

Supplementary material

Molecular, and Therapeutic Insights of Alpha-Lipoic Acid as a Potential Molecule for Disease Prevention

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#Amit Kumar Tripathi and Anup Kumar Ray have equal contribution.

Table S1 List of ongoing clinical trials on ALA

S. No.	Condition & (Number of Participants)	Phase 1, 2, 3 or 4 & (Status)	Dose, Duration	Principal Investigator affiliation	Duration (months)	Clinical trial registry number
1	Adolescent Migraine (60)	4 (recruiting)	300 mg once daily for 12 weeks	Dr. Monalisa Jena, M.D., All India Institute of Medical Sciences, Bhubaneswar	18	NCT04064814
2	Non-Alcoholic Fatty Liver Disease (120)	4 (Not yet recruiting)	600 mg twice daily for 12 weeks	Dr. Monalisa Jena, M.D., All India Institute of Medical Sciences, Bhubaneswar	18	NCT04475276
3	Diabetic Peripheral Neuropathy (150)	4 (Not yet recruiting)	480 mg once daily for 12 weeks.	Yuhan Corporation	18	NCT04846673
4	Ischemic Stroke (120)	3 (recruiting)	600 mg/day for 12 weeks	Kangho Choi, MD, PhD Chonnam National University Hospital	41	NCT04041167
5	Head and neck squamous cell carcinoma (18)	1 (recruiting)	1200 mg/day & 1800 mg/day for 2 weeks	Jessica Mcdermott, MD, University of Colorado, Denver	28	NCT04042935

6	Multiple Sclerosis (118)	2 (recruiting)	1200 mg daily for 104 weeks	Rebecca I. Spain, MD MSPH VA Portland Health Care System, Portland, OR	62	NCT03161028
7	Cystinuria (50)	2 (recruiting)	1200 mg daily for 156 weeks	Thomas Chi, MD University of California, San Francisco	78	NCT02910531
8	Ischemic Heart Failure (300)	4 (Not yet recruiting)	600 mg/day for 52 weeks	Shanghai Zhongshan Hospital	48	NCT03491969
9	Amyotrophic Lateral Sclerosis (150)	NA (recruiting)	600 mg/day for 4 weeks	Zhi-Ying Wu, MD&PhD, Second Affiliated Hospital, School of Medicine, Zhejiang University	25	NCT04518540
10	Diabetic Cardio-myopathies (100)	NA (recruiting)	600 mg/day for 12 weeks	Emile FERRARI, PUPH, Centre HospitalierUniversita ire de Nice	24	NCT04141475
11	Cervical Shortening Preterm Birth (54)	NA (Not yet recruiting)	-	Fabio Facchinetti, MD, University of Modena and Reggio Emilia	14	NCT03952533

12	Obstructive Sleep Apnea (106)	1 (Not yet recruiting)	600 mg/day for 6 weeks	Glen Foster, Associate Professor, University of British Columbia	51	NCT04021550
13	Cardiovascular Diseases (60)	NA (recruiting)	300 mg -	Song-Young Park, Principal Investigator, University of Nebraska	13	NCT03629613
14	Sterility Infertility (100)	4 (recruiting)	-	Johnny Awwad, Professor of Obstetrics and Gynecology, American University of Beirut Medical Center	52	NCT03177122
15	Cystic Fibrosis (80)	NA (recruiting)	600 mg/day -	Ryan Harris, Principal Investigator, Augusta University	80	NCT02690064
16	Hypertension (72)	NA (recruiting)	-	Joel Douglas Trinity, PhD, VA Salt Lake City Health Care System, Salt Lake City, UT	95	NCT02034422

Table S2 Mulliken Charges of S and R Enantiomers

Sl. No.	Atoms	Mulliken Charges	
		SLA	RLA
1.	S1	0.05462	-0.04592
2.	S2	0.00477	0.02971
3.	O3	-0.40623	-0.40486
4.	O4	-0.43985	-0.44299
5.	C5	0.09472	0.38019
6.	C6	-0.41138	-0.78243
7.	C7	-0.35334	-0.40062
8.	C8	-0.17923	-0.02894
9.	C9	-0.4496	-0.47207
10.	C10	-0.57508	-0.47107
11.	C11	-0.6146	-0.63832
12.	C12	0.58247	0.59196
13.	H13	0.22042	0.24489
14.	H14	0.1483	0.15042
15.	H15	0.1695	0.16702
16.	H16	0.15799	0.15592
17.	H17	0.17501	0.17946
18.	H18	0.15059	0.12795
19.	H19	0.1443	0.13428
20.	H20	0.15434	0.15723
21.	H21	0.16574	0.16575
22.	H22	0.20778	0.20144
23.	H23	0.20822	0.2078
24.	H24	0.20157	0.1987
25.	H25	0.20183	0.20786
26.	H26	0.38713	0.38663