Phytochemical profiling by FTIR and GC-MS analysis of several fractions of Methanolic extract of aerial parts of *A.Cordata*

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Abstract: Using GCMS and FTIR analyses, the methanolic extract of A. cordata was phytochemically profiled. Using VLC and increasing polarity solvents like hexane, chloroform, and ethylacetate, methanolic extracts can be fractionated. The results of the FTIR study showed the existence of the functional groups =CH-H, C-O, O-H, C-O-C, and C-O-C. For GC-MS, a Shimadzu QP2012 was utilised, and for FTIR, a KBr pellet approach. 4,6-Nonadecadien-1-ol-acetate (17.85%), Bicyclo(3,1)Hexan-3-ol, 4-methyl-1-(1-methylethyl)-(32.73%), 2,2-Dibromocholestane (16.28%), and Heptadecenal (27.65%) were all found in the Hexane fraction by GC-MS. Acetic acid (11.74%), 1,3, Bis-T-Butylperoxy-pthalan (3.71%), pentanoic acid, 2-(aminooxy)(25.808%), betacarotene (43.34%), and dihydrotachysterol (15.417%) are the main substances in the chloroform fraction. All of the chemicals, as well as antioxidant, antiproliferative, antibacterial, inhibitory, and flavouring agents, are known to have a variety of biological effects.

Keywords: *A.cordata*, Methanolic extract, VLC fractionisation, FTIR, GC-MS analysis.

Introduction:

Individual and societal health are greatly benefited by medicinal plants. In the underdeveloped world, plant-based traditional medicines help close to 3.4 billion people. This amounts to about 88% of the world's population, whose primary healthcare is predominantly provided by traditional medicine. As long as it is demonstrated to be safe and effective, traditional medicine is supported by the World Health Organization (WHO). (G. & P., 2017). Many disorders are treated with medicinal plants in Ayurveda, Unani, and other medical systems. Drugs derived from natural sources often show less negative effects. The indigenous population of this subcontinent has a long history of using herbal medicines as a result. Due to the large variety of native flora, herbal remedies are utilised for general treatment, especially in villages (Sajia Afrin et al., 2019). In recent years, the technical platform of choice for secondary metabolite profiling in both plant and non-plant species has solidly established itself as gas chromatography mass spectrometry (GC-MS). (2014) Kanthal et al.

Malphigiaceae member *Aspidopterys cordata* (Heyne ex Wall) *A. Juss* alternatives: Hiraea cordata

Herbacious Climbing juvenile sections of shrubs with white tomentose. broad oval or oribiculate leaves. Flowers with a yellowish hue; terminal tomentose long flowers; 11–14 mm in fruits; slender, filiform; calyx 5-partite; lobes oval or elliptic; glabrous; petals 5; stamens 10; filaments 2–5 mm long; ovary vilous. Found sporadically in woods in the districts of Mahabubnagar, Adilabad, Nizamabad, Medak, and Ranga Reddy. 2015's (T. Pullaiah) (2016) K.N. Reddy and C. Sudhakar Reddy. However, as the biochemicals of this plant have not yet been documented, an effort is made in this study to file Phytochemical Profiling by GC-MS analysis. This plant's methanolic extract has been found to have outstanding high phenolic content, flavonoid content, and antioxidant activity. Dr. K. Sunitha and P. Udaya Chandrika, 2022

Materials and Procedures

Collecting and identification of plants:

At the Kinnerasani Wild Life Sanctuary in the Telangana district of Bhadradri Kothagudem, Aspidopterys cordata was found. The plant has been verified by botanist Dr. K. Venkata Ratnam, Assistant Professor in the Department of Botany at Rayalaseema University in Kurnool; a specimen of the plant has been submitted (RU/BD/VSN-092) for future use. Dr. K. Sunitha and P. Udaya Chandrika, 2022

Extraction: Plant material's aerial portions were gathered, cleaned with water, dried in the shade, and then sonicated at 40 KHz for 45 minutes at 45 ^{o}C. The supernatant solutions were filtered, then decanted, concentrated in a Rotary evaporator, and conserved in a dessicator. (Dr. K. Sunitha and P. Udaya Chandrika, 2021)

Fractionisation: Methanolic extracts of both plants are prepared as a slurry, adsorbed on to silica gel, and then introduced over the adsorbent. A moderate vacuum of 20 to 70 mm hg is then applied, and the fractions are collected into the volumetric flask. The solvent is gradually added until the resulting fraction is colourless. Using ethylacetate and chloroform, the procedure is repeated. Rotavapour is used to concentrate the fractions once they have been separately collected. Analytical tests were conducted on the additional residues that were collected following separation utilising columns (GCMS and FTIR) 2018 (Maurya et al.)

FTIR: The KBr disc method (Vmax in cm-1) was used to prepare the samples, and Perkin Elmer Spectrum Version 10.03.08 was used to generate the FT-IR spectra. Using an IR press, the plant extract was pelletized after being mixed with KBR (1:10). After inserting the pellet into the sample slit, the transmittance was calculated. Payal Mittal and others, 2020

GC-MS: With GC-MS, it is simple to identify a compound's molecular mass and elemental makeup. High resolution electron impact mass spectroscopy was used. For the GC-MS study, a Shimadzu QP2012 30 X 0.32 mm X 1.8 m column was employed. For GC-MS detection, an electron system with an ionisation energy of -70eV was employed. The carrier gas was helium gas (99.9995%) with a split ratio of 10:1, a constant flow rate of 1.491 ml/min, and an injection volume of 1.0 ml. Injector temperature: 1400 °C The ion source is 2000°C in temperature. The oven's temperature was set to increase from 1100 ° C to 2400 ° C for 8 minutes at a rate of 100 ° C. At 70 eV, mass spectra were gathered throughout a 0.5 second scan period. The GC ran for 24.35 minutes in its entirety. By comparing each component's average peak area to the total areas, the relative percentage quantity for each component was determined. In order to handle mass spectra and chromatographs, GCMS solution version 2.53 was employed, and it was contrasted with NIST Library 2011 version. The components

of the test substance were identified, together with their names and structures. P. T. Srinivasan and colleagues (2016) Table 1 displays the substances found in the A. cordata extracts by GC-MS analysis.

Results:

The functional groups identified by FTIR analysis in the hexane, chloroform, and ethylacetate fractions were included in tables 1, 2, and 3, respectively. Six bio chemicals were found in the hexane fraction during GC-MS analysis. Heptacosonoic acid, 14-methyl, Methyl ester(2.64%), 4,6-Nonadecadien-1-ol-acetate(17.85%), Bicyclo(3,1)Hexan-3-ol, 4-methyl-1-(1-methylethyl)-(32.73%), 2,2-Dibromocholestane(16.28%), 2-Dodecen-1-yl(-)succinic anhydride2.85%), Heptadecenal(27.65%) and the biological activities of these compounds are shown in Table. 6. The chloroform fraction presented in the table 6 contains the phytocompounds 1,3, Bis-T-Butylperoxypthalan (3.717%) and Acetic acid (11.74%) in the highest concentrations. 5. The majority of the ethylacetate fraction in the table includes the following compounds: Undecanoic acid (7.026%), Pentanoic acid, 2-(aminooxy) (25.808%), Betacarotene (43.34%), Dihydrotachysterol (15.417%), and Eicosonoic acid (2.105%).

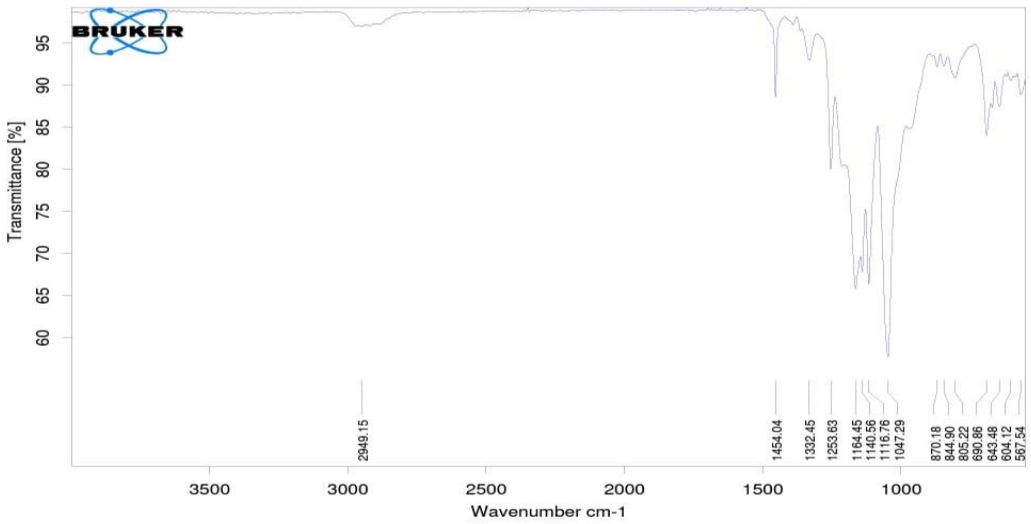

Fig.1 FTIR spectra of Hexane Fraction of *A.cordata*

Table.1 Functional groups identified by FTIR of *A.cordata* Hexane Fraction

Wave number cm^{-1}	Functional group
2949	C-H
1454	O-H
1332	C-N
1253	C-O
1164	C-O
1140	C-O-C
1116	C-O
1047	C-O
870	=C-H
844	C-C
805	=C-H

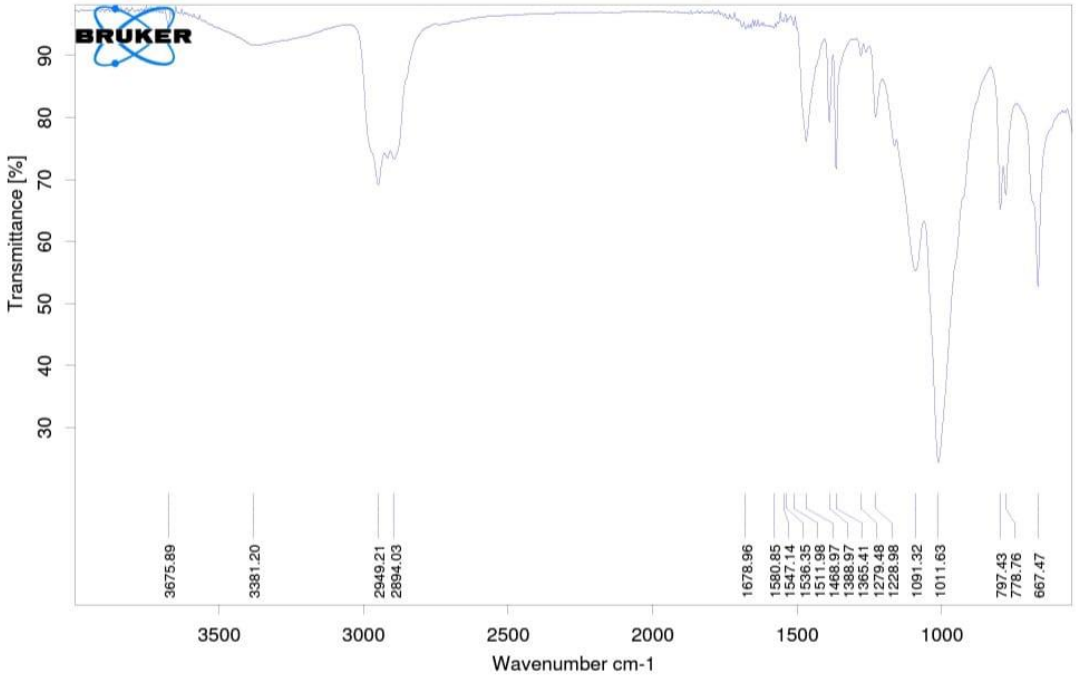

Fig.2 FTIR spectra of Chloroform Fraction of *A.cordata*

Table.2 Functional groups identified by FTIR of *A.cordata* Chloroform Fraction

Wave number cm^{-1}	**Functional group**
3675	
3381	O-H
2949	=C-H
2894	O-H
1678	=C-H(aromatic)
1580	N-H
1547	C-C(aromatic)
1536	C-C(alkene)
1511	C=C
1468	C=C
1388	C-H
1365	C-H
1279	C-N
1228	C-N
1091	C-O
797	C-C
778	C-C
667	C-Cl

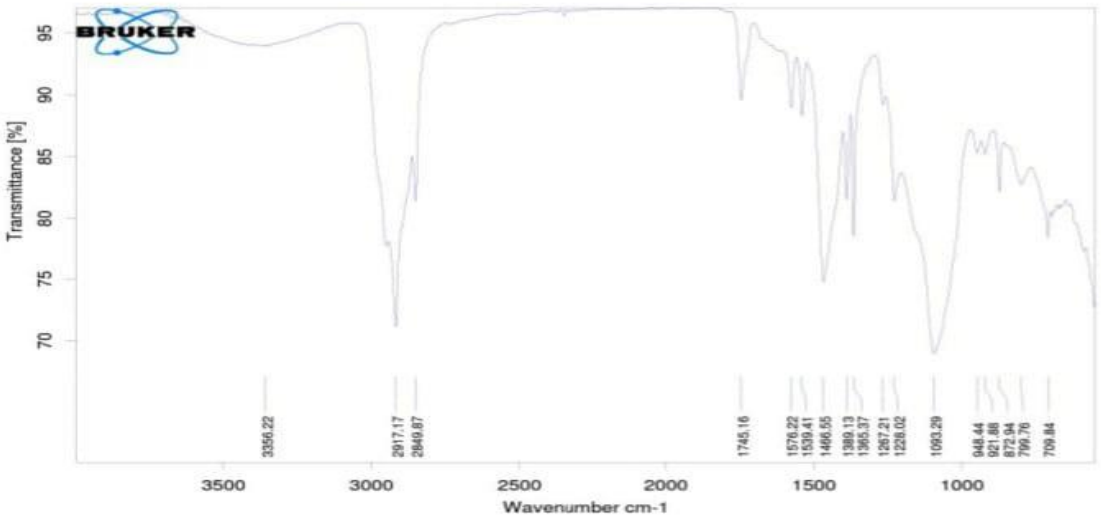

Fig.3 FTIR spectra of Ethylacetate Fraction of *A.cordata*

Table.3 Functional groups identified by FTIR of *A.cordata* Ethylacetate Fraction

Wave number cm-1	Functional group
3356	O-H
2917	C-H
2849	C-H
1745	C=O
1576	C=N
1539	C=C
1466	C=C
1389	C-O
1365	N=O
1267	C-O
1228	C-N
1093	C-O
948	=CH-H
921	=CH-H
872	N-H
799	C-F

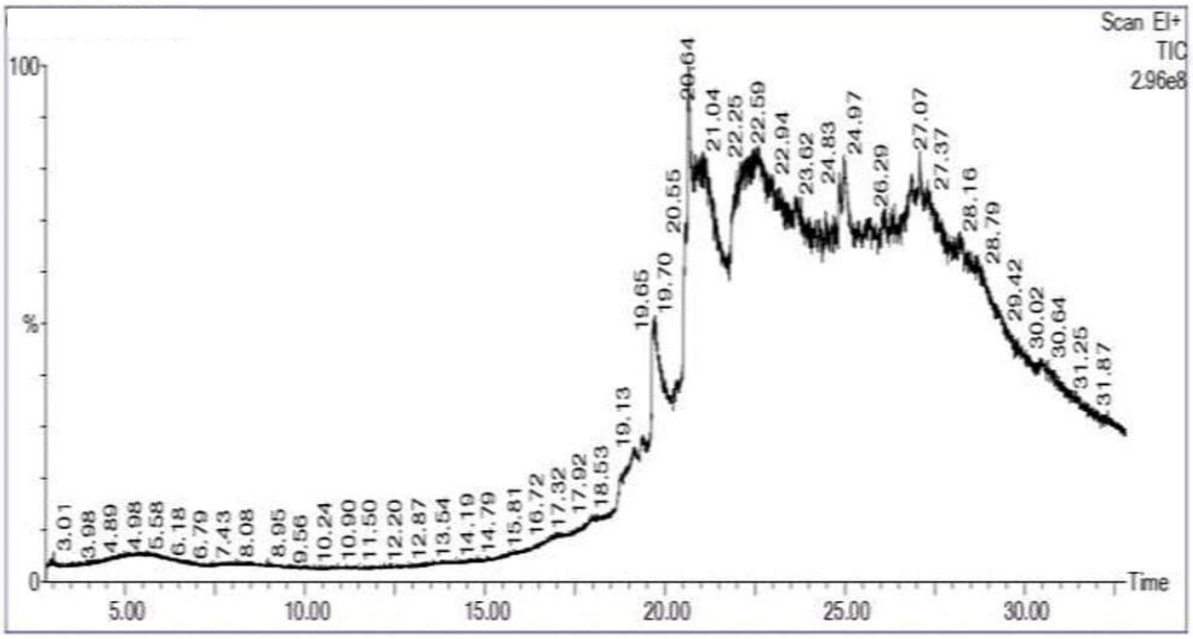

Fig.4 Methanolic extract of *A.cordata*-GCMS spectra of Hexane Fraction

Table.5: Biochemical compounds of *A.cordata* identified in GC-MS of Hexane Fraction:

Peak	Retention Time(RT)	Peak area (%)	Compound name	Biological activity
1	19.725	2.641	Heptacosonoic acid, 14-methyl, Methyl ester	Skin cancer Protein (Kandasamy et al., 2012)
2	20.661	17.853	4,6-Nonadecadien-1-ol-acetate	-
3	22.592	32.739	Bicyclo(3,1)Hexan-3-ol, 4-methyl-1-(1-methylethyl)-	Flavouring(National Center for Biotechnology Information (2023). PubChem Compound Summary for CID 12304610,
4	24.968	16.238	2,2-Dibromocholestane	
5	26.108	2.855	2-Dodecen-1-yl(-)succinic anhydride	Antineoplastic agents, Antioxidants, Antimicrobial(Rawal Jatin R & Sonawani Priya R, 2016)
6	27.073	27.675	Heptadecenal	Antibacterial and Antioxidant(Faridha Begum et al., 2016)

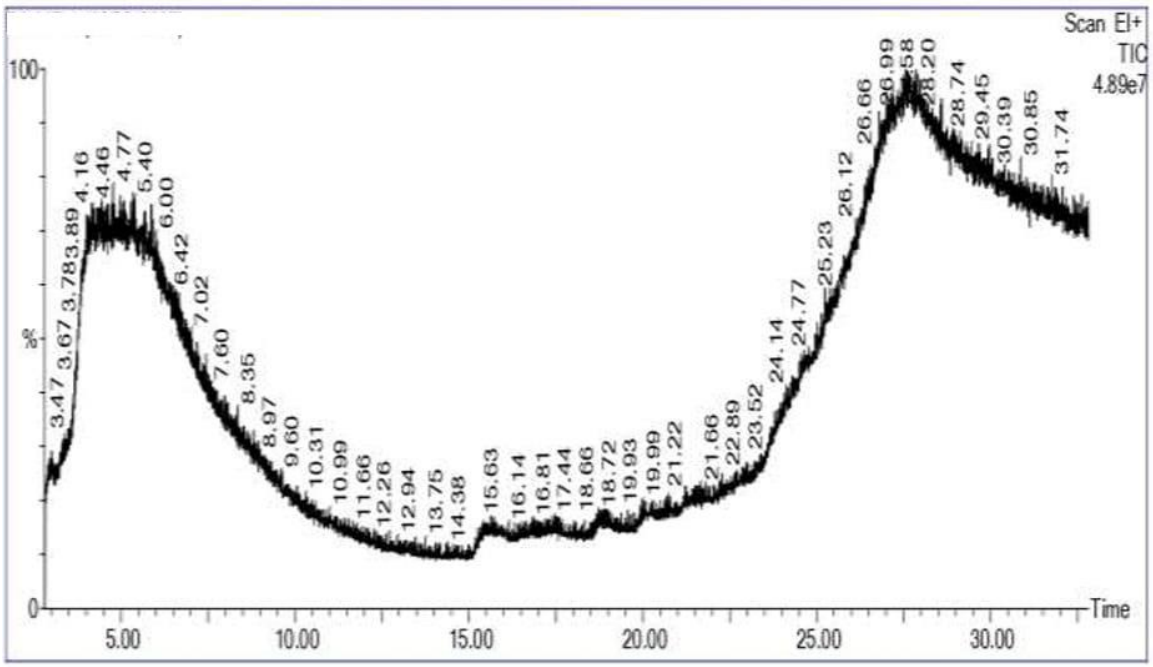

Fig.5 Methanolic extract of *A.cordata*-GCMS spectra of Chloroform Fraction

Table.5: Biochemical compounds of *A.cordata* identified in GC-MS of Chloroform Fraction

Peak	Retention Time(RT)	Peak area (%)	Compound name	Biological activity
1	4.189	15.096	Methylene chloride	Solvent
2	4.769	16.829	Dichloroacetaldehyde	-
3	4.979	11.747	Acetic acid	Antibacterial(Abdel Moneim, 2016)
4	5.4	15.839	Dichlroacetaldehyde	-
5	5.875	20.421	Methane-D, Trichloride	-
6	6.665	4.419	Dichloroacetaldehyde	-
7	7.045	1.486	Methylene chloride	-
8	26.66	1.65	Acetic acid, Dichloro	-
9	28.2	3.717	1,3, Bis-T-Butylperoxy-pthalan	Anti-tumor, catechol -o-methyl transferase, Glutathione transferase inhibitor(Sreedevi et al., 2022)
10	29.45	8.795	1,2,3-Propatriol, 1- Indol-4yl(Ether)	-

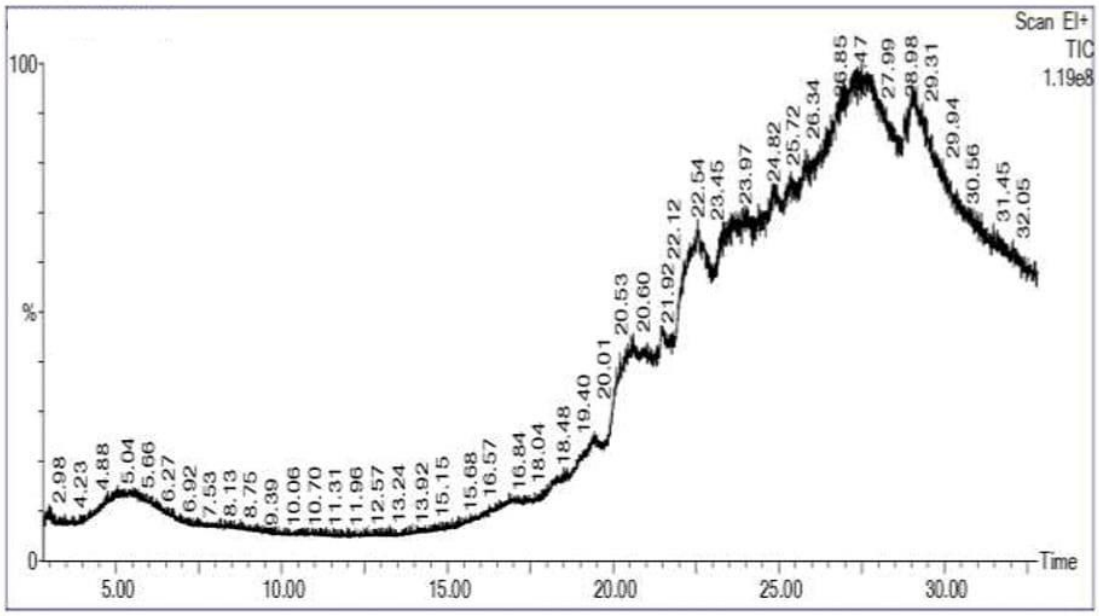

Fig.6 Methanolic extract of *A.cordata*-GCMS spectra of Ethylacetate Fraction

Table.6: Biochemical compounds of *A.cordata* identified in GC-MS of Ethylacetate Fraction

Peak	Retention Time(RT)	Peak area(%)	Compound name	Biological activity
1	20.53	1.506	3-isobutyldihydropyrazin-2-one	-
2	22.541	7.766	2,6-Dipyrazindiamine	-
3	23.817	7.026	Undecanoic acid	Antibacterial(Nisar et al., 2013)
4	23.972	3.126	9-bromonaldehyde	-
5	24.382	3.423	4-Flouro-1-methyl-5-carboxylic acid	-
6	24.822	4.887	Cholesta-8,24-dien-3-ol,4-methyl-(3 beta, 4alpha)	-
7	25.347	3.231	9-bromonaldehyde	-
8	25.808	6.183	Pentanoic acid, 2-(aminooxy)	Anticancer(Das et al., 2020)
9	27.493	43.384	Betacarotene	Antibacterial,Antioxidant (Basim et al., 2021; Stahl & Sies, 2005)
10	28.999	15.417	Dihydrotachysterol	Antiproliferative(Chen et al., 2000)
11	30.014	2.105	Eicosonoic acid	Inhibitory activity(Dang Khanh & Ahmad, 2007)
12	30.364	1.946	1-Monolinoleoglycerol Trimethyl ether	-

Discussion: Current studies on the analysis of different fractions by FTIR and GC-MS The numerous phytocompounds that are responsible for antioxidant, antiproliferative,

antibacterial, inhibitory, flavouring, etc. effects are found in methanolic extract of aerial portions of A. cordata. Future research has a lot of potential to identify and describe fresher restorative phytocompounds from A. cordata and assess their pharmacological effects.

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