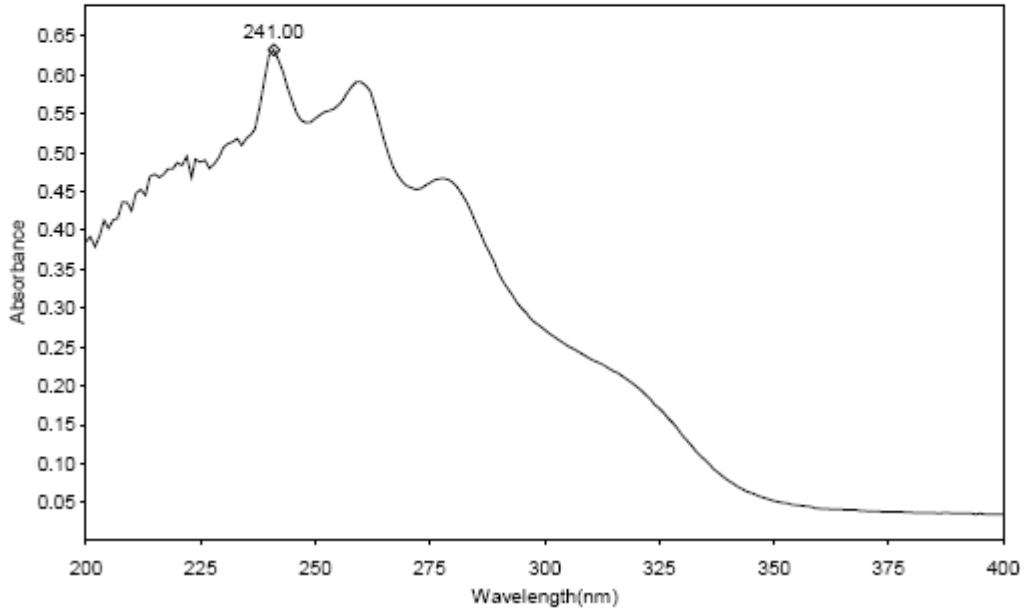

Figure S39. UV spectra of chaetoseminE

Compound **6**, white powder,ESI-MS (negative) *m/z* 219.33[M-H]$^-$, ^{1}H-NMR (400MHz, $CDCl_3$) δ12.78(1H, s, 5-OH), 6.34(1H, s, H-8), 6.02(1H, s, H-3), 3.88(s, 3H, 7-OCH_3), 2.34(s, 3H, 2-CH_3), 2.08(s, 3H, 6-CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ182.38(C-4), 166.29(C-2), 163.21(C-7), 158.36(C-5), 156.27(C-8a), 108.80(C-6), 108.77(C-3), 104.89(C-4a), 89.11(C-8), 55.79(7-OCH_3), 20.39(2-CH_3), 7.18(6-CH_3);

Compound **7**, white powder,ESI-MS (negative) *m/z* 249.33[M-H]$^-$, ^{1}H-NMR (400MHz, $CDCl_3$) δ13.03 (1H, s, 5-OH), 6.37(1H, s, H-8), 6.05(1H, s, H-3), 4.55(2H, s,$\mathbf{CH_2}OCH_3$) , 3.91(s, 3H, 7-OCH_3), 3.41(3H, s, $CH_2O\mathbf{CH_3}$) , 2.36(s, 3H, 2-CH_3)；

^{13}C-NMR (100MHz, $CDCl_3$) δ182.39(C-4), 166.59(C-2), 164.14(C-7), 160.5(C-5), 158.13(C-8a), 109.04(C-3), 108.88(C-6), 104.98(C-4a), 89.55(C-8), 61.54($\mathbf{CH_2}OCH_3$), 58.16($CH_2O\mathbf{CH_3}$), 56.12(7-OCH_3), 20.39(2-CH_3);

Compound **8**, white powder,ESI-MS (positive) m/z 236.92 [M+H]$^+$, ^{1}H-NMR (400MHz, C_5D_5N) δ13.78 (1H, s, 5-OH), 6.48(1H, s, H-8), 6.15(1H, s, H-3), 5.20(2H, s,$\mathbf{CH_2}$),3.76(3H, s, 7-OCH_3), 2.15(s, 3H, 2-CH_3); ^{13}C-NMR (100MHz, C_5D_5N) δ 183.24(C-4), 167.73(C-2), 164.66(C-7), 160.51(C-5), 158.29(C-8a), 113.96(C-6), 109.35(C-3), 105.74(C-4a), 90.66(C-8), 56.42(7-OCH_3), 52.47($\mathbf{CH_2}$), 20.28(2-CH_3);

Compound **9**, pale yellow powder,ESI-MS (negative) *m/z* 205.42[M-H]$^-$, ^{1}H-NMR (400MHz, $CDCl_3$) δ13.04 (1H, s, 5-OH), 6.38(1H, s, H-8), 6.13(1H, s, H-3), 2.33(s, 3H, 2-CH_3), 1.95(s, 3H, 6-CH_3); ^{13}C-NMR (100MHz, $CDCl_3$)δ181.73(C-4), 167.29(C-2), 162.00(C-7), 158.53(C-5), 155.38(C-8a), 107.84(C-3), 106.66(C-6), 103.06(C-4a), 92.77(C-8), 19.91(2-CH_3), 7.32(6-CH_3);

Compound **10**, white powder,ESI-MS (positive) m/z 221.00$[M+H]^+$, ^{1}H-NMR (400MHz, $CDCl_3$) δ12.77 (1H, s, 5-OH), 6.37(1H, s, H-6), 6.01(1H, s, H-3), 3.89(3H, s, 7-OCH_3), 2.38(s, 3H, 2-CH_3), 2.15(s, 3H, 8-CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ183.02(C-4), 166.79(C-2), 162.91(C-7), 160.15(C-5), 154.86(C-8a), 108.16(C-3), 104.54(C-4a), 103.63(C-8), 94.71(C-6), 55.94(7-OCH_3), 20.55(2-CH_3), 7.42(8-CH_3);

Compound **11**, white powder,ESI-MS (negative) m/z 368.25$[M-H]^-$, ^{1}H-NMR (400MHz, $CDCl_3$:CD_3OD = 1:1)δ 6.37 (1H, s, H-8), 5.99 (1H, s, H-3), 4.33 (2H, s, H-1′), 3.99 (3H, s, 7-OCH_3), 3.82 (2H, s, H-4′), 3.58 (2H, s, H-3′), 2.27 (3H, s, 2-CH_3), 1.82 (3H, s, H-7′); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.16(C-4), 171.36(C-6′), 167.64(C-2), 163.42(C-7), 159.35(C-5), 158.39(C-8a), 108.68(C-3), 104.64(C-4a), 99.78(C-6), 90.39(C-8), 56.18(7-OCH_3), 52.07(C-3′), 32.57(C-4′), 22.21(C-7′), 20.06 (2-CH_3);

Compound **12**, white powder,ESI-MS (negative) *m/z* 357.42$[M-H]^-$, ^{1}H-NMR (400MHz, $CDCl_3$) δ12.82 (1H, s, 5-OH), 6.32(1H, s, H-8), 6.01(1H, s, H-3), 5.20(1H, s, H-4′), 4.40(1H, s, H-7′), 3.84(3H, s, 7-OCH_3), 2.74(1H, m, H-2′) , 2.64(1H, m, H-1′a), 2.90(1H, m, H-1′b), 2.35(3H,s, 2-CH_3), 2.30 (2H, m, H-6′), 1.40(3H,d, 7′-CH_3), 1.09(3H,d, 2′- CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ193.54(C-5′), 182.37 (C-4) , 181.49(C-3′), 166.46 (C-2) , 163.18(C-7), 158.97(C-5), 156.73(C-8a) , 110.48 (C-6), 108.80 (C-3), 104.86 (C-4a) , 102.40(C-4′), 89.29 (C-8) , 75.35 (C-7′) , 55.78(7-OCH_3), 42.64(C-6′), 38.38(C-2′), 27.06 (C-1′), 20.34 (2-CH_3), 20.27(C-8′), 17.14(2′-CH_3);

Compound **13**, white powder,ESI-MS (negative) *m/z* 357.42[M-H]$^-$, ^{1}H-NMR (400MHz, $CDCl_3$)δ12.82 (1H, s, 5-OH), 6.32(1H, s, H-8), 6.01(1H, s, H-3), 5.09(1H, s, H-4′), 4.35(1H, s, H-7′),3.84(3H, s, 7-OCH_3), 2.74(1H, m, H-2′) , 2.70, 2.95(2H, m, H-1′), 2.35(s, 3H, 2-CH_3), 2.30 (2H, m, H-6′) 1.95(s, 3H, H-14),1.15(3H,d, 2′-CH_3) ;^{13}C-NMR (100MHz, $CDCl_3$) δ193.64(C-5′), 182.40 (C-4), 181.19(C-3′), 166.47 (C-2), 163.13(C-7), 158.83(C-5) , 156.73(C-8a), 110.48 (C-6), 108.80 (C-3), 104.82 (C-4a) , 102.99(C-4′), 89.23(C-8) , 75.56 (C-7′), 55.75 (7-OCH_3) , 42.53(C-6′) , 38.81 (C-2′) , 27.00(C-1′) , 20.34 (2-CH_3) , 20.25 (C-8′), 17.38(2′-CH_3);

Compound **14**, white powder, $[\alpha]_D^{21}$ = +33.86(*c* = 0.1, $CHCl_3$), ESI-MS (negative) m/z 425.42[M-H]$^-$, ^{1}H-NMR (400MHz, C_5D_5N) δ6.46(1H, s, H-8), 6.08(1H, s, H-3), 4.56(1H, m, H-3′), 3.97(2H, s, H-9), 3.79(3H, s, 7-OCH_3), 3.45(1H, dd, *J*= 16.4, 3.0HzH-4′a), 2.67 (1H, dd, *J*=16.4, 11.8 Hz,H-4′b),2.21(1H, s, 2-CH_3), 2.20(3H, s, 7′-CH_3), 1.39(3H, d, *J*=6.3 Hz, 3′-CH_3); ^{13}C-NMR (100MHz, C_5D_5N) δ 182.92(C-4), 171.62(C-1′), 168.10(C-2), 163.69(C-7), 161.49(C-8′), 161.02(C-6′), 158.24(C-5), 157.19(C-8a), 137.62(C-4a′), 116.07(C-5′), 111.09(C-7′), 110.12(C-6), 108.80(C-3), 105.08(C-4a), 101.01(C-8a′), 90.90(C-8), 75.59(C-3′), 56.18(7-OCH_3), 32.36(C-4′), 20.77(3′-CH_3), 19.82(2-CH_3), 19.39 (C-9), 8.49(7′-CH_3).

Compound **15**, white powder,ESI-MS (negative) *m/z* 333.33[M-H]$^-$, ^{1}H-NMR (400MHz, $CDCl_3$) δ12.85 (1H, s, 5-OH), 6.35(1H, s, H-8), 6.03(1H, s, H-3), 3.85(3H, s, 7-OCH_3), 3.37(1H, m, H-13), 2.51-2.93(5H, m, H-9, H-10, H-12), 2.34(s, 3H, 2-CH_3), 1.16(3H, d, *J*=6.0 Hz, H-14), 1.04(3H,d, *J*= 6.6Hz,10-CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ216.14(C-12), 182.40(C-4), 165.54(C-2), 163.13(C-7,

158.95(C-5), 156.80(C-8a), 110.23(C-7),108.86(C-3),104.93(C-4a),89.40(C-8), 63.94(C-13), 55.81(7-OCH_3), 48.65(C-12), 46.10(C-10), 25.39(C-9), 22.23(C-14), 20.39(2-CH_3), 15.51(10-CH_3).