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Data Article

In vitro studies data on anticancer activity of *Caesalpinia sappan L.* heartwood and leaf extracts on *MCF7* and *A549* cell lines

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ABSTRACT

This article contains data on in vitro cytotoxicity activity of chloroform, methanolic and water extracts of leaf and heartwood of *Caesalpinia sappan L.* a medicinal plant against Breast cancer (MCF-7) and Lung cancer (A-549) cells. This data shows that Brazilin A, a natural bioactive compound in heartwood of *Caesalpinia sappan L.*induced cell death in breast cancer (MCF-7) cells. The therapeutic property was further proved by docking the Brazilin A molecule against BCL-2 protein (an apoptotic inhibitor) using auto dock tools.

Specifications table

Subject area	Biology
More specific subject area	Screening for Anti Cancer Activity in medicinal plants and Ethno medicines

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Type of data	Tables, microscopy images, text file, graphs, Chromatogram figure, docking images
How data was acquired	Conducting of anticancer activity assays and cytotoxicity studies with methanol and water extracts of leaf and heartwood *of Caesalpinia sappan* L. on MCF-7 (Human breast cancer) and A549 (Human lung cancer) cell lines. The in vitro anti tumor activity was screened by assessing tumor volume, viable and nonviable tumor cell count, tumor weight, hematological parameters and biochemical estimations by MTT Assay and Flow cytometry studies.
Data format	Analyzed data
Experimental factors	Leaf and heart wood was extracted in chloroform, water and methanol solvents to study their cytotoxic effect on human cancer cell lines and determine the extracts IC_{50} value.
Experimental features	The effect of leaf and heartwood extracts prepared in water and methanol on MCF-7 (Human breast cancer) and A549 (Human lung cancer) and Identification of compounds from *Caesalpinia sappan L.,* leaf and heartwood water and methanol extracts through LC–MS () and Docking studies against a BCl2 (B-cell lymphoma 2) protein which regulates the apoptosis.
Data source location	Yogi Vemana University campus green house facility (N 14°.473′, E 78°.710)
Data accessibility	Data are available within this article

Value of the data

- The data can be further explored to develop and design anticancer drugs for human Lung and breast cancer treatment from *Caesalpinia sappan* L. plant as a source for drugs [1,2].
- These plant compounds can also be tried on other types of cancers for anticancer activity and compare with curing effect with the drugs currently in use, as plant based products are safer than synthetic drugs and with no side effects.

1. Data

The Dataset in this study shows the potential of leaf and heart wood extracts (chloroform, methanol and water) of *Caesalpinia sappan L.* (Family: *Caesalpiniaceae L.)* as anti cancer agents(Fig. 1 and Table 1) which can be used further for drug development and designing in pharmaceutical industry. The Protein BCL-2 was used for carrying out docking studies (Fig. 2) with the compounds from leaf and heartwood (Figs. 3–6) (Table 2).

2. Experimental design, materials and methods

2.1. Cell culture

The pure cultures of *MCF-7* (Breast cancer cell line) and *A549* (Lung Cancer), were obtained From National Centre for Cell Science, Pune, Maharashtra state,India. The cells were grown and maintained in RPMI – 1640 media, supplemented with 10% v/v foetal bovine serum, sodium carbonate with 100 mg/l penicillin, 50 mg/l streptomycin to prevent the bacterial contamination and incubated at 37 °C in a humidified atmosphere having 5% CO_2.

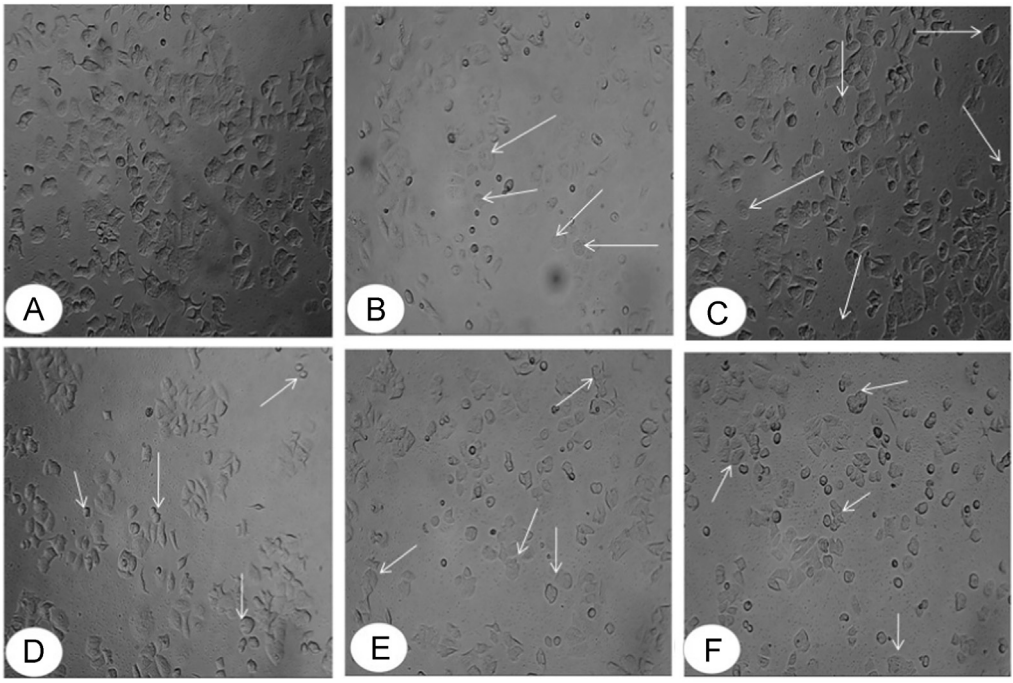


Fig. 1. Morphological changes in cells of MCF-7 after treatment with heartwood methanol extracts of *Caesalpinia sappan L.* A: Untreated Cell lines, B: +Ve Control (Campotheterin −40 μM), C: –Ve Control (DMSO), D–F: *Caesalpinia sappan L.* Heartwood methanol extracts, D: 50 μg/ml, E: 150 μg/ml, F: 250 μg/ml.

Table 1
Effect of *Caesalpinia sappan L.* leaf (L) and heartwood (H) extracts prepared in chloroform, methanol and water on MCF-7 (Human breast cancer) and A549 (Human lung cancer) cells, Camptothecin is taken as positive control.

Cell line	Plant sample	Camptothecin (50 uM)	50 μg/ml	150 μg/ml	250 μg/ml	350 μg/ml	450 μg/ml
A549 Cell line	L $CHCL_3$	57.48 ± 0.03	87.2 ± 0.03	86.37 ± 0.01	83.41 ± 0.02	71.56 ± 0.04	67.07 ± 0.00
	LH_2O	57.48 ± 0.03	86.87 ± 0.13	84.14 ± 0.02	92.55 ± 0.03	94.77 ± 0.01	97.48 ± 0.00
	L MET	57.48 ± 0.03	101.52 ± 0.00	89.50 ± 0.01	89.34 ± 0.07	86.00 ± 0.04	84.23 ± 0.02
	H H_2O	57.48 ± 0.03	81.06 ± 0.29	87.69 ± 0.00	88.35 ± 0.00	88.06 ± 0.03	96.82 ± 0.06
	H Met	57.48 ± 0.03	100.12 ± 0.00	80.69 ± 0.01	78.14 ± 0.06	78.02 ± 0.07	60.12 ± 0.07
MCF7 Cell line	L $CHCL_3$	56.32 ± 0.02	98.84 ± 0.07	102.17 ± 0.01	108.63 ± 0.06	112.24 ± 0.01	102.64 ± 0.01
	LH_2O	56.32 ± 0.02	105.10 ± 0.00	104.76 ± 0.00	102.24 ± 0.02	97.82 ± 0.03	96.39 ± 0.14
	L MET	56.32 ± 0.02	107.68 ± 0.01	96.33 ± 0.05	85.54 ± 0.19	63.96 ± 0.05	46.19 ± 0.00
	H H_2O	56.32 ± 0.02	107.00 ± 0.00	93.12 ± 0.01	62.51 ± 0.01	37.89 ± 0.02	12.04 ± 0.00
	H Met	56.32 ± 0.02	101.15 ± 0.01	52.31 ± 0.00	4.01 ± 0.00	2.31 ± 0.00	1.22 ± 0.01

2.2. Anticancer assay

Soxhlet extraction method [3] was used for extraction of heart wood and powdered leaf sample of *Caesalpinia sappan L.* The cytotoxic activity of these extracts was tested against MCF7 and A549 cell lines and determined by MTT assay. This assay was performed in a 96-well culture plate according to a previously published protocol [4]. Percentage of viability was checked by calculating simulation

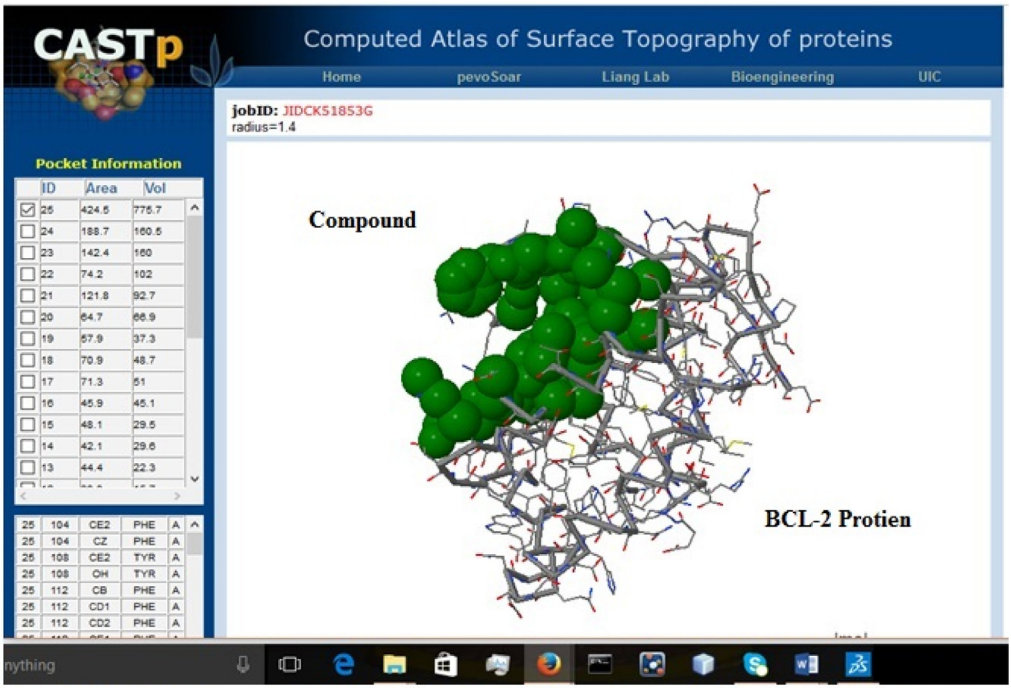


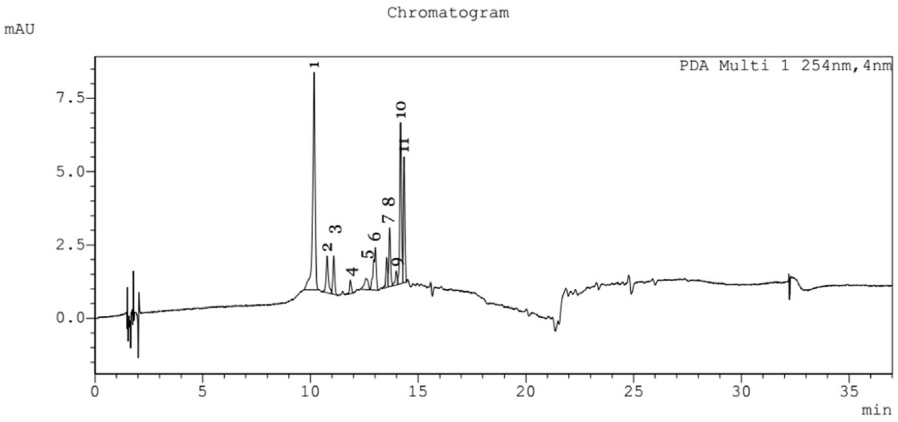
Fig. 2. The 3D structure of Docked molecule (Brazilin A from *Caesalpinia sappan L.* heartwood extract) binding to receptors of BCL-2 protein, an anti apoptotic protein selected as target molecule.

index using the following formulae.

$$\text{Stimulation index} = \frac{\text{Absorbance with plant extract}}{\text{Absorbance without plant extract}}$$

$$\%\ \text{of viability} = \text{Stimulation index} \times 100$$

The plant extract were subjected to LC–MS (SHIMADZU LCMS-2020) chromatography and UPLC–MS chromatography to identify the compounds in them (Figs. 3–6). BCL-2 protein is an anti apoptotic protein selected as target molecule. The 3D structure of the compounds present in the sample was



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%
1	10.171	9.696	10.368	59470	35.019
2	10.774	10.571	10.987	9676	5.698
3	11.085	10.987	11.296	7815	4.602
4	11.859	11.595	11.989	2656	1.564
5	12.585	12.341	12.768	4806	2.830
6	13.018	12.768	13.163	14028	8.261
7	13.539	13.333	13.600	5654	3.329
8	13.680	13.600	13.813	11438	6.735
9	13.980	13.813	14.048	3183	1.875
10	14.183	14.048	14.283	29988	17.659
11	14.346	14.283	14.464	21105	12.428
Total				169819	100.000

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BG Mode:Averaged 0.000-9.708(1-3531)

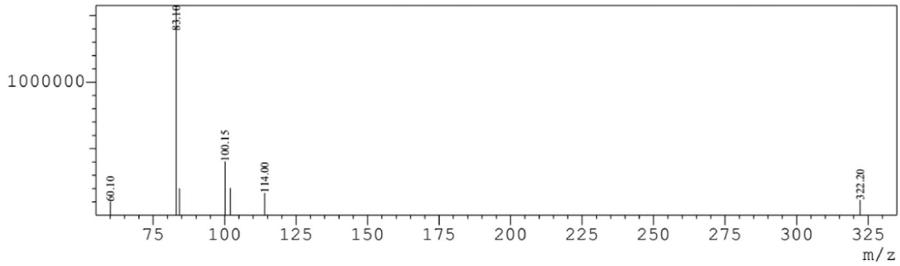
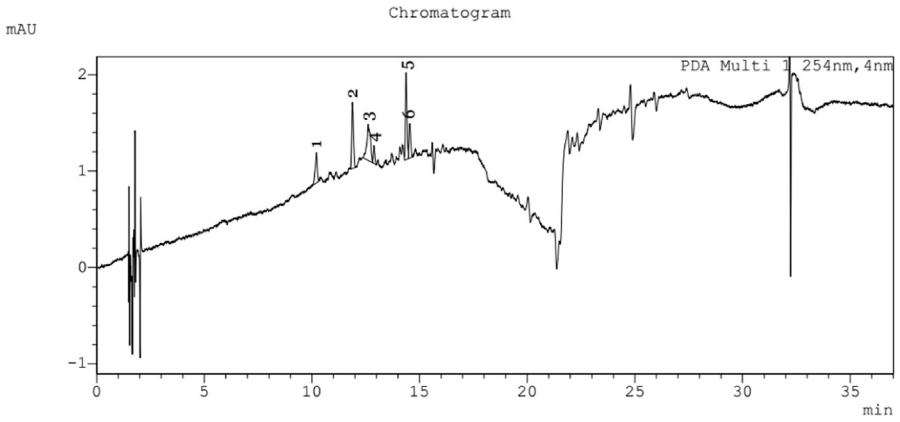


Fig. 3. LCMS chromatogram of *Caesalpinia sappan L.* heartwood methanol extract. 10 μL of sample was loaded in eclipse XDB C18 column (150*4.6 mm and 5μ pore size), with 1.0 mL/min flow rate of Methanol:Water (80:20) as mobile phase. Mass spectra was performed by ESI (Electro spray Ionization), the formation of positive and negative ions occurs in high yield which is useful for determination of compounds.



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%
1	10.206	10.027	10.336	2159	12.352
2	11.883	11.765	12.021	3632	20.782
3	12.603	12.384	12.811	4311	24.667
4	12.879	12.811	13.003	916	5.242
5	14.373	14.293	14.485	4645	26.577
6	14.539	14.485	14.656	1814	10.379
Total				17476	100.000

Q1 Scan Negative-
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BG Mode:Averaged 0.003-9.771(2-3554)

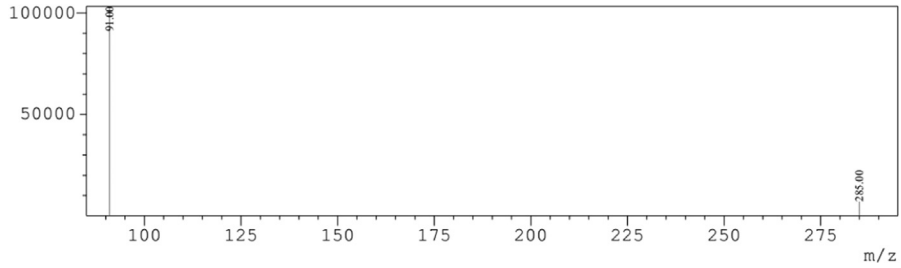
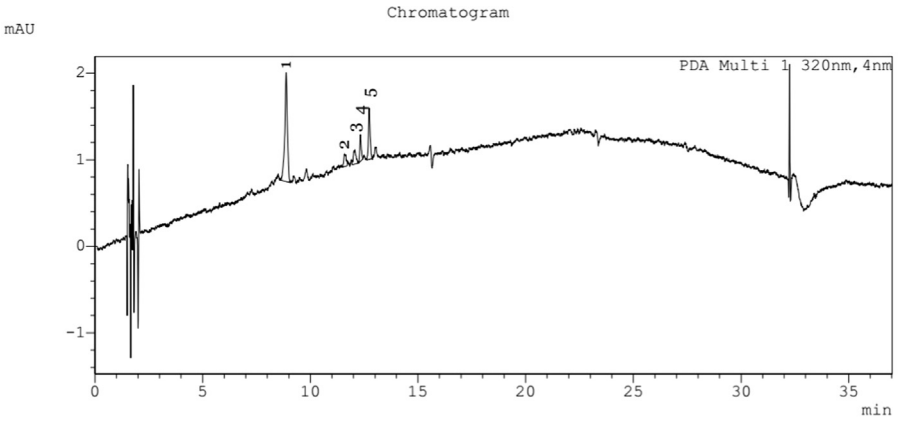


Fig. 4. LCMS chromatogram of *Caesalpinia sappan L.* heartwood water extract. 10 μL of sample was loaded in eclipse XDB C18 column (150*4.6 mm and 5μ pore size), with 1.0 mL/min flow rate of Methanol: Water (80:20) as mobile phase. Mass spectra was performed by ESI (Electro spray Ionization), the formation of positive and negative ions occurs in high yield which is useful for determination of compounds.



Peak Table

PDA Ch1 320nm

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%
1	8.871	8.640	9.077	10457	59.191
2	11.579	11.499	11.712	1182	6.692
3	12.065	11.936	12.203	1363	7.716
4	12.318	12.235	12.437	1490	8.433
5	12.730	12.608	12.853	3174	17.968
Total				17666	100.000

Q1 Scan Negative-
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BG Mode:Averaged 1.015-8.500(370-3092)

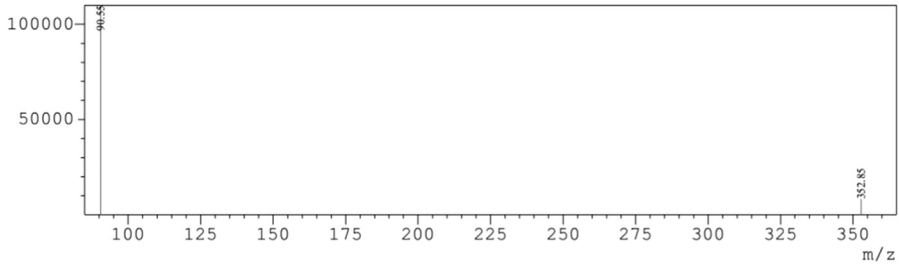
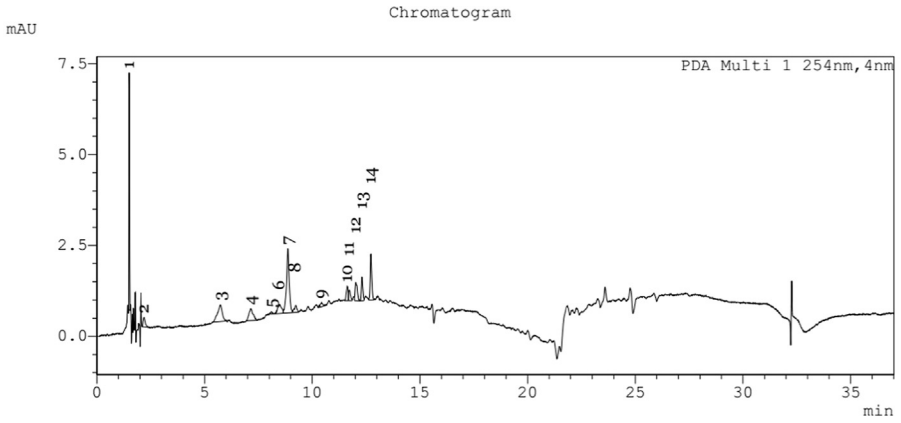


Fig. 5. LCMS chromatogram of *Caesalpinia sappan L.* leaf methanol extract. 10 μL of sample was loaded in eclipse XDB C18 column (150*4.6 mm and 5μ pore size), with 1.0 mL/min flow rate of Methanol: Water (80:20) as mobile phase. Mass spectra was performed by ESI (Electro spray Ionization), the formation of positive and negative ions occurs in high yield which is useful for determination of compounds.



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%
1	1.497	1.440	1.547	13753	20.878
2	2.194	2.101	2.379	1790	2.718
3	5.742	5.376	6.005	6967	10.576
4	7.152	6.933	7.445	4270	6.482
5	8.096	8.032	8.192	335	0.508
6	8.484	8.235	8.651	3248	4.931
7	8.875	8.651	9.088	15617	23.707
8	9.244	9.088	9.365	1523	2.311
9	10.411	10.261	10.677	1133	1.719
10	11.628	11.499	11.680	2330	3.538
11	11.723	11.680	11.861	1709	2.595
12	12.022	11.957	12.203	3671	5.572
13	12.313	12.203	12.416	3120	4.737
14	12.724	12.608	12.864	6409	9.729
Total				65876	100.000

Q1 Scan Negative-
If(SpPrTab==SpPrTab)Spectrum Mode:Averaged 1.394-1.713(508-624)
BG Mode:Averaged 0.003-1.334(2-486)

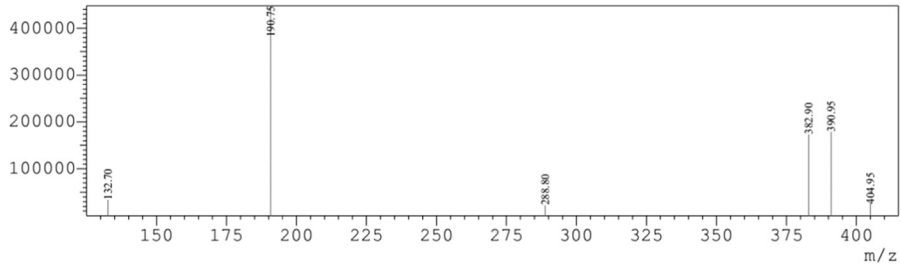
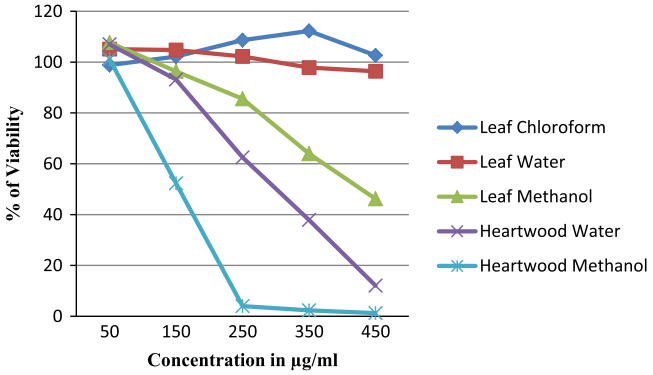


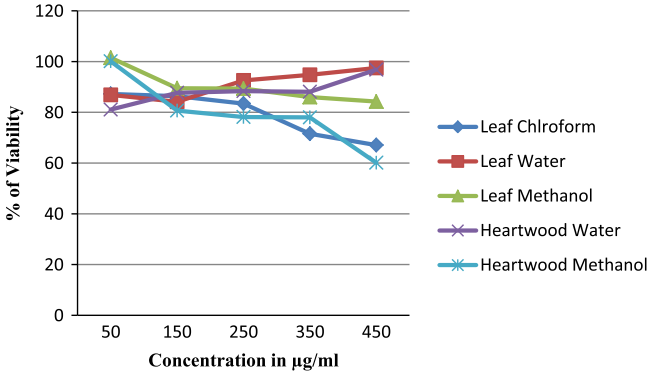
Fig. 6. LCMS chromatogram of *Caesalpinia sappan L.* leaf water extract. 10 μL of sample was loaded in eclipse XDB C18 column (150*4.6 mm and 5μ pore size), with 1.0 mL/min flow rate of methanol:water (80:20) as mobile phase. Mass spectra was performed by ESI (Electro spray Ionization), the formation of positive and negative ions occurs in high yield which is useful for determination of compounds.

Table 2
Binding energy of various secondary metabolites in methanolic extract of *Caesalpinia sappan L* with BCL-2 Protein by using auto dock software.

S NO	Secondary metabolites	Binding energy (kcal/mol)
1.	4-O-methylsappanol	−6.6
2.	Protosappanin B,	−6.9
3.	protosappanin A,	−7
4.	caesalpin J,	−6.6
5.	BrazilinA	−7
6.	BrazilinB	−7
7.	BrazilinC	−7
8.	Brazilein.	−6.9



Graph 1. MTT analysis with different concentration of *Caesalpinia sappan L.* leaf and heart wood extracts in chloroform, water and methanol on MCF-7 (Human breast cancer) cell line. *L – leaf and H – heartwood.



Graph 2. MTT analysis with different concentration of *Caesalpinia sappan L.* leaf and heart wood extracts in chloroform, water and methanol on A549 (Human lung cancer) cell line. *L – leaf and H – heartwood. .

drawn in chemsketch tool. Further docking studies was carried out using auto dock [5] using bioactive molecule (Fig. 2) (Graphs 1 and 2).

Acknowledgements

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.05.050.

References

[1] Nurzijah Ika, et al., Secang (*Caesalpinia sappan L.*) heartwood ethanolic extract shows activity as doxorubicin co-chemotherapeutic agent by apoptosis induction on T47D breast cancer cells, Indones. J. Cancer Chemoprev. 3 (2) (2017) 376–383.
[2] Rachmady Rahmawaty, et al., Antiproliferative effect of secang heartwood ethanolic extract (*Caesalpinia sappan L.*) on HER2-positive breast cancer cells, Indones. J. Cancer Chemoprev. 7 (1) (2017) 1–5.
[3] Bukke Arunkumar Naik, Fathima Nazneen Hadi, Chandramati Shankar Produtur, Comparative study of in vitro antibacterial activity of leaves, bark, heart wood and seed extracts of *Caesalpinia sappan L.*, Asian Pac. J. Trop. Dis. 5 (11) (2015) 903–907. http://dx.doi.org/10.1016/S2222-1808(15)60954-9.IS.
[4] P. Senthilraja, K. Kathiresan, in vitro cytotoxicity MTT assay in Vero, HepG2 and MCF-7 cell lines study of Marine Yeast, J. Appl. Pharm. Sci. 5 (03) (2015) 080–084.
[5] G.M. Morris, R. Huey, W. Lindstrom, M.F. Sanner, R.K. Belew, D.S. Goodsell, A.J. Olson, Autodock4 and AutoDockTools4: automated docking with selective receptor flexibility, J. Comput. Chem. 16 (2009) 2785–2791.