Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Inhibition of amyloid fibril formation of β-lactoglobulin by the natural and synthetic curcuminoids

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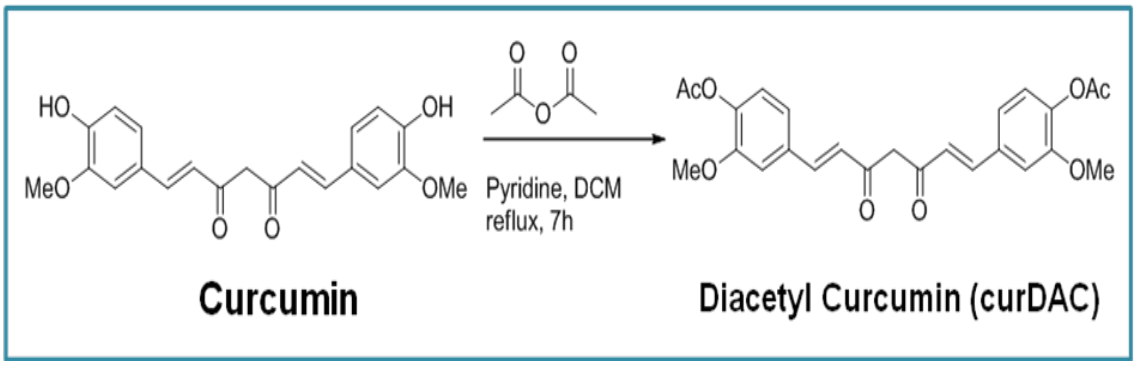
1. Synthesis of curcumin derivatives

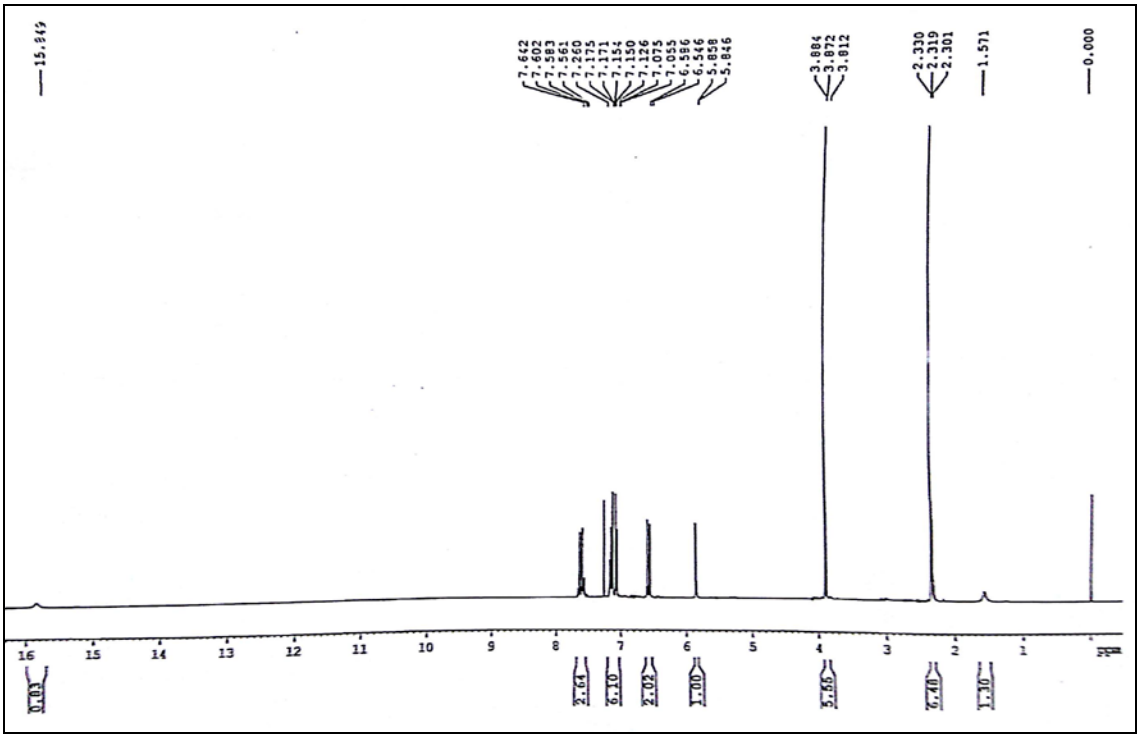
IOC, PY derivatives were synthesized and characterized according to S. Maity *et al.* [1]. The derivative DAC was also synthesized in the lab. These curcumin derivatives were further characterized by ^{1}H-NMR, ^{13}C-NMR and ESI-MS.

2. Synthesis of diacetyl curcumin (DAC)

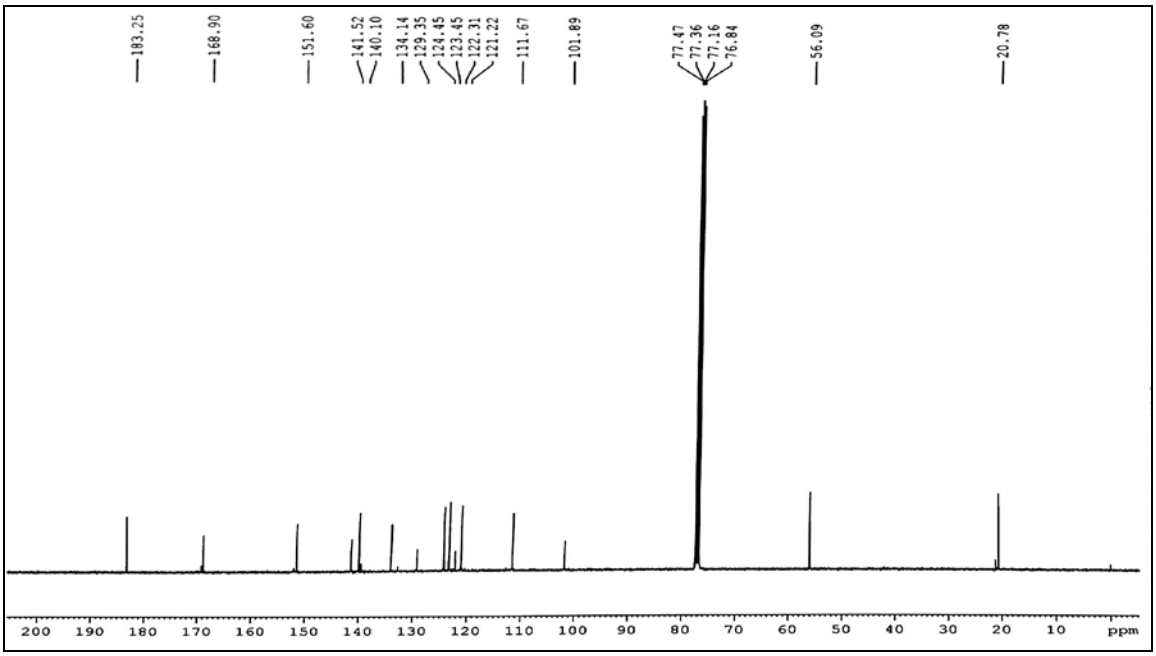
400 mg of purified curcumin (1.09 mmol) was dissolved in 100 ml of CH_2Cl_2 containing 1 ml of pyridine and 1 ml of acetic anhydride. The solution was kept at reflux under stirring for 7 hours and then was neutralized with 0.1 N HCl and was extracted with CH_2Cl_2. The residue obtained after solvent removal was dissolved in ethyl acetate and washed with water. The organic portion was collected, dried over anhydrous sodium sulfate and concentrated under vacuum. Crude product was purified by column chromatography on a silica column (100-200 mesh) to afford diacetyl curcumin (DAC). The solvent system used was ethyl acetate /hexane, 70%. Yield - 80%. ^{1}H NMR spectrum in $CDCl_3$ (500 MHz): δ = 2.33 (s, 6H, CH_3COO-), 3.88 (s, 6H, CH_3O), 5.86 (s, 1H), 6.56 (d, J = 15.6 Hz, 2H), 7.06 (d, J = 8.4 Hz, 2H), 7.12 (s, 2H), 7.15 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 16.0 Hz, 2H), 15.84 (broad enolic OH). ^{13}C NMR ($CDCl_3$, 100 MHz) 183.25, 168.9, 151.6, 141.52, 140.10, 134.14, 129.35, 124.45, 123.45, 122.31, 121.22, 111.67, 101.89, 56.809, 20.78; ESI-MS(ES+)m/z: [M+] calcd for $C_{24}H_{27}O_8$ 452.459; found 455.2439.



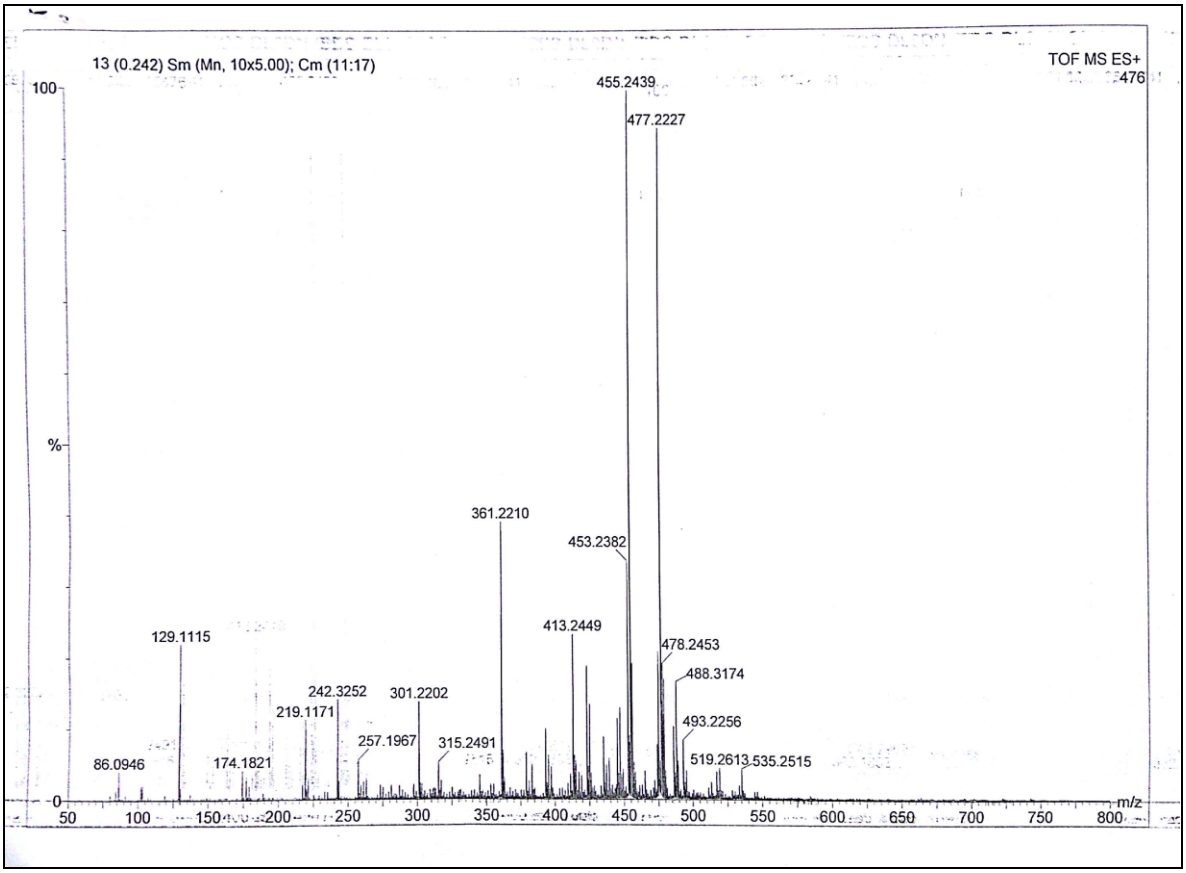
3. ^{1}H-NMR of DAC



4. ^{13}C-NMR of DAC



5. ESI-MS of DAC



6. CD- Calculations

Table- 1

Structural integrity of native and incubated β-lg in absence and presence of curcumin derivatives as determined by CDNN 2.1 software.

Sample	α-helix	β-sheet	β-turn	Random coil
Native β-lg	28.7	18.8	19.8	32.7
β-lg (incubated)	16.28	29.65	17.56	36.49
β-lg(incubated) with (1:0.5) curcumin	16.31	29.22	17.53	36.51
β-lg(incubated) with (1:1) curcumin	16.45	29.09	17.52	37.45
β-lg(incubated) with (1:0.5)DAC	16.89	28.09	16.35	39.35
β-lg(incubated) with (1:1)DAC	17.01	27. 57	16.1	39.86
β-lg(incubated) with (1:0.5) IOC	17.56	26.63	16.01	40.29
β-lg(incubated) with (1:1)IOC	18.74	25.36	15.69	41.1
β–lg(incubated) with (1:0.5)PY	19.57	24.7	14.7	41.4
β-lg(incubated) with (1:1) PY	22.78	22.54	13.67	41.99

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7. References:

1. S. Maity, S. Pal, S. Sardar, N. Sepay, H. Parvej, J. Chakraborty and U. C. Halder, RSC Adv., 2016, **6**, 112175.