WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 6, 1091-1106. Research Article ISSN 2277–7105

ANTISEIZURE LEAD IDENTIFICATION FROM MALVASTRUM COROMANDELIANUM USING SOXHLET EXTRACTION, HR-LCMS AND IN SILICO APPROACHES

Porselvi R.*, Dr. K. B. Ilango, Beenamol I., Dhivakar S., Nithish Kumar R., Pravisha S., Sanchitha K.

Shree Venkateshwara College of Paramedical Sciences, College of Pharmacy, Gobi-638455.

Article Received on 15 Feb. 2026,
Article Revised on 05 March 2026,
Article Published on 16 March 2026,

https://doi.org/10.5281/zenodo.19046577

***Corresponding Author**

Porselvi R.

Shree Venkateshwara College of Paramedical Sciences, College of Pharmacy, Gobi-638455.

How to cite this Article: Porselvi R.*, Dr. K. B. Ilango, Beenamol I., Dhivakar S., Nithish Kumar R., Pravisha S., Sanchitha K.. (2026). Antiseizure Lead Identification From Malvastrum Coromandelianum Using Soxhlet Extraction, Hr-Lcms And In Silico Approaches. World Journal of Pharmaceutical Research, 15(6), 1091–1106.

ABSTRACT

Malvastrum coromandelianum, a promising traditional herbal medicine from Malvaceae family has long been recognized for its medicinal attributes. Though it is traditionally used for many diseases including neurological disorders, yet its Anticonvulsant property was not explained. This research used a special technique called HR-LCMS provides a powerful platform for precise, unambiguous structural elucidation and quantitative profiling of the complex mixture of phytoconstituents present in the plant's stem extract and In-Silico Docking to predict their binding affinity towards the neurological target. The substances identified by HR-LCMS were tested against important targets like GABA-A receptors. D2 receptors and NMDA (N-methyl-D-aspartate) receptors through molecular docking. Many flavonoids and phenolic compounds obtained from the stem extract showed strong binding affinities and favourable ADMET properties, suggesting they might help manage seizures. Hence, this synergistic methodologies accelerated the process of identification of compounds and their therapeutic potential for the treatment of seizures, making the search for new medicines from the natural sources more efficient.

KEYWORDS: Soxhlet extraction, HR-LCMS, anticonvulsant, epilepsy, molecular docking, *Malvastrum coromandelianum*.

INTRODUCTION

Affecting millions of people worldwide, Epilepsy is chronic neurological disorder that is characterized by unprovoked, recurrent seizures, remains a significant global health burden. The limitations of current antiepileptic drugs (AEDs)-frequently manifesting as pharmaco-resistence or dose-related adverse effect profiles necessitate the exploration of novel, often phytotherapeutic interventions with therapeutic indices.[1,2,10,17,19]

The traditional medicinal plant, *Malvastrum coromandelianum* is recognized for its rich phytochemical repertoire, which encompasses diverse classes of secondary metabolites such as flavonoids, alkaloids, terpenoids, tannins, saponins and other phenolic derivatives. These compounds are frequently implicated in neuroprotective and antiseizure pharmacological properties. Despite its ethnobotanical utility, there hasn't been enough scientific study on how effectively it can prevent seizure.[3,4,5,6,12,18]

Figure 1.

MATERIALS AND METHODS

Plant Collection & Authentication

The fresh plant of *Malvastrum coromandelianum* (L.) Garcke were collected from local area in Thiruvannamalai district. It was identified and authenticated by Dr. P. RADHA, Research Officer (Botany), Sci II & i/c SIDDHA MEDICINAL PLANTS GARDEN, METTUR.

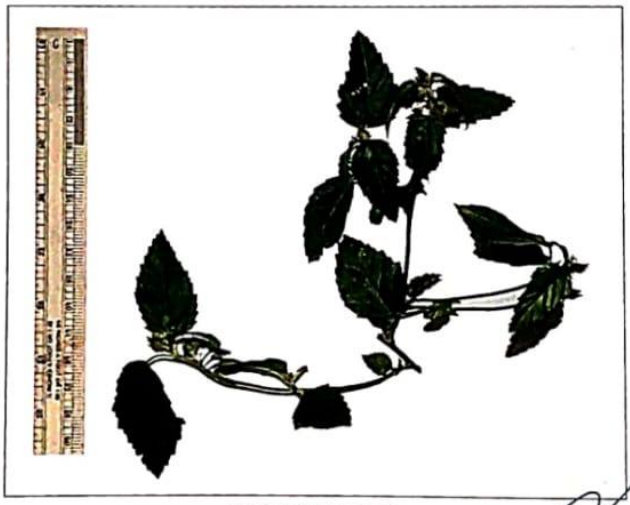
சித்த மருத்துவ மூலிகைத் தோட்டம்
(மத்திய சித்த மருத்துவ ஆராய்ச்சிக் குழுமம்)
(ஆயுஷ் அமைச்சகம், இந்தியஅரசு.)
सिद्ध औषधीय पादप उद्यान, कावेरीनगर, मेट्टूर बांध
SIDDHA MEDICINAL PLANTS GARDEN
(Central Council for Research in Siddha),
Ministry of Ayush, Govt. of India,
No. 17, SDO Quarters, Opp. Ulavar Santhai, Cauvery Nagar, Mettur Dam, Tamilnadu-636 401
Phone No. 04298 – 243 773 E-mail: smpgmettur@gmail.com

Date: 14.11.2025

AUTHENTICATION CERTIFICATE FOR 141125168

Certified that the drug/material submitted by **Mr. DHIVAKAR. S (Reg. No. 560021523017),** Bachelor of Pharmacy, Department of Pharmaceutical Chemistry, Shree Venkateshwara College of Paramedical Science, College of Pharmacy, Gobi is identified as:

Sl. No.	Botanical Name	Family	Part	Code
1.	*Malvastrum coromandelianum* (L.) Garcke	Malvaceae	Aerial parts	M141125168C



M141125168C

डॉ.पि. राधा/Dr. P. RADHA
प्रभारी अनुसंधान अधिकारी (वनस्पति विज्ञान) वैज्ञानिक II
Research Officer (Botany) Sci II & I/c
सिद्ध औषधीय पादप उद्यान/ Siddha Medicinal Plants Garden
(केन्द्रीय सिद्ध अनुसंधान परिषद, आयुष मंत्रालय, भारत सरकार)
(CCRS, Ministry of Ayush, Govt. Of India)
मेट्टूर बांध, तमिलनाडु/ Mettur Dam, Tamil Nadu-636 401.

Dr. P. Radha
Research Officer (Botany) Sci II/ I/C
Siddha Medicinal Plants Garden
Date:

Preparation of plant extract

The stems has been washed with tap water and shade-dried for upto 7-10 days, then powdered. About 25gms of the powder were extracted with 250ml of 95% of Ethanol using Soxhlet for 6-8hrs. The extract was then concentrated and stored for further investigation.[7,13]

Preliminary High Resolution – Liquid Chromatography Mass Spectrometry

The hyphenated technique, which enables a selective and sensitive identification and quantification of wide range of compounds in a complex mixture. The chemical profiling of *Malvastrum coromandelianum* stem extract was carried out using an Agilent TOF/Q-TOF mass spectrometer (Model G6550A) equipped with a Dual AJS ESI ion source. The instrument was operated in positive electrospray ionization (ESI+) mode under the AutoMS2 acquisition method.[8,9,14,15]

In Silico approaches for target validation

The modern drug discovery pipeline is significantly enhanced by chemo-informatics tools, which facilitate the rapid, high-throughput screening of natural product scaffolds against targets associated to epilepsy. In silico methodologies, including Swiss ADME and AutoDock Vina and predictive ADMET pharmacokinetics/pharmacodynamics assessments are crucial for identifying lead compounds exhibiting optimal binding affinities and favourable drug-likeness characteristics.[16,20,21]

RESULT AND DISCUSSION

The Anticonvulsant assay was performed and the results are shown in (Table 1,2,3,4). Ethanolic extract of *Malvastrum coromandelianum* showed significant activity.

Table 1: HR-LCMS Identified Phytoconstituents from *Malvastrum coromandelianum*.

S.No	RT	Mass	Name	Formula
1	2.577	122.0371	Benzoic acid	C7H6O2
2	4.277	164.0477	p-Coumaric acid	C9H8O3
3	4.277	164.0477	Enol-phenylpyruvate	C9H8O3
4	2.577	168.0426	2,6-Dihydroxyphenylacetate	C8H8O4
5	4.887	194.0585	Ferulic acid	C10H10O4
6	2.73	110.0371	Resorcinol	C6H6O2
7	4.887	194.0585	Kakuol	C10H10O4
8	1.237	504.0904	3-Methylellagic acid 8-(2acetylrhamnoside)	C23H20O13
9	3.938	318.0745	Brompheniramine	C16H19BrN2
10	3.982	359.103	Quinoline-3-carboxamides	C21H14FN3O2
11	3.999	125.9996	Ethyl hydrogen sulfate	C2H6O4S
12	1.53	166.0316	6-Methylmercaptopurine	C6H6N4S

13	4.334	422.0322	Chloramphenicol succinate	C15H16Cl2N2O8
14	4.906	188.0129	4-Sulfobenzyl alcohol	C7H8O4S
15	5.089	400.0498	Bis(glycerophospho)-glycerol	C9H22O13P2
16	5.159	532.1409	Trichotomine	C30H20N4O6
17	5.413	359.1086	Clovamide	C18H17NO7
18	5.737	290.0813	(-)-Epicatechin	C15H14O6
19	5.956	313.0981	Amoxapine	C17H16ClN3O
20	6.001	349.072	m-Carboxyphenyl phenylacetamidomethylphosphonate	C16H16NO6P
21	6.281	564.1524	Kaempferol 3-rhamnoside 7-xyloside	C26H28O14
22	5.748	174.0902	Diethyl succinate	C8H14O4
23	5.917	334.1075	Byakangelicin	C17H18O7
24	6.001	464.099	Demeclocycline	C21H21ClN2O8
25	6.281	434.0871	Guajavarin	C20H18O11
26	4.334	446.0407	Benzobicyclon	C22H19ClO4S2
27	7.228	850.2008	ent-Fisetinidol-(4beta->8)catechin-(6->4beta)-ent-fisetinidol	C45H38O17
28	7.542	448.1042	Quercitrin	C21H20O11
29	7.905	430.187	Phenethyl rutinoside	C20H30O10
30	7.969	448.1039	Luteolin 4'-O-glucoside	C21H20O11
31	8.334	460.3589	omega-hydroxy behenic	C22H44O3
32	10.394	460.3587	(3beta,5alpha,6beta,9alpha,22E,24R) -23-Methylergosta-7,22-diene3,5,6,9-tetrol	C29H48O4
33	10.779	594.1416	7-O-(4-Hydroxycinnamoyl) astragalin	C30H26O13
34	7.833	328.2272	Corchorifatty acid F	C18H32O5
35	11.02	258.0909	O-Desmethylangolensin	C15H14O4
36	11.082	220.1143	1D-1-Guanidino-3-amino-1,3dideoxyscyllo-inositol	C7H16N4O4
37	11.337	330.2431	9,10-Dihydroxy-12,13epoxyoctadecanoate	C18H34O5
38	18.234	682.2483	Bruceoside A	C32H42O16
39	21.03	453.2877	Sambutoxin	C28H39NO4
40	21.337	481.3195	LysoPE(0:0/18:0)	C23H48NO7P
41	22.108	294.1888	Sodium Tetradecyl Sulfate	C14H30O4S
42	22.294	280.2417	Linalyl caprylate	C18H32O2
43	22.474	326.1929	4-Dodecylbenzenesulfonic acid	C18H30O3S
44	24.791	464.3528	Castasterone	C28H48O5
45	24.819	666.4385	Notoginsenoside T2	C37H62O10
46	25.075	338.2115	[6]-Gingerdiol 3-acetate	C19H30O5
47	25.417	598.4014	Idoxanthin	C40H54O4
48	25.561	564.3965	Alloxanthin	C40H52O2
49	25.614	382.2407	Sarcostin	C21H34O6
50	25.918	912.5414	Ritterazine A	C54H76N2O10
51	26.299	566.4122	3-Hydroxy-b,e-caroten-3'-one	C40H54O2
52	27.151	974.5773	Megalomicin C2	C49H86N2O17
53	27.453	750.4872	Salinomycin	C42H70O11
54	28.17	703.5183	PE(15:0/18:1(9Z))	C38H74NO8P
55	29.028	474.3735	Bryodulcosigenin	C30H50O4

56	29.118	514.4787	Muricadienin	C35H62O2
57	1.195	234.1492	Benzoylagmatine	$C_{12}H_{18}N_4O$
58	2.71	336.1798	Apovincamine	$C_{21}H_{24}N_2O_2$
59	3.084	285.1259	Isothipendyl	$C_{16}H_{19}N_3S$
60	3.088	307.1688	Alcaftadine	$C_{19}H_{21}N_3O$
61	3.454	426.1746	(Z)-Narceine imide	$C_{23}H_{26}N_2O_6$
62	3.473	264.1369	Vulgarin	$C_{15}H_{20}O_4$
63	4.077	299.141	Metochlopramide	$C_{14}H_{22}ClN_3O_2$
64	4.29	337.1421	Talampanel	$C_{19}H_{19}N_3O_3$
65	4.507	386.0846	O-Feruloylgalactarate	$C_{16}H_{18}O_{11}$
66	4.845	381.1669	Cis-zeatin-O-glucoside	$C_{16}H_{23}N_5O_6$
67	5.255	265.0825	5'-Dehydroadenosine	$C_{10}H_{11}N_5O_4$
68	5.363	200.0623	Tegafur	$C_8H_9FN_2O_3$
69	6.5	313.1198	Angustine	$C_{20}H_{15}N_3O$
70	6.557	434.1057	Knipholone	$C_{24}H_{18}O_8$
71	6.967	295.1337	GYKI 52895	$C_{17}H_{17}N_3O_2$
72	7.93	262.1094	Oil Orange SS	$C_{17}H_{14}N_2O$
73	8.158	202.1117	N-Methyl-1H-indole-3-propanamide	$C_{12}H_{14}N_2O$
74	8.579	292.1916	(S)-3-Octanol glucoside	$C_{14}H_{28}O_6$
75	8.62	350.194	(1S,2R,4R,8S)-p-Menthane-2,8,9triol 2glucoside	$C_{16}H_{30}O_8$
76	8.863	572.3055	Ganoderic acid H	$C_{32}H_{44}O_9$
77	9.673	484.1716	Dukunolide E	$C_{26}H_{28}O_9$
78	9.965	249.1289	Epinastine	$C_{16}H_{15}N_3$
79	10.757	287.1416	CI Basic red 9	$C_{19}H_{17}N_3$
80	10.931	200.0396	Camalexin	$C_{11}H_8N_2S$
81	10.984	548.2738	Antimycin A1	$C_{28}H_{40}N_2O_9$
82	12.186	311.1409	Domoic acid	$C_{15}H_{21}NO_6$
83	12.245	204.0723	Tetramisole	$C_{11}H_{12}N_2S$
84	12.353	268.158	Daimuron	$C_{17}H_{20}N_2O$
85	12.588	293.1897	Amitraz	$C_{19}H_{23}N_3$
86	12.642	325.1554	Monocrotaline	$C_{16}H_{23}NO_6$
87	13.324	329.1872	Europine	$C_{16}H_{27}NO_6$
88	15.246	316.1902	(S)-alpha-Terpinyl glucoside	$C_{16}H_{28}O_6$
89	15.409	292.1552	Vellosimine	$C_{19}H_{20}N_2O$
90	15.593	318.2052	L-Citronellol glucoside	$C_{16}H_{30}O_6$
91	15.897	428.2954	Hydroxyprogesterone caproate	$C_{27}H_{40}O_4$
92	16.852	618.3191	BILA 2185BS	$C_{35}H_{46}N_4O_4S$
93	17.537	584.3138	Caracurine V	$C_{38}H_{40}N_4O_2$
94	17.624	608.245	Somniferine	$C_{36}H_{36}N_2O_7$
95	9.673	484.1716	Dukunolide E	$C_{26}H_{28}O_9$
96	9.965	249.1289	Epinastine	$C_{16}H_{15}N_3$
97	10.757	287.1416	CI Basic red 9	$C_{19}H_{17}N_3$
98	10.931	200.0396	Camalexin	$C_{11}H_8N_2S$
99	10.984	548.2738	Antimycin A1	$C_{28}H_{40}N_2O_9$
100	12.186	311.1409	Domoic acid	$C_{15}H_{21}NO_6$
101	12.245	204.0723	Tetramisole	$C_{11}H_{12}N_2S$

102	12.353	268.158	Daimuron	$C_{17}H_{20}N_2O$
103	12.588	293.1897	Amitraz	$C_{19}H_{23}N_3$
104	12.642	325.1554	Monocrotaline	$C_{16}H_{23}NO_6$
105	13.324	329.1872	Europine	$C_{16}H_{27}NO_6$
106	15.246	316.1902	(S)-alpha-Terpinyl glucoside	$C_{16}H_{28}O_6$
107	15.409	292.1552	Vellosimine	$C_{19}H_{20}N_2O$
108	15.593	318.2052	L-Citronellol glucoside	$C_{16}H_{30}O_6$
109	15.897	428.2954	Hydroxyprogesterone caproate	$C_{27}H_{40}O_4$
110	16.852	618.3191	BILA 2185BS	$C_{35}H_{46}N_4O_4S$
111	17.537	584.3138	Caracurine V	$C_{38}H_{40}N_4O_2$
112	17.624	608.245	Somniferine	$C_{36}H_{36}N_2O_7$

Table 2: Summary of ADME and Drug-Likeness Prediction.

S.No	Phytoconstituent	PubChe m ID	SMILES	Lipinski Violation
1.	Benzoic acid	243	C1=CC=C(C=C1)C(=O)O	Yes; 0 violation
2.	p-Coumaric acid	637542	C1=CC(=CC=C1/C=C/C(=O)O)O	Yes; 0 violation
3.	Enol-phenylpyruvate	641637	C1=CC=C(C=C1)/C=C(/C(=O)O)\O	Yes; 0 violation
4.	Ferulic acid	445858	COC1=C(C=CC(=C1)/C=C/C(=O)O)O	Yes; 0 violation
5.	3-Methylellagic acid 8-(2-acetylrhamnoside)	73157205	CC1C(C(C(C(O1)OC2=C(C=C3C4=C2OC(=O)C5=CC(=C(C(=C54)OC3=O)OC)O)O)OC(=O)C)O)O	No; 2 violations: MW>500, NorO>10
6.	Bis(glycerophospho)glycerol	440144	C(C(COP(=O)(O)OCC(COP(=O)(O)OCC(CO)O)O)O)O	No; 2 violations: NorO>10, NHorOH>5
7.	Trichotomine	442120	C1[C@H](N2C(=CC(=C2O)C3=CC4=C5C(=C6C=CC=CC6=N5)C[C@H](N4C3=O)C(=O)O)C7=C1C8=CC=CC=C8N7)C(=O)O	Yes; 1 violation: MW>500
8.	Clovamide	6443790	C1=CC(=C(C=C1C[C@@H](C(=O)O)NC(=O)/C=C\C2=CC(=C(C=C2)O)O)O)O	Yes; 1 violation: NHorOH>5
9.	(-)-Epicatechin	72276	C1[C@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	Yes; 0 violation
10.	Kaempferol 3rhamnoside 7-xyloside	14334866	CC1C(C(C(C(O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)OC4C(C(C(CO4)O)O)O)O)C5=CC=C(C=C5)O)O)O	No; 3 violations: MW>500, NorO>10, NHorOH>5
11.	Diethyl succinate	31249	CCOC(=O)CCC(=O)OCC	Yes; 0 violation

12.	Byakangelicin	10211	CC(C)([C@@H](COC1=C2C(=C(C3=C1OC(=O)C=C3)OC)C=CO2)O)O	Yes; 0 violation
13.	Guajavarin	5481224	C1[C@@H]([C@@H]([C@H]([C@@H](O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC(=C(C=C4)O)O)O)O)O	No; 2 violations: NorO>10, NHorOH>5
14.	ent-Fisetinidol-(4beta>8)-catechin-(6->4beta)ent-fisetinidol	442680	C1[C@@H]([C@H](OC2=C(C(=C(C(=C21)O)[C@@H]3[C@H]([C@H](OC4=C3C=CC(=C4)O)C5=CC(=C(C=C5)O)O)O)O)[C@@H]6[C@H]([C@@H](OC7=C6C=CC(=C7)O)C8=CC(=C(C=C8)O)O)O)C9=CC(=C(C=C9)O)O)O	No; 3 violations: MW>500, NorO>10, NHorOH>5
15.	Quercitrin	5280459	C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC(=C(C=C4)O)O)O)O)O	No; 2 violations: NorO>10, NHorOH>5
16	Phenethyl rutinoside	14312558	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC=CC=C3)O)O)O)O)O)O	Yes; 1 violation: NHorOH>5
17.	Luteolin 4'-O-glucoside	5319116	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O	No; 2 violations: NorO>10, NHorOH>5
18.	7-O-(4-Hydroxycinnamoyl) astragalin	131752827	C1=CC(=CC=C1/C=C/C(=O)OC2=CC(=C3C(=C2)OC(=C(C3=O)OC4C(C(C(C(O4)CO)O)O)O)C5=CC=C(C=C5)O)O)O	No; 3 violations: MW>500, NorO>10, NHorOH>5
19	Corchorifatty acid F	44559173	CC/C=C\CC(C(/C=C/C(CCCCCCCC(=O)O)O)O)O	Yes; 0 violation
20.	1D-1-Guanidino-3amino-1,3-dideoxyscyllo-inositol	5459885	[C@@H]1([C@@H]([C@H]([C@@H]([C@H]([C@@H]1O)O)O)N=C(N)N)O)N	Yes; 1 violation: NHorOH>5
21.	9,10-Dihydroxy-12,13epoxyoctadecanoate	11954063	CCCCCC1C(O1)CC(C(CCCCCCCC(=O)O)O)O	Yes; 0 violation
22.	Bruceoside A	441789	C[C@H]1[C@@H]2C[C@@H]3[C@@]45CO[C@@]([C@@H]4[C@H](C(=O)O3)OC(=O)C=C(C)C)([C@H]([C@@H]([C@@H]5[C@]2(C=C(C1=O)O[C@H]6[C@@H]([C@H]([C@@H]([C@H](O6)CO)O)O)O)C)O)O)C(=O)OC	No; 3 violations: MW>500, NorO>10, NHorOH>5
23.	Sambutoxin	54710553	CCC(C)CC(C)/C=C(\C)/[C@H]1[C@@H](CC[C@H](O1)C2=C(C(=CN(C2=O)C)C3=CC=C(C=C3)O)O)C	Yes; 0 violation
24.	LysoPE(0:0/18:0)	53480667	CCCCCCCCCCCCCCCCCC(=O)O[C@H](CO)COP(=O)(O)OCCN	Yes; 0 violation

25.	Linalyl caprylate	61435	CCCCCCCC(=O)OC(C)(CCC=C(C)C)C=C	Yes; 1 violation: MLOGP>4.15
26.	Castasterone	133534	C[C@@H]([C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC(=O)[C@@H]4[C@@]3(C[C@H]([C@H](C4)O)O)C)C)[C@H]([C@@H]([C@@H](C)C(C)C)O)O	Yes; 0 violation
27.	Notoginsenoside T2	131752528	C/C(=C\C(C1C(O1)(C)C)OC)/C2CCC3(C2C(CC4C3(CC(C5C4(CCC(C5(C)C)O)C)OC6C(C(C(C(O6)CO)O)O)O)C)O)C	No; 2 violations: MW>500, NHorOH>5
28.	[6]-Gingerdiol 3-acetate	131752857	CCCCCC(CC(CCC1=CC(=C(C=C1)O)OC)OC(=O)C)O	Yes; 0 violation
29.	Sarcostin	46173994	C[C@@H]([C@@]1(CC[C@]2([C@@]1([C@@H](C[C@H]3[C@]2(CC=C4[C@@]3(CC[C@@H](C4)O)C)O)O)C)O)O)O	Yes; 1 violation: NHorOH>5
30.	(3beta,5alpha,6beta,9alpha,22E,24R)-23Methylergosta-7,22diene-3,5,6,9-tetrol	131751468	CC(C)C(C)/C(=C/C(C)C1CCC2C1(CCC3(C2=CC(C4(C3(CCC(C4)O)C)O)O)O)C)/C	Yes; 0 violation
31.	Bryodulcosigenin	441813	C[C@H](CCC(C(C)(C)O)O)[C@H]1CC[C@@]2([C@@]1(CC(=O)[C@@]3([C@H]2CC=C4[C@H]3CC[C@@H](C4(C)C)O)C)C)C	Yes; 1 violation: MLOGP>4.15
32	Benzoylagmatine	439689	C1=CC=C(C=C1)C(=O)NCCCCN=C(N)N	Yes; 0 violation
33	Apovincamine	71204	CC[C@@]12CCCN3[C@@H]1C4=C(CC3)C5=CC=CC=C5N4C(=C2)C(=O)OC	Yes; 0 violation
34	(Z)-Narceine imide	5459241	CN(C)CCC1=CC2=C(C(=C1/C=C\3/C4=C(C(=C(C=C4)OC)OC)C(=O)N3)OC)OCO2	Yes; 0 violation
35	Vulgarin	94253	C[C@H]1[C@@H]2CC[C@@]3([C@@H]([C@H]2OC1=O)[C@](C=CC3=O)(C)O)C	Yes; 0 violation
36	O-Feruloylgalactarate	14104340	COC1=C(C=CC(=C1)/C=C/C(=O)O[C@H]([C@H]([C@H]([C@@H](C(=O)O)O)O)O)O)C(=O)O)O	No; 2 violations: NorO>10, NHorOH>5
37	Cis-zeatin-O-glucoside	5280589	C/C(=C/CNC1=NC=NC2=C1NC=N2)/CO[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O	No; 2 violations: NorO>10, NHorOH>5
38	5'-Dehydroadenosine	443234	C1=NC(=C2C(=N1)N(C=N2)[C@H]3[C@@H]([C@@H]([C@H](O3)C=O)O)O)N	Yes; 0 violation

39	Angustine	441983	C=CC1=CN=CC2=C1C=C3C4=C(CCN3C2=O)C5=CC=CC=C5N4	Yes; 0 violation
40	Knipholone	442753	CC1=CC(=C2C(=C1C3=C(C(=C(C=C3O)OC)C(=O)C)O)C(=O)C4=C(C2=O)C(=CC=C4)O)O	Yes; 0 violation
41	N-Methyl-1H-indole-3 propanamide	151412	CC(=O)N[C@@H](CC1=CNC2=CC=CC=C21)C(=O)NC	Yes; 0 violation
42	(S)-3-Octanol 036.	22269604	CCCCCC(CC)OC1C(C(C(C(O1)CO)O)O)O	Yes; 0 violation
43	(1S,2R,4R,8S)-pMenthane 2,8,9-triol 2glucoside	73075552	CC1CCC(CC1OC2C(C(C(C(O2)CO)O)O)O)O)C(C)(CO)O	Yes; 1 violation: NHorOH>5
44	Ganoderic acid H	73657194	CC(CC(=O)CC(C)C(=O)O)C1CC(=O)C2(C1(C(C(=O)C3=C2C(=O)CC4C3(CCC(C4(C)C)O)C)OC(=O)C)C)C	Yes; 1 violation: MW>500
45	Dukunolide E	131751857	CC1(C2CC(=O)OC2(C3(C4=C5C(CCC6C5(O6)CC3(C1=O)O)(C(OC4=O)C7=COC=C7)C)O)C)C	Yes; 0 violation
46	Camalexin	636970	C1=CC=C2C(=C1)C(=CN2)C3=NC=CS3	Yes; 0 violation
47	Antimycin A1	12550	CCCCCCC1C(C(OC(=O)C(C(OC1=O)C)NC(=O)C2=C(C(=CC=C2)NC=O)O)C)OC(=O)CC(C)C	No; 2 violations: MW>500, NorO>10
48	Phenethylamine glucuronide	191195	C1=CC=C(C=C1)CCN[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)C(=O)O)O)O)O	Yes; 0 violation
49	Prolyl-Histidine	9856353	C1C[C@H](NC1)C(=O)N[C@@H](CC2=CN=CN2)C(=O)O	Yes; 0 violation
50	Monocrotaline	9415	C[C@H]1C(=O)O[C@@H]2CCN3[C@@H]2C(=CC3)COC(=O)[C@]([C@]1(C)O)(C)O	Yes; 0 violation
51	Europine	5462451	C[C@@H]([C@](C(=O)OCC1=CCN2[C@H]1[C@H](CC2)O)(C(C)(C)O)O)OC	Yes; 0 violation
52	(S)-alpha-Terpinyl glucoside	13325862	CC1=CCC(CC1)C(C)(C)OC2C(C(C(C(O2)CO)O)O)O	Yes; 0 violation
53	Vellosimine	11266327	C/C=C\1/CN2[C@H]3C[C@@H]1[C@H]([C@@H]2CC4=C3NC5=CC=CC=C45)C=O	Yes; 0 violation
54	L-Citronellol glucoside	14239337	CC(CCC=C(C)C)CCOC1C(C(C(C(O1)CO)O)O)O	Yes; 0 violation

Table 3: Binding Affinities (kcal/mol) of Selected Compounds Towards D2 (6VMS), -GABA (6X3W), and GluN1/GluN2A NMDA receptor (7EOT).

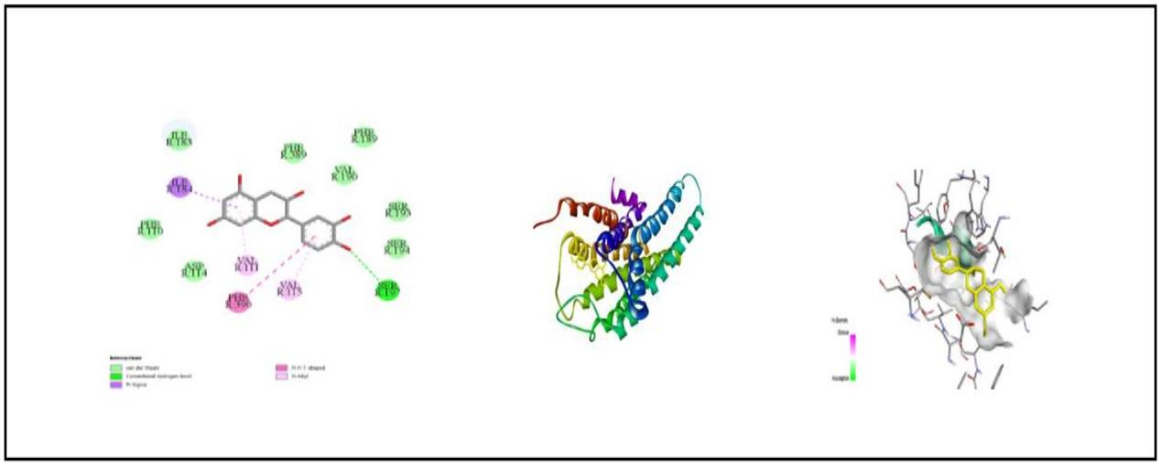
S.NO	COMPOUND NAME	D2 (6VMS)	GABA (6X3W)	NMDA (7EOT)
1	(-)-Epicatechin	-8.1	-6.6	-7.7
2	[6]-Gingerdiol 3-acetate	-7.0	-5.8	-6.3
3	9,10-Dihydroxy-12,13epoxyoctadecanoate	-6.2	-5.3	-5.9
4	Benzoic Acid	-5.5	-5.3	-5.3
5	Byakangelicin	-7.8	-6.0	-6.8
6	Castasterone	-9.2	-7.2	-6.8
7	Corchorifatty acid F	-6.3	-4.9	-5.9
8	Diethyl succinate	-5.2	-4.2	-4.6
9	Enol-phenylpyruvate	-6.3	-5.4	-5.3
10	Ferulic acid	-6.5	-5.6	-6.2
11	p-Coumaric acid	-6.4	-5.6	-5.8
12	Sambutoxin	-9.3	-6.0	-5.8
13	Benzoylagmatine	-7.1	-5.8	-6.3
14	Apovincamine	-8.2	-6.4	-6.6
15	(Z)-Narceine imide	-8.5	-5.8	-7.1
16	Vulgarin	-8.5	-6.2	-7.5
17	5'-Dehydroadenosine	-7.0	-6.1	-6.5
18	Angustine	-9.9	-7.0	-7.3
19	Knipholone	-9.2	-6.8	-7.8
20	N-Methyl-1H-indole-3 propanamide	-7.5	-6.4	-6.7
21	Camalexin	-6.7	-5.6	-5.8
22	Phenethylamine glucuronide	-7.6	-6.6	-6.9
23	Prolyl-Histidine	-6.1	-5.5	-6.1
24	Monocrotaline	-7.7	-6.8	-6.3
25	Europine	-6.2	-5.2	-5.6
26	Vellosimine	-8.6	-6.5	-7.6
	STANDARDS			
1	phenobarbital	-6.7		
2	Diazepam		-6.4	
3	Galantamine			-6.7

Table 4: Summary of ADME and Drug-Likeness Prediction.

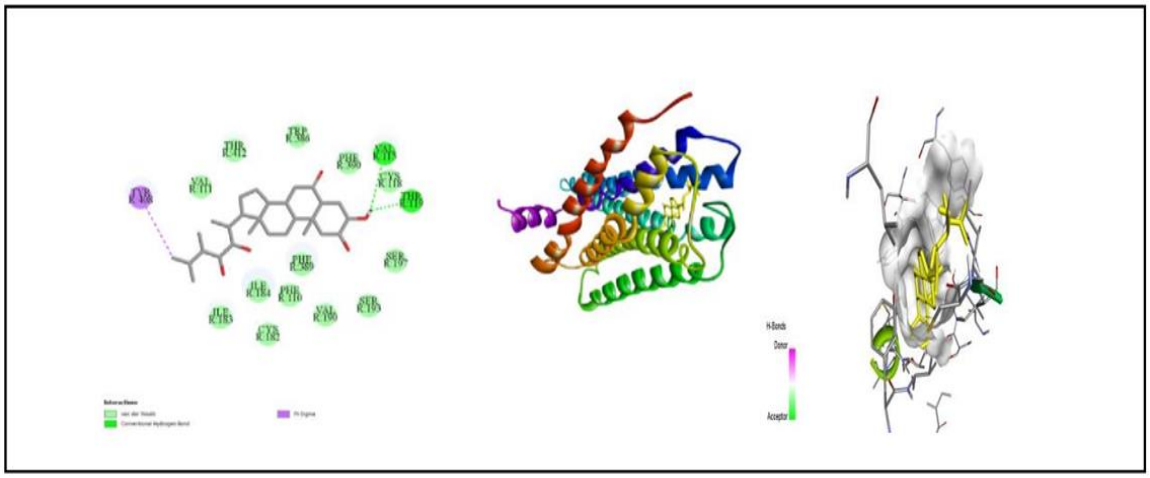
S.NO	Compound	Docking score	Amino acid Interaction	Conventional Hydrogen Interaction
1.	Sambutoxin	-9.3	ASPA:114, VALA:111, VALA:115, PHEA:189, ILEA:184, TYRA:408, SERA:193, SERA:194, PHEA:389, HISA:393, PROA:187, ASNA:186, ALAA:185, ILE:397, ASNA:396, VALA:190, PHEA:390, SERA:197.	ASP:114

2.	(–)-Epicatechin	–8.1	ILER: 184, PHE R:390, VALR: 111, VAL R:115, PHE R:110, ASP R:114, PHE R:189, PHER: 389, VAL R:190, SER R:193, SERR: 194, SERR: 197	SERA: 197
3.	Castasterone	-9.2	THR 110, CYS 118, TYR 408, VAL 111, VAL 115, TRP 386, THR 412, PHE 390, PHE 389, PHE 110, ILE 183, ILE 184, CYS 182, VAL 190, SER 193, SER 197	THR 110, CYS 118
4.	(Z)-Narceine imide	−8.5	VAL A:91, PHE A:110, VAL A:111, THR A:119, CYS A:118, SER A:193, SER A:197, SER A:194, VAL A:190, VAL A:115, PHE A:38 HIS A:393, TYR A:408, THR A:412, ILE A:184, TRP A:386, PHE A:390, ASP A:114	THRA:119, THRA:412
5.	Angustine	-9.9	ASP A:114, THR A:412, ILE A:183, ILE A:184, VAL A:115, TRP A:386, CYS	ASP A:114 ILE A:184.
			A:118, THR A:119, SER A:197, SER A:194, SER A:193, PHE A:389, PHE A:390, VAL A:190.	
6.	Knipholone	-9.2	PHE R:389, TYR R:408, ILE R:184, ILE R:183, VAL R:190, PRO R:187, ILE R:397, PRO R:405, ILE R:403, HIS R:393, ASN R:396, ASN R:186, ALA R:185, THR R:412	ASN R:186, ASN R:396 , ILER:403, HISR:393

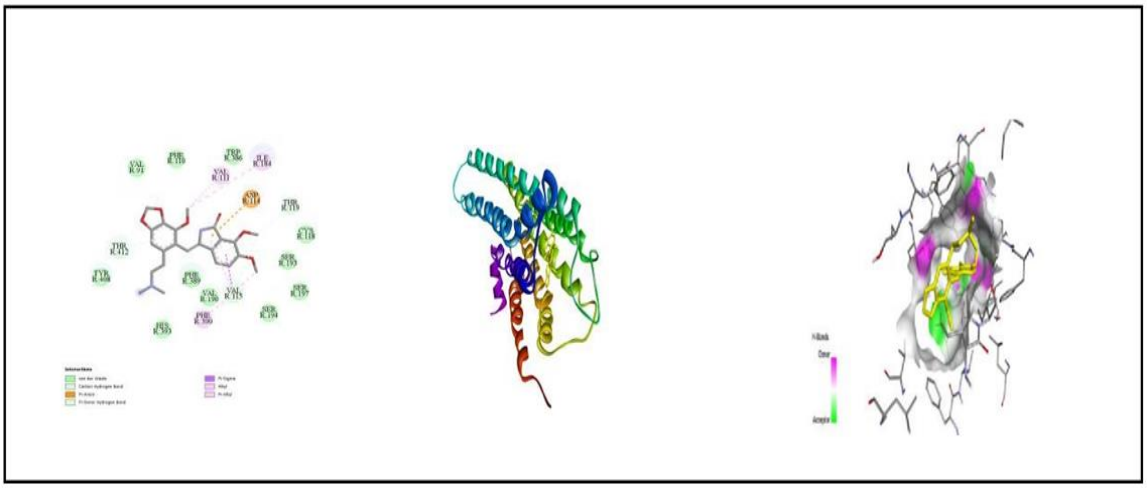
Among the six tested compounds, Angustine exhibited the strongest binding affinity with a docking score of –9.9, followed by Sambutoxin (–9.3), Castasterone (–9.2), and Knipholone(–9.2). These top-performing ligands formed multiple hydrophobic and aromatic interactions with key residues such as PHE 389/390 (Phenylalanine), ILE 184 (Isoleucin), VAL 115 (Valine), and TRP 386 (Tryptophan), indicating stable binding within the active site. Hydrogen bonding varied among the compounds, with Sambutoxin interacting through ASP114 (Aspartic acid), (–)-Epicatechin via SER197 (Serine), Castasterone forming hydrogen bonds with THR110 (Threonine) and CYS118 (Cysteine), (Z)-Narceine imide interacting with THR119 and THR412, Angustine forming bonds with ASP114 and ILE184, and Knipholone engaging ASN186 (Asparagine), ASN396, ILE403, and HIS393 (Histidine) Overall, Angustine, Sambutoxin, Castasterone, and Knipholone demonstrated the most favorable binding profiles due to their strong docking scores and extensive interactions with critical residues.



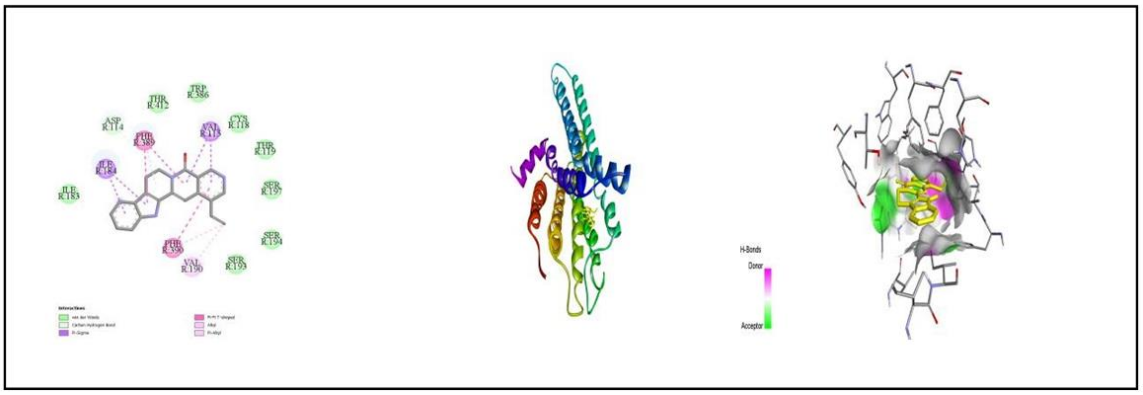
Molecular docking of (-)-Epicatechin with d2 (PDB: 6vms)



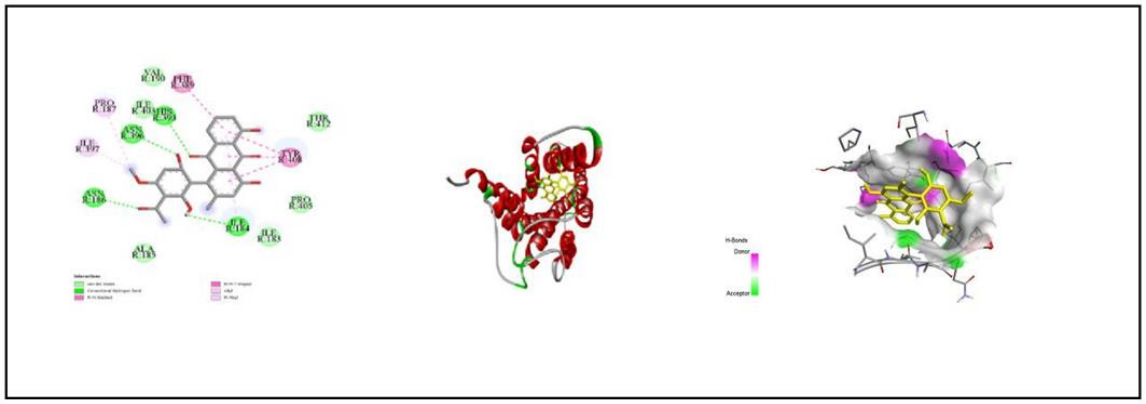
Molecular docking of Castasterone with d2 (PDB: 6vms)



Molecular docking of (Z)-Narceine imide with d2 (PDB: 6vms).



Molecular dockingof Angustine with d2 (PDB: 6vms)



Molecular docking Knipholone with d2 (PDB: 6vms)

CONCLUSION

This research scientifically validates the traditional claim of *Malvastrum coromandelianum* as a therapeutic agent for neurological disorders. Through HR-LCMS analysis, we successfully profiled 112 phytoconstituents, identifying potential bioactive leads including Angustine, Sambutoxin, and Catasterone. In Silico docking studies revealed that these natural compounds exhibit superior binding affinities towards critical epilepsy targets (D2, GABA-A, and NMDA receptors) compared to standard synthetic drugs like Phenobarbital and Diazepam. The study concludes that the stem extract of *Malvastrum coromandelianum* acts as a reservoir of multi-target anticonvulsant agent with favourable drug-likeness properties. These findings provide a strong rationale for the isolation of these specific metabolites and subsequent in vivo preclinical trials to develop novel, plant-based pharmacotherapies for epilepsy management.

ACKNOWLEDGMENTS

The autors are grateful to Shree Venkateshwara College Of Pharmacy for providing the

facilities to accomplish this work.

REFERENCES

1. Potnis, V.V., Albhar, K.G., Nanaware, P.A., & Pote, V.S. A review on epilepsy and its management. *Journal of Drug Delivery and Therapy,* 2020; *10*(3): 273-279.
2. Sumadewi, K.T., Harkitasari, S., & Tjandra, D.C. Biomolecular mechanisms of epileptic seizures and epilepsy: A review. *Acta Epileptologica,* 2023; *5*(1): 28.
3. Sivarajan, V.V., & Pradeep, A.K. *Malvaceae of Southern Peninsular India: A Taxonomic Monograph,* 1996; 210-230. India: Daya Publishing House.
4. Wirat, C. Medicinal plants in Asia and the Pacific for parasitic infections: Botany, ethnopharmacology, molecular basis, and future prospects. *Academic Press,* 2020; 267-274.
5. Saxena, S., Rawat, D.S., & Rao, P.B. *Malvastrum coromandelianum* (L.) Gracke: An invasive weed with multiple ethnopharmacological properties. *International Journal of Pharmacognosy and Phytochemical Research,* 2020; *12:* 16-22.
6. Devi, S., & Kumar, V. Comprehensive structural analysis of cis-and trans-tiliroside and quercetin from *Malvastrum coromandelianum* and their antioxidant activities. *Arabian Journal of Chemistry,* 2020; *13*(1): 1720-1730.
7. Torres-Rodriguenz, A., Darvishzadeh, R., Skidmore, A.K., Franzel-Lutein, E., Knaken, B., & Schuur, B. High-throughput Soxhlet extraction method applied for analysis of lignocelluloses and non-structural substances. *MethodsX,* 2024; *12:* 102644.
8. Rochat, B. From targeted quantification to untargeted metabolomics: Why LC-high-resolution-MS will become a key instrument in clinical labs. *TrAC Trends in Analytical Chemistry,* 2016; *84:* 151-164.
9. Sorapalli, S.K., Kagitha, K.B., Doddi, N.S., Alla, M., Nagidi, M., & Gope, E.R. A review of liquid chromatography-mass spectrometry and its applications in chemical analysis. *Journal of Pharma Insights and Research,* 2024; *2*(6): 25-32.
10. Thijs, R.D., Surges, R., O'Brien, T.J., & Sander, J.W. Epilepsy in adults. *The Lancet,* 2020; *396*(10252): 689-701.
11. Newman, D.J., & Cragg, G.M. Natural products as sources of new drugs over the nearly four decades from 1981 to 2019. *Journal of Natural Products,* 2020; *83*(3): 770-803.
12. Devi, S., & Kumar, V. Structural elucidation of flavonoids from *Malvastrum coromandelianum* and their antioxidant activities. *Arabian Journal of Chemistry,* 2020; *13*(1): 1720-1730.

13. Chemat, F., Abert-Vian, M., Fabiano-Tixier, A.S., Strube, J., & Vorobiev, E. Green extraction of natural products. *Ultrasonics Sonochemistry*, 2021; *70:* 105436.
14. Sorapalli, S.K., Kagitha, K.B., Doddi, N.S., et al. A review of liquid chromatography-mass spectrometry and its applications. *Journal of Pharma Insights and Research*, 2024; *2*(6): 25-32.
15. Myers, O.D., Sumner, S.J., Li, S., Barnes, S., & Du, X. One-step forward: Advances in LC-MS-based metabolomics. *Analytical Chemistry*, 2020; *92*(1): 110-120.
16. Huang, S.Y., & Zou, X. Advances and challenges in ensemble docking. *Proteins: Structure, Function, and Bioinformatics*, 2022; *90*(1): 91-103.
17. Dillon, C. A comprehensive review of plant-based therapies for epilepsy: Efficacy, mechanisms, and bioavailability. *Neuropharmacology*, 2021; *180:* 108308.
18. Kumar, V., & Devi, S. Chemical and pharmacological aspects of *Malvastrum coromandelianum*: Focus on potential neuroprotective properties. *Journal of Ethnopharmacology*, 2021; *267:* 113484.
19. Xu, J., & Zhou, Y. Phytochemicals in epilepsy therapy: Their mechanism of action and pharmacological potentials. *Pharmacological Research*, 2022; *182:* 106357.
20. Yasir M, Choe J, Han JH, Chun W. Molecular Basis of GABA Aminotransferase Inhibition in Epilepsy: Structure, Mechanisms, and Drug Development. Current Issues in Molecular Biology, Dec. 11, 2025; 47(12): 1032.
21. Lolam V, Roy A. Developmental mechanisms underlying pediatric epilepsy. Frontiers in Neurology, Jun. 3, 2025; 16: 1586947.