Supplementary Information (SI)

SPECTROSCOPIC (FTIR, UV-VIS AND NMR), THEORETICAL INVESTIGATION AND MOLECULAR DOCKING OF SOME SUBSTITUTED 1,8-DIOXODECAHYDROACRIDINE DERIVATIVES

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Keywords: 1, 8-dioxodecahydroacridine derivatives; FT-IR; UV-Vis; NMR; Global Reactivity Descriptors; Molecular docking

RUNNING TITLE: SPECTROSCOPIC AND THEORETICAL INVESTIGATION OF SUBSTITUTED 1,8-DIOXODECAHYDROACRIDINE DERIVATIVES

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Fig.S1: Experimental NMR plot of MTDOSA

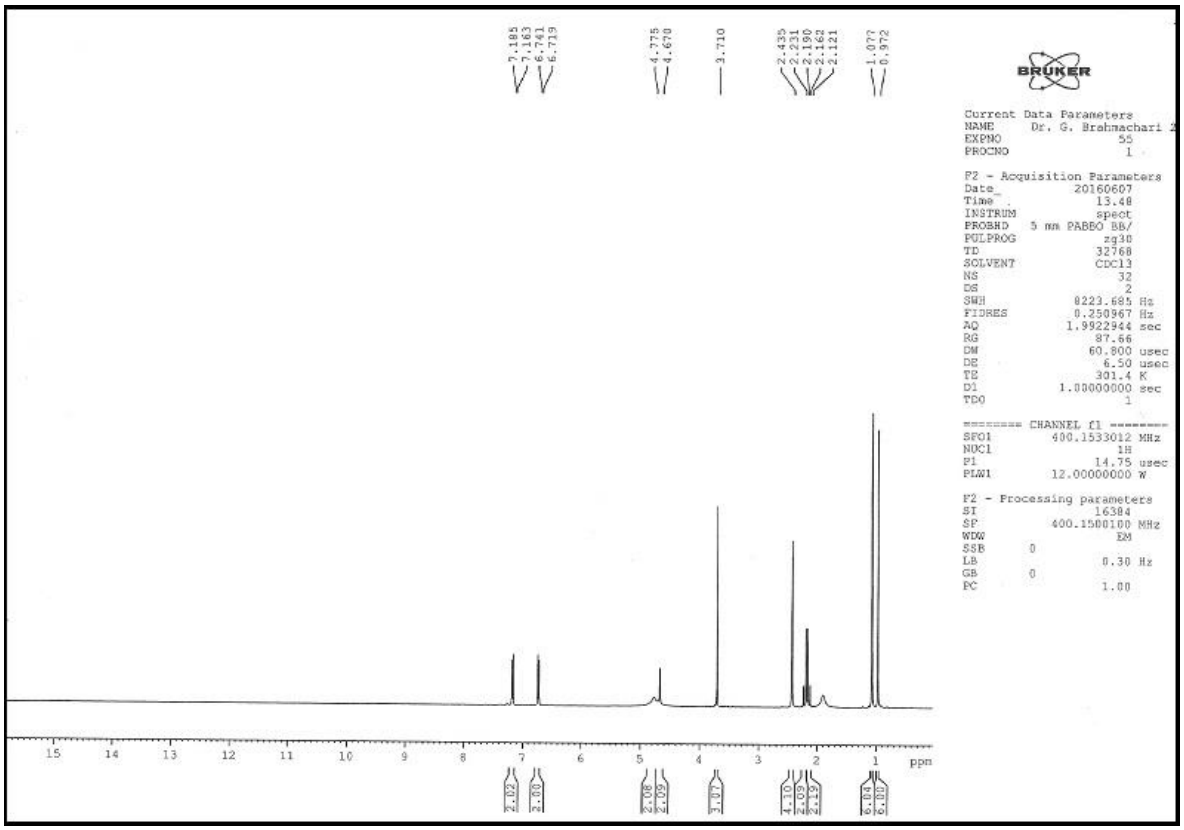

Fig.S1(a)

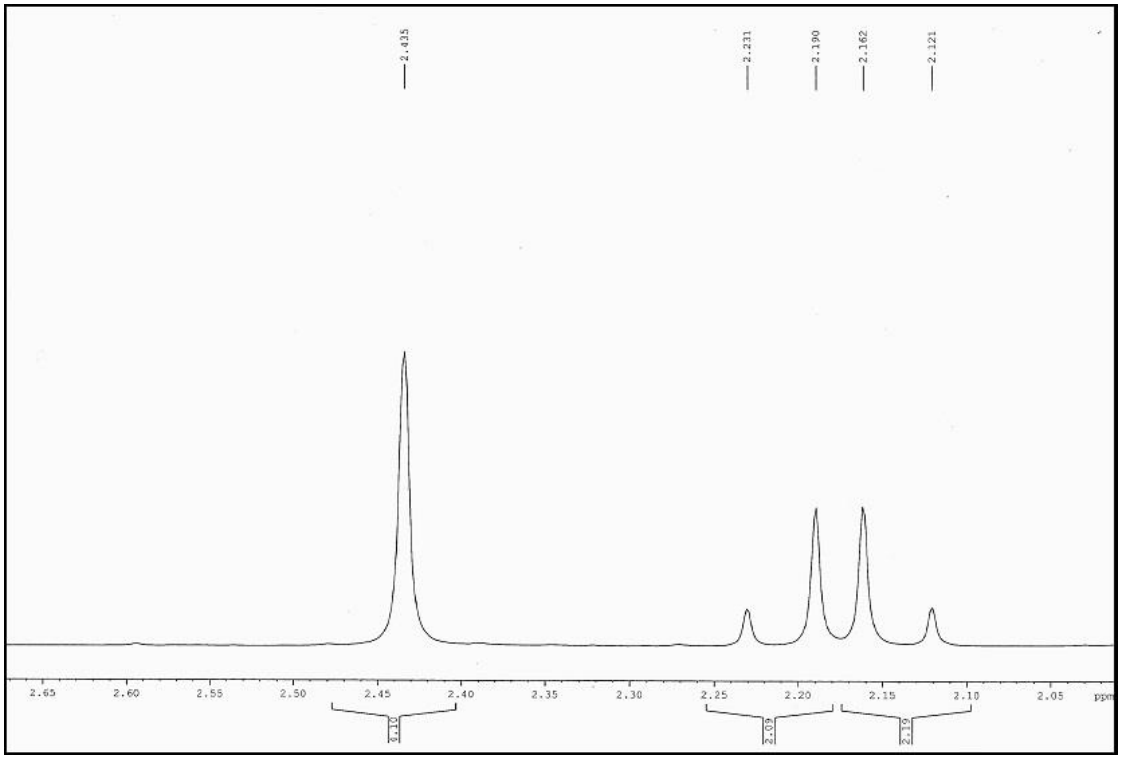

Fig. S1(b) (extended scale-I)

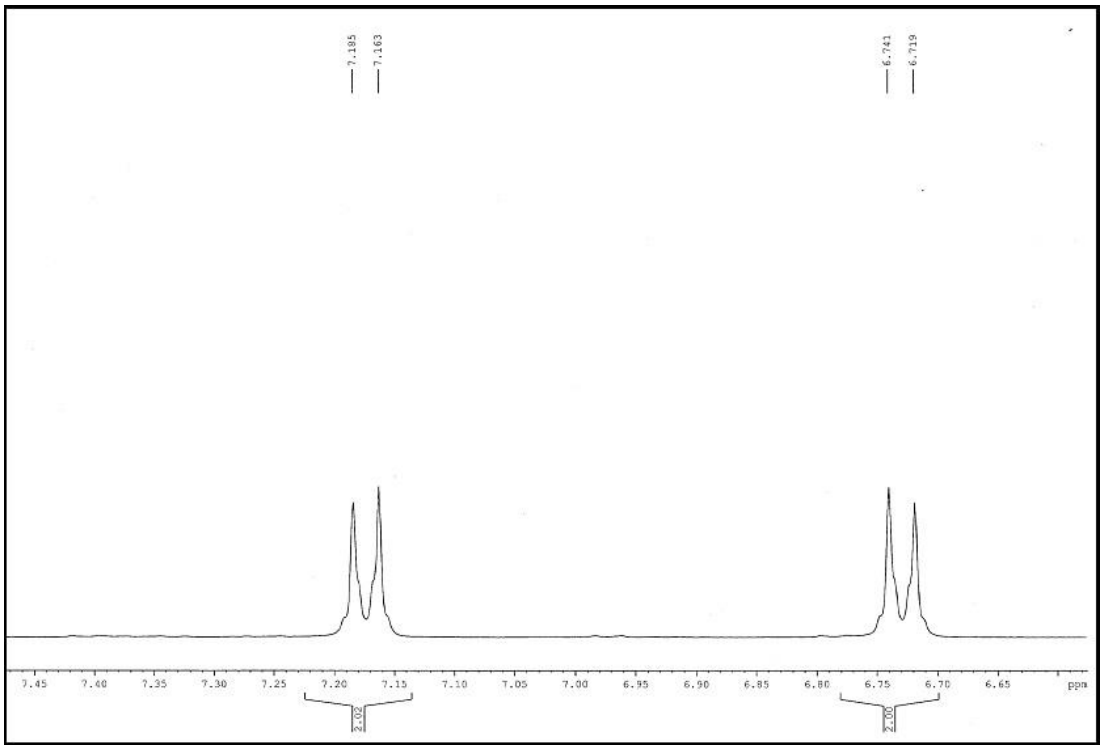

Fig. S1(c) (extended scale-II)

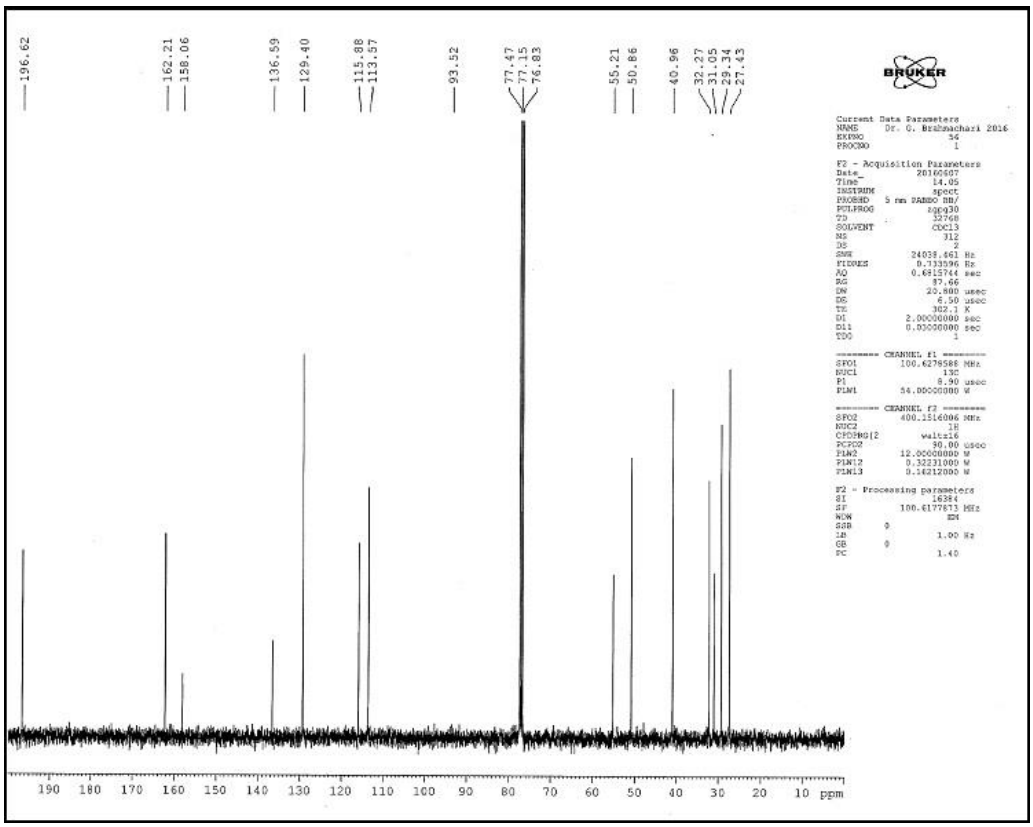

Fig. S1 (d) ^{13}C NMR MTDOSA

Fig.S2: Experimental NMR plot of NTDOSA

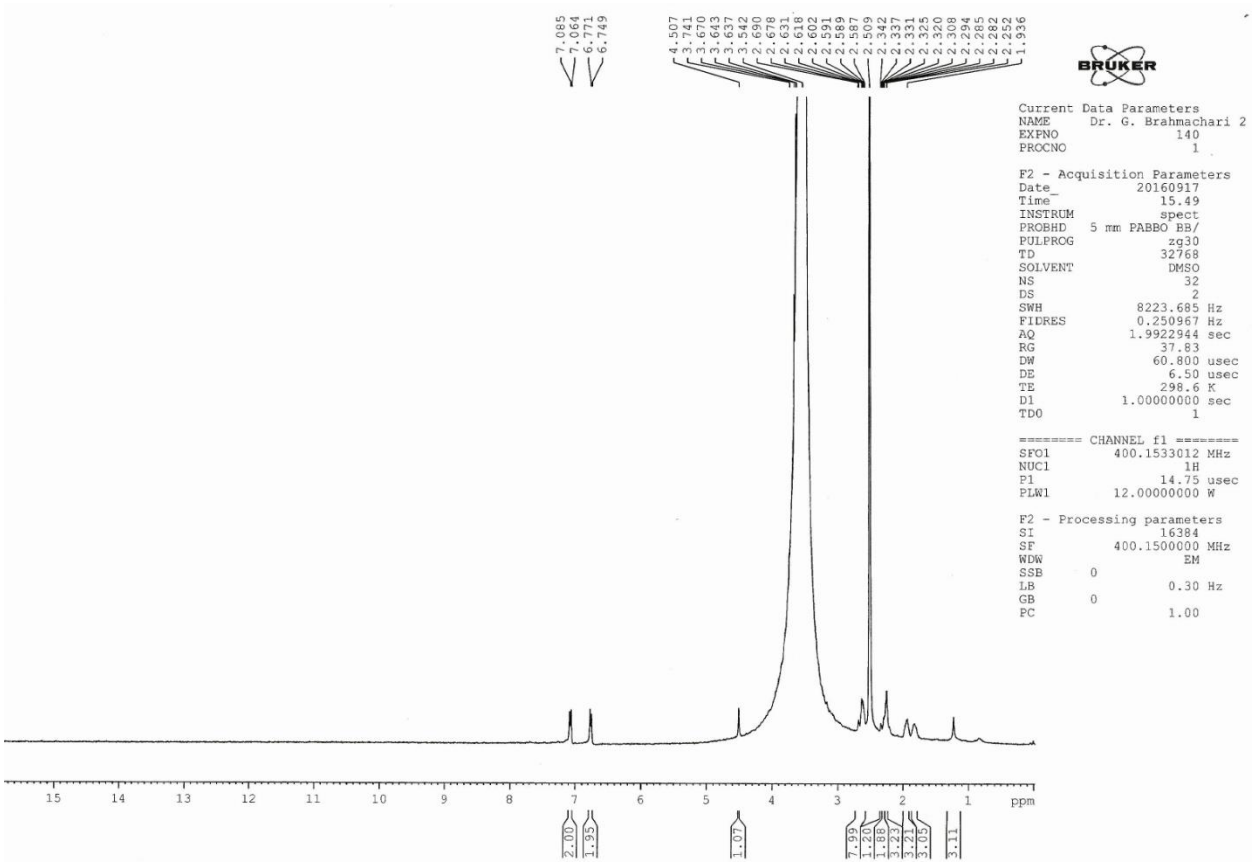

Fig. S2(a)

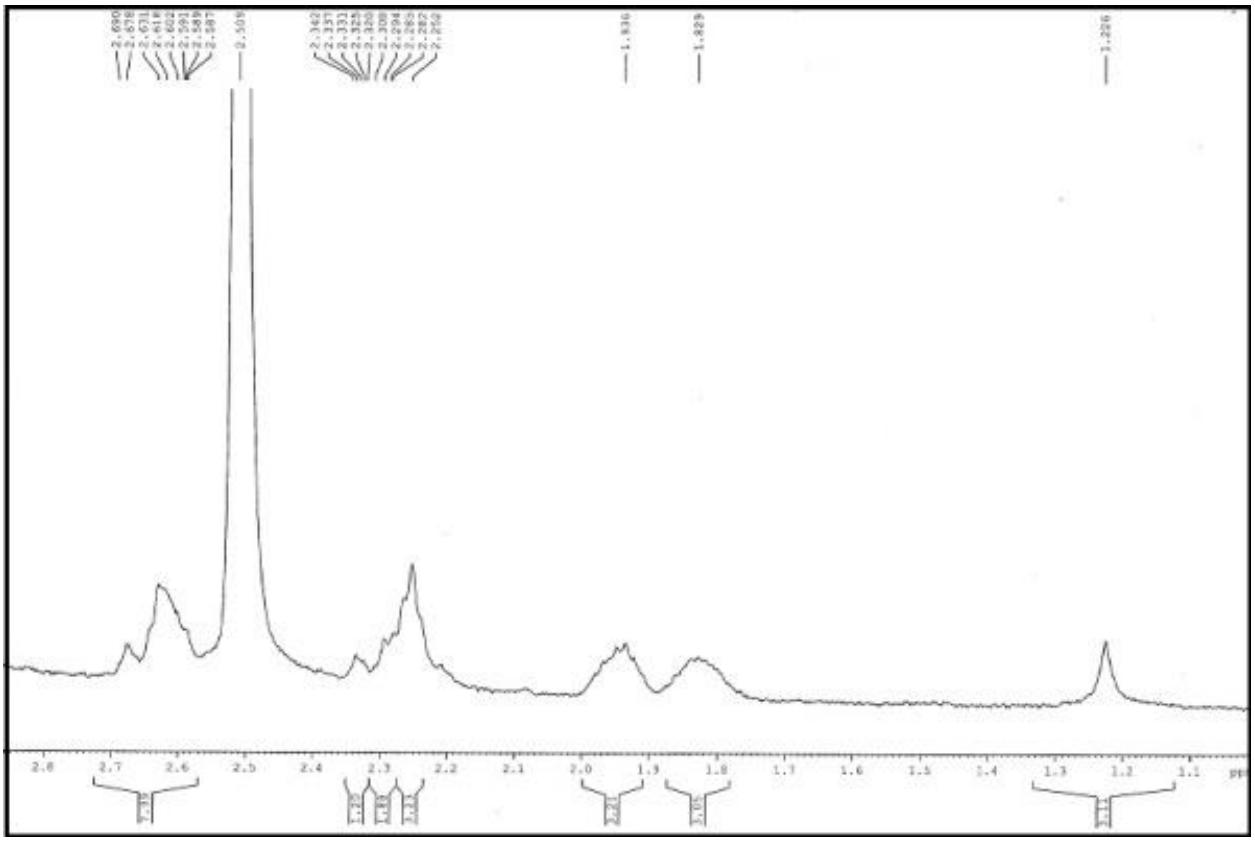

Fig. S2(b) (extended scale-I)

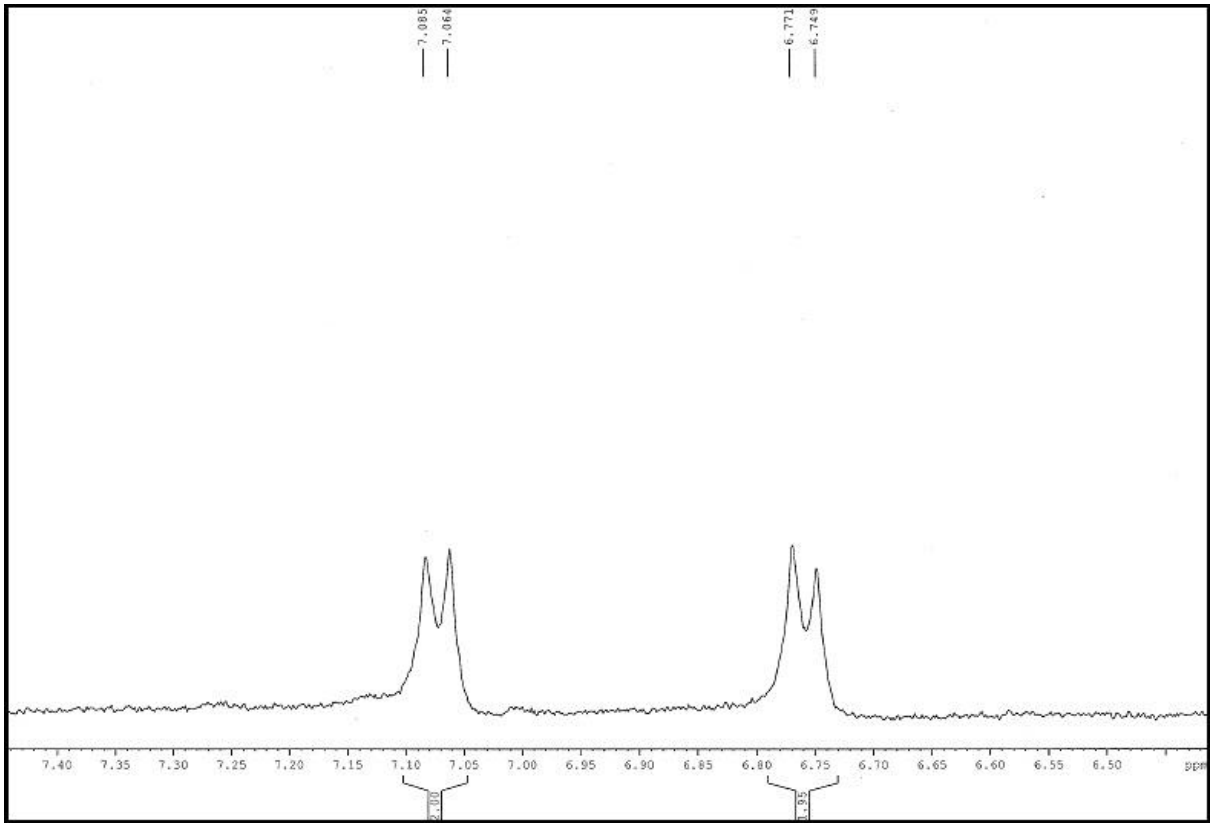

Fig. S2(c) (extended scale-II)

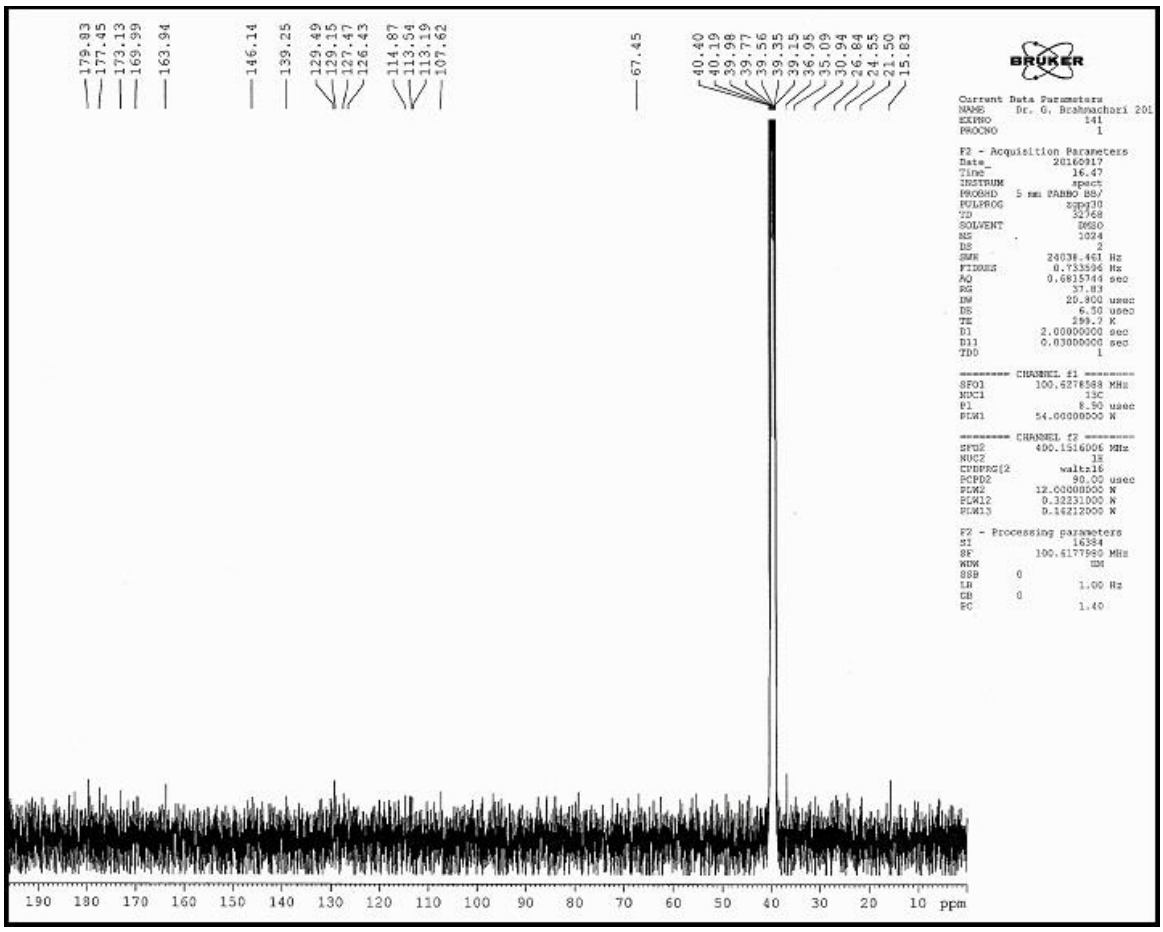

Fig. S2(d) ^{13}C NMR NTDOSA

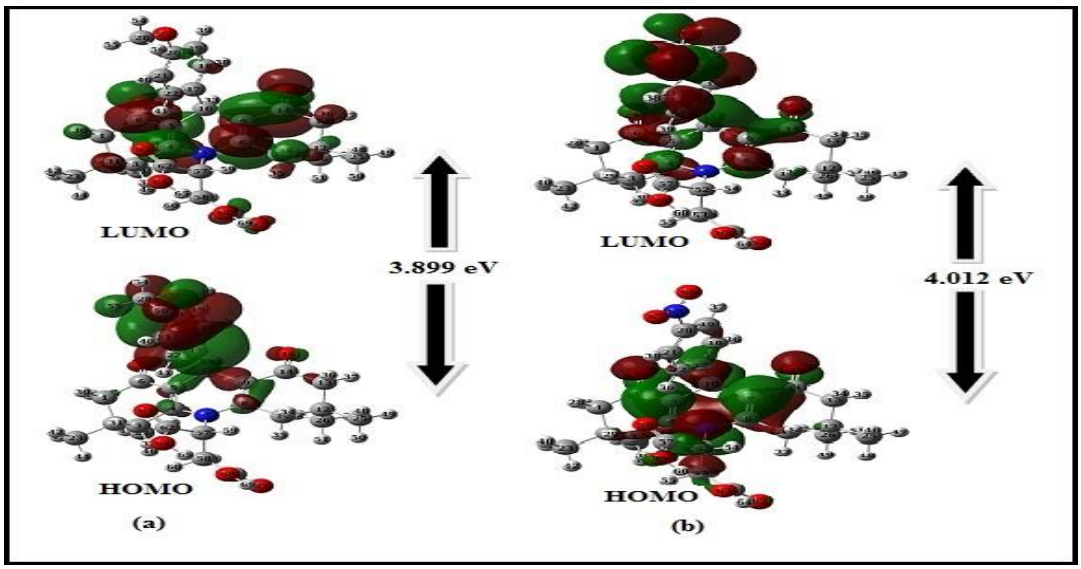

Fig.S3: HOMO, LUMO plots of (a) MTDOSA (b) NTDOSA molecules

Table S-I: Optimized geometric parameter for MTDOSA.

Parameter	DFT/B3LYP6311++G(d,p)	Parameter	DFT/B3LYP6311++G(d, p)
Bond length, *Å*		C58-C66-O68	111.28
C1-C2	1.537	O67-C66-O68	121.96
C1-C6	1.518	C66-O68-H69	109.02
C1-H29	1.093	Dihedral Angle (in degree)	
C1-H30	1.098	C6-C1-C2-C3	53.25
C2-C3	1.546	C6-C1-C2-C23	171.72

C2-H23	1.538	C6-C1-C2-C24	-67.97
C2-H24	1.541	H29-C1-C2-C3	175.71
C3-C4	1.515	H29-C1-C2-C23	-65.82
C3-H31	1.096	H29-C1-C2-C24	54.49
C3-H32	1.090	H30-C1-C2-C3	-65.83
C4-C5	1.355	H30-C1-C2-C23	52.64
C4-N7	1.416	H30-C1-C2-C24	172.94
C5-C6	1.476	C2-C1-C6-C5	-33.75
C5-C10	1.511	C2-C1-C6-O15	147.79
C6-O15	1.220	H29-C1-C6-C5	-158.30
N7-C8	1.415	H29-C1-C6-O15	23.24
N7-C57	1.461	H30-C1-C6-C5	86.87
C8-C9	1.354	H30-C1-C6-O15	-91.58
C8-C11	1.516	C1-C2-C3-C4	-59.60
C9-C10	1.515	C1-C2-C3-H31	71.40
C9-C14	1.475	C1-C2-C3-H32	-173.19
C10-C17	1.534	C23-C2-C3-C4	-168.84
C10-H33	1.093	C23-C2-C3-H31	-47.84
C11-C12	1.547	C23-C2-C3-H32	67.57
C11-H34	1.099	C24-C2-C3-C4	71.36
C11-H35	1.093	C24-C2-C3-H31	-167.63
C12-C13	1.536	C24-C2-C3-H32	-52.22
C12-C25	1.537	C1-C2-C23-H42	-58.56
C12-C26	1.541	C1-C2-C23-H43	61.42
C13-C14	1.519	C1-C2-C23-H44	-179.06
C13-H36	1.098	C3-C2-C23-H42	59.32
C13-H37	1.092	C3-C2-C23-H43	179.31
C14-O16	1.221	C3-C2-C23-H44	-61.17
C17-C18	1.402	C24-C2-C23-H42	-179.73
C17-C22	1.393	C24-C2-C23-H43	-59.74

C18-C19	1.386	C24-C2-C23-H44	59.77
C18-H38	1.083	C1-C2-C24-H45	59.66
C19-C20	1.399	C1-C2-C24-H46	-179.43
C19-H39	1.084	C1-C2-C24-H47	-60.34
C20-C21	1.395	C3-C2-C24-H45	-59.76
C20-O27	1.369	C3-C2-C24-H46	61.14
C21-C22	1.398	C3-C2-C24-H47	-179.77
C21-H40	1.082	C23-C2-C24-H45	-179.43
C22-H41	1.083	C23-C2-C24-H46	-58.53
C23-H42	1.093	C23-C2-C24-H47	60.56
C23-H43	1.094	C2-C3-C4-C5	26.53
C23-H44	1.095	C2-C3-C4-N7	-151.00
C24-H45	1.092	H31-C3-C4-C5	-94.64
C24-H46	1.095	H31-C3-C4-N7	87.82
C24-H47	1.094	H32-C3-C4-C5	148.43
C25-H48	1.094	H32-C3-C4-N7	-29.09
C25-H49	1.094	C3-C4-C5-C6	-3.83
C25-H50	1.094	C3-C4-C5-C10	176.63
C26-H51	1.094	N7-C4-C5-C6	173.66
C26-H52	1.092	N7-C4-C5-C10	-5.87
C26-H53	1.093	C3-C4-CN7-C8	159.64
O27-C28	1.418	C3-C4-N7-C57	-23.90
C28-H54	1.089	C5-C4-N7-C8	-17.94
C28-H55	1.095	C3-C4-N7-C57	158.50
C28-H56	1.096	C4-C5-C6-C1	7.42
C57-C58	1.576	C4-C5-C6-O15	-174.13
C57-H59	1.089	C10-C5-C6-C1	-173.01
C57-C62	1.551	C10-C5-C6-O15	4.43
C58-H60	1.093	C4-C5-C10-C9	26.43
C58-H61	1.087	C4-C5-C10-C17	-99.03

C58-C66	1.511	C4-C5-C10-H33	143.46
C62-O63	1.197	C6-C5-C10-C9	-153.12
C62-O64	1.346	C6-C5-C10-C17	81.41
O64-H65	0.973	C6-C5-C10-H33	-36.08
C66-O67	1.198	C4-N7-C8-C9	17.88
C66-O68	1.372	C4-N7-C8-C11	-159.18
O68-H69	0.97	C57-N7-C8-C9	-158.71
Bond Angle (in degree)		C57-N7-C8-C11	24.21
C2-C1-C6	113.48	C4-N7-C57-C58	79.23
C2-C1-H29	111.82	C4-N7-C57-H59	-163.69
C2-C1-H30	109.44	C4-N7-C57-C62	-52.58
C6-C1-H29	107.99	C8-N7-C57-C58	-104.31
C6-C1-H30	106.73	C8-N7-C57-H59	12.76
H29-C1-H30	107.06	C8-N7-C57-C62	123.87
C1-C2-C3	107.84	N7-C8-C9-C10	6.00
C1-C2-C23	109.97	N7-C8-C9-C14	-173.13
C1-C2-C24	110.42	C11-C8-C9-C10	-177.07
C3-C2-C23	108.77	C11-C8-C9-C14	3.79
C3-C2-C24	110.83	N7-C8-C11-C12	151.92
C23-C2-C24	108.98	N7-C8-C11-H34	-86.85
C2-C3-C4	114.11	N7-C8-C11-H35	20.39
C2-C3-H31	108.66	C9-C8-C11-C12	-25.08
C2-C3-H32	107.77	C9-C8-C11-H34	96.13
C4-C3-H31	108.34	C9-C8-C11-H35	-146.62
C4-C3-H32	110.87	C8-C9-C10-C5	-26.41
H31-C3-H32	106.83	C8-C9-C10-C17	99.90
C3-C4-C5	121.87	C8-C9-C10-H33	-143.40
C3-C4-N7	118.33	C14-C9-C10-C5	152.75
C5-C4-N7	119.74	C14-C9-C10-C17	-80.94
C4-C5-C6	120.89	C14-C9-C10-H33	35.75

C4-C5-C10	122.20	C8-C9-C14-C13	-8.69
C6-C5-C10	116.90	C8-C9-C14-O16	172.84
C1-C6-C5	117.96	C10-C9-C14-C13	172.14
C1-C6-O15	120.76	C10-C9-C14-O16	-6.32
C5-C6-O15	121.27	C5-C10-C17-C18	-149.36
C4-N7-C8	118.69	C5-C10-C17-C22	41.44
C4-N7-C57	122.68	C9-C10-C17-C18	96.70
C8-N7-C57	118.52	C9-C10-C17-C22	-82.49
N7-C8-C9	120.31	H33-C10-C17-C18	-20.96
N7-C8-C11	117.41	H33-C10-C17-C22	159.84
C9-C8-C11	122.22	C8-C11-C12-C13	48.17
C8-C9-C10	121.61	C8-C11-C12-C25	167.80
C8-C9-C14	120.79	C8-C11-C12-C26	-72.65
C10-C9-C14	117.58	H34-C11-C12-C13	-73.62
C5-C10-C9	109.09	H34-C11-C12-C25	45.99
C5-C10-C17	113.38	H34-C11-C12-C26	165.54
C5-C10-H33	107.89	H35-C11-C12-C13	171.34
C9-C10-C17	111.93	H35-C11-C12-C25	-69.03
C9-C10-H33	107.96	H35-C11-C12-C26	50.52
C17-C10-H33	106.34	C11-C12-C13-C14	-53.15
C8-C11-C12	114.22	C11-C12-C13-H36	66.10
C8-C11-H34	109.20	C11-C12-C13-H37	-175.49
C8-C11-H35	110.59	C25-C12-C13-C14	-172.02
C12-C11-H34	108.14	C25-C12-C13-H36	-52.76
C12-C11-H35	107.58	C25-C12-C13-H37	65.45
H34-C11-H35	106.80	C26-C12-C13-C14	67.63
C11-C12-C13	108.10	C26-C12-C13-H36	-173.11
C11-C12-C25	108.90	C26-C12-C13-H37	-54.70
C11-C12-C26	110.34	C11-C12-C25-H48	-60.27
C13-C12-C25	110.11	C11-C12-C25-H49	179.88

C13-C12-C26	110.41	C11-C12-C25-H50	60.38
C25-C12-C26	108.96	C13-C12-C25-H48	57.10
C12-C13-C14	113.47	C13-C12-C25-H49	-61.75
C12-C13-H36	109.58	C13-C12-C25-H50	178.75
C12-C13-H37	111.68	C26-C12-C25-H48	179.32
C14-C13-H36	106.80	C26-C12-C25-H49	59.47
C14-C13-H37	107.98	C26-C12-C25-H50	-60.02
H36-C13-H37	107.02	C11-C12-C26-H51	-61.40
C9-C14-C13	117.88	C11-C12-C26-H52	59.50
C9-C14-O16	121.44	C11-C12-C26-H53	179.41
C13-C14-O16	120.66	C13-C12-C26-H51	179.15
C10-C17-C18	119.85	C13-C12-C26-H52	-69.50
C10-C17-C22	122.16	C13-C12-C26-H53	59.89
C18-C17-C22	117.98	C25-C12-C26-H51	58.11
C17-C18-C19	121.23	C25-C12-C26-H52	179.02
C17-C18-H38	119.21	C25-C12-C26-H53	-61.04
C19-C18-H38	119.55	C12-C13-C14-C9	34.93
C18-C19-C20	120.17	C12-C13-C14-O16	-146.59
C18-C19-H39	121.12	H36-C13-C14-C9	-85.90
C20-C19-H39	118.70	H36-C13-C14-O16	92.56
C19-C20-C21	119.46	H37-C13-C14-C9	158.29
C19-C20-O27	115.94	H37-C13-C14-O16	-22.23
C21-C20-O27	124.61	C10-C17-C18-C19	-179.00
C20-C21-C22	119.67	C10-C17-C18-H38	0.66
C20-C21-H40	121.28	C22-C17-C18-C19	-0.21
C22-C21-H40	119.05	C22-C17-C18-H38	179.88
C17-C22-C21	121.49	C10-C17-C22-C21	179.05
C17-C22-H41	120.36	C10-C17-C22-H41	-1.88
C21-C22-H41	118.14	C18-C17-C22-C21	-0.15
C2-C23-H42	111.35	C18-C17-C22-H41	178.91

C2-C23-H43	110.68	C17-C18-C19-C20	-0.14
C2-C23-H44	111.17	C17-C18-C19-H39	-179.66
H42-C23-H43	107.88	H38-C18-C19-C20	-179.81
H42-C23-H44	108.02	H38-C18-C19-H39	0.67
H43-C23-H44	107.59	C18-C19-C20-C21	0.01
C2-C24-H45	112.19	C18-C19-C20-O27	-179.77
C2-C24-H46	110.79	H39-C19-C20-C21	179.52
C2-C24-H47	110.41	H39-C19-C20-O27	-0.24
H45-C24-H46	108.08	C19-C20-C21-C22	0.07
H45-C24-H47	107.59	C19-C20-C21-H40	-179.44
H46-C24-H47	107.59	O27-C20-C21-C22	179.81
C12-C25-H48	111.39	O27-C20-C21-H40	0.30
C12-C25-H49	110.59	C19-C20-O27-C28	178.73
C12-C25-H50	111.16	C21-C20-O27-C28	-1.02
H48-C25-H49	107.79	C20-C21-C22-C17	0.02
H48-C25-H50	108.12	C20-C21-C22-H41	-179.07
H49-C25-H50	107.63	H40-C21-C22-C17	179.54
C12-C26-H51	110.76	H40-C21-C22-H41	0.45
C12-C26-H52	112.20	C20-O27-C28-H54	-179.53
C12-C26-H53	110.27	C20-O27-C28-H55	-60.75
H51-C26-H52	108.11	C20-O27-C28-H56	61.70
H51-C26-H53	107.73	N7-C57-C58-H60	-109.09
H52-C26-H53	107.60	N7-C57-C58-H61	9.67
C20-O27-C28	118.42	N7-C57-C58-C66	129.19
O27-C28-H54	105.93	H59-C57-C58-H60	134.60
O27-C28-H55	111.50	H59-C57-C58-H61	-106.63
O27-C28-H56	111.56	H59-C57-C58-C66	12.89
H54-C28-H55	109.28	C62-C57-C58-H60	22.28
H54-C28-H56	109.24	C62-C57-C58-H61	141.04
H55-C28-H56	108.24	C62-C57-C58-C66	-99.43

N7-C57-C58	114.08	N7-C57-C62-O63	-1.65
N7-C57-H59	105.57	N7-C57-C62-O64	-179.67
N7-C57-H62	112.82	C58-C57-C62-O63	-133.63
C58-C57-H59	106.90	C58-C57-C62-O64	48.34
C58-C57-C62	113.74	H59-C57-C62-O63	111.37
H59-C57-C62	102.45	H59-C57-C62-O64	-66.64
C57-C58-H60	111.06	C57-C58-C66-O67	-124.96
C57-C58-H61	109.01	C57-C58-C66-O68	55.32
C57-C58-C66	114.52	H60-C58-C66-O67	111.28
H60-C58-H61	107.90	H60-C58-C66-O68	-68.43
H60-C58-C66	107.28	H61-C58-C66-O67	4.19
H61-C58-C66	106.77	H61-C58-C66-O68	176.08
C57-C62-O63	124.04	C57-C62-O64-H65	5.02
C57-C62-O64	115.14	O63-C62-O64-H65	-173.07
O63-C62-O64	120.79	C58-C66-O68-H69	-179.57
C62-O64-H65	112.85	O67-C66-O68-H69	-0.16
C58-C66-O67	126.75		

Table S-II: Optimized geometric parameters for NTDOSA.

Parameter	DFT/B3LYP6311++G(d,p)	Parameter	DFT/B3LYP6311++G(d,p)
Bond length, $\AA$		O66-C65-O67	124.27
C1-C2	1.538	Dihedral Angle (in degree)	
C1-C6	1.517	C6-C1-C2-C3	52.83
C1-H27	1.092	C6-C1-C2-C23	171.23
C1-H28	1.092	C6-C1-C2-C24	-68.48
C2-C3	1.548	H27-C1-C2-C3	175.40

C2-C23	1.538	H27-C1-C2-C23	-66.19
C2-C24	1.541	H27-C1-C2-C24	54.09
C3-C4	1.514	H28-C1-C2-C3	-66.22
C3-H29	1.096	H28-C1-C2-C23	52.093
C3-H30	1.090	H28-C1-C2-C24	172.48
C4-C5	1.355	C2-C1-C6-C5	-32.48
C4-N7	1.415	C2-C1-C6-O15	159.65
C5-C6	1.476	H27-C1-C6-C5	-157.13
C5-C10	1.510	H27-C1-C6-O15	24.73
C6-O15	1.221	H28-C1-C6-C5	88.20
N7-C8	1.4132	H28-C1-C6-O15	-89.93
N7-C52	1.4637	C1-C2-C3-C4	-49.73
C8-C9	1.355	C1-C2-C3-H29	71.34
C8-C11	1.516	C1-C2-C3-H30	-173.20
C9-C10	1.515	C23-C2-C3-C4	-169.93
C9-C14	1.475	C23-C2-C3-H29	-47.85
C10-C17	1.534	C23-C2-C3-H30	66.59
C10-H31	1.091	C24-C2-C3-C4	71.35
C11-C12	1.547	C24-C2-C3-H29	-167.56
C11-H32	1.099	C24-C2-C3-H30	-52.12
C11-H33	1.094	C1-C2-C23-H40	-58.56
C12-C13	1.573	C1-C2-C23-H41	61.44
C12-C25	1.537	C1-C2-C23-H42	-179.09
C12-C26	1.542	C3-C2-C23-H40	59.39
C13-C14	1.517	C3-C2-C23-H41	179.40
C13-H34	1.098	C3-C2-C23-H42	-61.13
C13-H35	1.092	C24-C2-C23-H40	-179.40
C14-O16	1.221	C24-C2-C23-H41	-59.73
C17-C18	1.400	C24-C2-C23-H42	59.72
C17-C22	1.400	C1-C2-C24-H43	59.75

C18-C19	1.389	C1-C2-C24-H44	-179.33
C18-H36	1.082	C1-C2-C24-H45	-60.28
C19-C20	1.391	C3-C2-C24-H43	-59.85
C19-H37	1.081	C3-C2-C24-H44	61.05
C20-C21	1.391	C3-C2-C24-H45	-179.88
C20-N65	1.475	C23-C2-C24-H43	-179.38
C21-C22	1.390	C23-C2-C24-H44	-58.47
C21-H38	1.081	C23-C2-C24-H45	60.57
C22-H39	1.083	C2-C3-C4-C5	26.26
C23-H40	1.093	C2-C3-C4-N7	-151.12
C23-H41	1.093	H29-C3-C4-C5	-94.96
C23-H42	1.095	H29-C3-C4-N7	87.64
C24-H43	1.092	H30-C3-C4-C5	148.09
C24-H44	1.094	H30-C3-C4-N7	-29.29
C24-H45	1.094	C3-C4-C5-C6	-2.74
C25-H46	1.094	C3-C4-C5-C10	177.47
C25-H47	1.094	N7-C4-C5-C6	174.61
C25-H48	1.095	N7-C4-C5-C10	-5.16
C26-H49	1.094	C3-C4-N7-C8	159.78
C26-H50	1.093	C3-C4-N7-C52	-24.86
C26-H51	1.093	C5-C4-N7-C8	-17.68
C52-C53	1.574	C5-C4-N7-C52	157.69
C52-H54	1.092	C4-C5-C6-C1	5.82
C52-C57	1.552	C4-C5-C6-O15	-176.03
C53-H55	1.094	C10-C5-C6-C1	-174.38
C53-H56	1.087	C10-C5-C6-O15	3.75
C53-C61	1.511	C4-C5-C10-C9	24.95
C57-O58	1.198	C4-C5-C10-C17	-100.29
C57-O59	1.344	C4-C5-C10-H31	142.27
O59-H60	0.974	C6-C5-C10-C9	-154.83

C61-O62	1.198	C6-C5-C10-C17	79.91
C61-O63	1.371	C6-C5-C10-H31	-37.51
O63-H64	0.970	C4-N7-C8-C9	17.54
N65-O66	1.226	C4-N7-C8-C11	-159.31
N65-O67	1.227	C52-N7-C8-C9	-157.99
Bond Angle (in degree)		C52-N7-C8-C11	25.14
C2-C1-C6	113.55	C4-N7-C52-C53	79.63
C2-C1-H27	111.84	C4-N7-C52-H54	-163.25
C2-C1-H28	109.48	C4-N7-C52-C57	-52.35
C6-C1-H27	108.02	C8-N7-C52-C53	-105.01
C6-C1-H28	106.68	C8-N7-C52-H54	12.10
H27-C1-H28	106.95	C8-N7-C52-C57	123.01
C1-C2-C3	107.96	N7-C8-C9-C10	5.38
C1-C2-C23	109.92	N7-C8-C9-C14	-173.33
C1-C2-C24	110.48	C11-C8-C9-C10	-177.89
C3-C2-C23	108.67	C11-C8-C9-C14	3.38
C3-C2-C24	110.45	N7-C8-C11-C12	151.56
C23-C2-C24	108.97	N7-C8-C11-H32	-87.17
C2-C3-C4	113.11	N7-C8-C11-H33	29.99
C2-C3-H29	108.67	C9-C8-C11-C12	-25.25
C2-C3-H30	107.76	C9-C8-C11-H32	96.01
C4-C3-H29	108.39	C9-C8-C11-H33	-146.81
C4-C3-H30	110.77	C8-C9-C10-C5	-24.99
H29-C3-H30	106.85	C8-C9-C10-C17	101.23
C3-C4-C5	121.67	C8-C9-C10-H31	-142.35
C3-C4-N7	118.40	C14-C9-C10-C5	153.77
C5-C4-N7	119.87	C14-C9-C10-C17	-79.99
C4-C5-C6	121.13	C14-C9-C10-H31	36.42
C4-C5-C10	122.31	C8-C9-C14-C13	-7.80
C6-C5-C10	116.55	C8-C9-C14-C16	173.90

C1-C6-C5	118.04	C10-C9-C14-C13	173.41
C1-C6-O15	121.98	C10-C9-C14-O16	-4.87
C5-C6-O15	120.94	C5-C10-C17-C18	-138.92
C4-N7-C8	118.74	C5-C10-C17-C22	41.97
C4-N7-C52	122.51	C9-C10-C17-C18	97.10
C8-N7-C52	118.58	C9-C10-C17-C22	-81.99
N7-C8-C9	120.46	H31-C10-C17-C18	-22.39
N7-C8-C11	117.42	H31-C10-C17-C22	160.49
C9-C8-C11	122.02	C8-C11-C12-C13	48.43
C8-C9-C10	121.68	C8-C11-C12-C25	168.02
C8-C9-C14	120.94	C8-C11-C12-C26	-72.36
C10-C9-C14	117.35	H32-C11-C12-C13	-73.34
C5-C10-C9	109.29	H32-C11-C12-C25	46.24
C5-C10-C17	113.35	H32-C11-C12-C26	165.85
C5-C10-H31	108.07	H33-C11-C12-C13	171.53
C9-C10-C17	111.66	H33-C11-C12-C25	-68.87
C9-C10-H31	108.01	H33-C11-C12-C26	50.72
C17-C10-H31	106.20	C11-C12-C13-C14	-52.92
C8-C11-C12	114.23	C11-C12-C13-H34	66.35
C8-C11-H32	109.14	C11-C12-C13-H35	-175.29
C8-C11-H33	110.47	C25-C12-C13-C14	-171.74
C12-C11-H32	108.20	C25-C12-C13-H34	-52.46
C12-C11-H33	107.67	C25-C12-C13-H35	65.88
H32-C11-H33	106.82	C26-C12-C13-C14	67.84
C11-C12-C13	108.11	C26-C12-C13-H34	-172.87
C11-C12-C25	108.88	C26-C12-C13-H35	-54.51
C11-C12-C26	110.34	C11-C12-C25-H46	-60.29
C13-C12-C25	110.08	C11-C12-C25-H47	179.87
C13-C12-C26	110.38	C11-C12-C25-H48	60.38
C25-C12-C26	109.02	C13-C12-C25-H46	58.05

C12-C13-C14	113.53	C13-C12-C25-H47	-61.77
C12-C13-H34	109.60	C13-C12-C25-H48	178.73
C12-C13-H35	111.73	C26-C12-C25-H46	179.27
C14-C13-H34	106.76	C26-C12-C25-H47	59.45
C14-C13-H35	107.93	C26-C12-C25-H48	-60.03
H34-C13-H35	106.93	C11-C12-C26-H49	-61.32
C9-C14-C13	117.95	C11-C12-C26-H50	59.61
C9-C14-O16	121.18	C11-C12-C26-H51	179.54
C13-C14-O16	120.83	C13-C12-C26-H49	179.23
C10-C17-C18	119.58	C13-C12-C26-H50	-59.81
C10-C17-C22	121.48	C13-C12-C26-H51	60.10
C18-C17-C22	118.92	C25-C12-C26-H49	58.19
C17-C18-C19	120.94	C25-C12-C26-H50	179.14
C17-C18-H36	119.29	C25-C12-C26-H51	-60.93
C19-C18-H36	119.75	C12-C13-C14-C9	34.15
C18-C19-C20	118.77	C12-C13-C14-O16	-147.55
C18-C19-H37	121.48	H34-C13-C14-C9	-86.73
C20-C19-H37	119.74	H34-C13-C14-O16	91.55
C19-C20-C21	121.68	H35-C13-C14-C9	158.59
C19-C20-N65	119.20	H35-C13-C14-O16	-23.11
C21-C20-N65	119.11	C10-C17-C18-C19	-178.81
C20-C21-C22	118.81	C10-C17-C18-H36	0.73
C20-C21-H38	119.79	C22-C17-C18-C19	0.31
C22-C21-H38	121.38	C22-C17-C18-H36	179.86
C17-C22-C21	120.86	C10-C17-C22-C21	178.78
C17-C22-H39	120.39	C10-C17-C22-H39	-1.99
C21-C22-H39	118.73	C18-C17-C22-C21	-0.32
C2-C23-H40	111.37	C18-C17-C22-H39	178.89
C2-C23-H41	110.67	C17-C18-C19-C20	0.012
C2-C23-H42	111.15	C17-C18-C19-H37	-179.79

H40-C23-H41	107.88	H36-C18-C19-C20	-179.56
H40-C23-H42	108.03	H36-C18-C19-H37	0.65
H41-C23-H42	107.55	C18-C19-C20-C21	-0.29
C2-C24-H43	112.27	C18-C19-C20-N65	179.90
C2-C24-H44	110.78	H37-C19-C20-C21	179.49
C2-C24-H45	110.36	H37-C19-C20-N65	-0.31
H43-C24-H44	108.05	C19-C20-C21-C22	0.28
H43-C24-H45	107.58	C19-C20-C21-H38	-179.47
H44-C24-H45	107.57	N65-C20-C21-C22	-179.91
C12-C25-H46	111.39	N65-C20-C21-H38	0.33
C12-C25-H47	110.56	C19-C20-N65-O66	0.01
C12-C25-H48	111.15	C19-C20-N65-O67	-179.85
H46-C25-H47	107.78	C21-C20-N65-O66	-179.80
H46-C25-H48	108.14	C21-C20-N65-O67	0.33
H47-C25-H48	107.68	C20-C21-C22-C17	-0.02
C12-C26-H49	110.78	C20-C21-C22-H39	-179.19
C12-C26-H50	112.23	H38-C21-C22-C17	179.78
C12-C26-H51	110.25	H38-C21-C22-H39	0.55
H49-C26-H50	108.10	N7-C52-C53-H55	-107.87
H49-C26-H51	107.70	N7-C52-C53-H56	10.99
H50-C26-H51	107.58	N7-C52-C53-C61	130.24
N7-C52-C53	114.06	H54-C52-C53-H55	135.81
N7-C52-H54	105.56	H54-C52-C53-H56	-105.31
N7-C52-C57	112.32	H54-C52-C53-C61	13.93
C53-C52-H54	106.94	C57-C52-C53-H55	23.19
C53-C52-C57	114.21	C57-C52-C53-H56	142.06
H54-C52-C57	102.47	C57-C52-C53-C61	-98.68
C52-C53-H55	111.13	N7-C52-C57-O58	-3.19
C52-C53-H56	108.95	N7-C52-C57-O59	178.86
C52-C53-C61	114.29	C53-C52-C57-O58	-135.10

H55-C53-H56	107.98	C53-C52-C57-O59	46.95
H55-C53-C61	107.49	H54-C52-C57-O58	109.63
H56-C53-C61	106.71	H54-C52-C57-O59	-68.31
C52-C57-O58	125.45	C52-C53-C61-O62	-122.93
C52-C57-O59	115.45	C52-C53-C61-O63	57.14
O58-C57-O59	120.92	H55-C53-C61-O62	113.21
C57-O59-H60	113.01	H55-C53-C61-O63	-66.70
C53-C61-O62	126.68	H56-C53-C61-O62	2.42
C53-C61-O63	111.22	H56-C53-C61-O63	-177.65
O62-C61-O63	122.09	C52-C57-O59-H60	5.16
C61-O63-H64	109.16	O58-C57-O59-H60	-172.84
C20-N65-O66	117.88	C53-C61-O63-H64	179.76
C20-N65-O67	117.85	O62-C61-O63-H64	-0.15

Table. S-III: Vibrational analysis of prominent modes of MTDOSA at the B3LYP/6-311++G (d,p) level.

Cal. Frequency, cm^{-1}	Scaled Frequency, cm^{-1}	Exp. FTIR Frequency, cm^{-1}	Assignment
3753	3630	3630	ν_{as}[O-H)(99)]
3644	3523	3312	ν_{s}[O-H)(99)]
3203	3097	3069	ν_{as} [C-H)R1(94)]
3195	3090		ν_{as} [C-H)R1(98)]
3188	3083		ν_{s} [C-H)R1(89)]
3180	3075		ν_{as} [C-H)R1(98)]
3148	3045		ν_{as} [C-H) CH_2 (98)]
3127	3024		ν_{as} [C-H) CH_3-O (91)]
3104	3002	3002	ν_{as} [C-H)R2 (91)]
3099	2997		ν_{as} [C-H)CH_3-R4 (76)]
3098	2996		ν_{as} [C-H)CH_3-R2(64)]
3097	2995		ν[C57-H59 (94)]
3090	2988		ν_{s} [C-H)CH_3-R4 (54)]
3089	2987		ν_{as} [C-H)CH_3-R2(83)]
3085	2983		ν_{as} [C-H)CH_3-R4(68)]
3083	2981		ν [C-H)R2 (54)]
3083	2981		ν_{as} [C-H){R2(44)+CH_3-R2(26)}]
3081	2979		ν_{as} [(C-H){R2+R3+CH_3-R2}(70)]
3080	2979		ν_{as} [(C-H){R2+R3+CH_3-R2}(70)]
3077	2976		ν_{as} [C-H)CH_3-R4(89)]
3075	2974		ν_{as} [C-H)CH_3-R2(84)]

3061	2960	2959	ν_{as} [C-H)R4 (69)]
3058	2957		ν_{s} [C-H)CH_2 (87)]
3055	2954		ν_{as} [C-H)CH_3-O-R1(100)]
3043	2943		ν_{s} [C-H)R2 (79)]
3026	2926		ν_{s} [C-H)CH_3-R4 (87)]
3023	2923		ν_{s} [C-H)CH_3-R2 (31)]
3016	2916		ν_{s} [C-H)CH_3-R4 (71)]
3015	2915		ν_{as} [C-H)CH_3-R2(78)]
3007	2908		ν_{s} [C-H)R2 (73)]
3004	2905		ν_{s} [C-H)R24(76)]
2999	2900		ν_{s} [C-H)CH_3-O-R1(91)]
2985	2886	2877	ν_{s} [C-H)R4 (72)]
1846	1785	1808	ν_{s} [(O=C)COOH(74)]
1836	1776	1731	ν_{s} [(O=C)COOH(82)]
1722	1665	1668	ν_{s} [(O=C)R2+R4(89)]
1716	1660		ν [(O=C)R4(64)]
1678	1622	1618	ν_{s} [(C=C)R3(68)]
1648	1593	1600	ν_{as} [C-C)R1(62)]+ β [(H-C-C)R1(19)]
1627	1573	1575	ν_{as} [(C=C)R3(71)]
1616	1563	1556	ν_{as} [C-C)R1(43)]
1540	1489	1510	β [(H-C-C)R1(48)]
1514	1464		β_O [(H-C-H)CH_3-R2(48)]
1513	1463	1461	β_O [(H-C-H)CH_3-R4(59)]
1507	1457		β_O [(H-C-H)CH_3-R4(55)]
1506	1456		β_O [(H-C-H)CH_3-R2(51)]
1505	1456		β_O [(H-C-H)CH_3-0-R1(72)]
1500	1450		β_O [(H-C-H)CH_3-R2+R2(39)]
1498	1449		β_O [(H-C-H)CH_3-R4+R4(52)]
1491	1442		β_O [(H-C-H)CH_3-O-R1(73)]
1490	1441		β_O [(H-C-H)CH_3-R2+R2(54)]
1489	1440	1440	β_O [(H-C-H)CH_3-R4(34)]
1483	1434	1434	β_O [(H-C-H)CH_3-R2+R2(56)]
1481	1433		β_O [(H-C-H)R4+CH_2(43)]
1475	1427		β_O [(H-C-H)R4+CH_2(64)]
1474	1426		β_O [(H-C-H)CH_3-O-R1(84)]
1463	1415		β_O [(H-C-H)CH_3-R4+R4(73)]
1461	1413		β_O [(H-C-H)CH_3-R2+R2(61)]
1455	1407		β [(H-C-C)R1(30)]
1439	1391		τ_i[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(22)]
1424	1377		β_O [(H-C-H)CH_3-R4(42)]
1423	1376		β_O [(H-C-H)CH_3-R1+R1(74)]
1403	1356	1360	β_O [(H-C-H)CH_3-R4(79)]
1402	1357		β_O [(H-C-H)CH_3-R1(22)]
1385	1339	1328	τ_i[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(18)]
1361	1316		β [(H-O-C)COOH(63)]
1352	1308		ν_{s} [C6-C5+C14-C9) (20)]
1346	1301	1301	β_O [(H-C-H)CH_2-R4(23)]
1340	1295		ν_{s} [(C-C)R1 (20)]+ β [(H-C-C)R1(57)]
1318	1275	1260	β [(H-O-C)COOH(19)]
1268	1226	1233	ν [O27-C20) (34)]
1264	1222		ν_{as} [(N-C)R3 (17)]
1249	1208		ν [N7-C57) (20)]
1235	1195	1194	β_O [(H-C-C)CH_2(34)]

1204	1164	1163	β [(H-C-C)R1(58)]
1201	1161		τ_i[(H-C-O-C)CH3-O-R1(48)]
1183	1143		ν [(O-C) COOH(17)]
1168	1130	1137	β_O [(H-C-H)CH_3-O-R1(19)]+ τ_i[(H-C-O-C)CH3-O-R1(54)]
1146	1108	1106	ν [(O-C) COOH(26)]+ β [(H-O-C)COOH(19)]
1142	1104		β_O [(H-C-C)R2(21)]
1139	1101		β_O [(H-C-C)R1(25)]
1136	1099		β [(H-C-C)R1(34)]
1123	1086		ν [(C-C) R1+R2(20)]
1063	1028	1031	ν [O27-C28) (72)]
1036	1002		τ_i[(H-C-C-C)CH3-R4+R4(21)]
1034	999	998	τ_i[(H-C-C-C)CH3-R2(21)]
1027	993		β [(H-C-C)R1(19)]+ β [(C-C-C)R1(60)]
985	953		τ_i[(H-C-C-C)R1(86)]
968	936	934	τ_i[(H-C-C-C)R1(51)]
948	917		τ_i[(H-C-C-C)CH_3-R1(20)]
944	913	910	β [(C-C-N)R1+R2+R3(20)]
905	875	882	τ_i[(H-C-C-C)R2(26)]
864	836	845	τ_i[(H-C-C-C)R1(24)]
826	799	806	τ_i[(H-C-C-C)R1(66)]
784	758	776	ν [O27-C20) (18)]
760	735	722	τ_o [(O-C-O-C)COOH(41)]
688	665	685	τ_i[(H-O-C-C)COOH(20)]
666	644	651	τ_i[(H-O-C-C)COOH(38)]
644	623	637	τ_o [{(O15-C1-C5-C6)(R2+(O-C-O-C)(COOH)}(18)]
642	621	606	β [(O-C-O)COOH(20)]
597	577	567	τ_i[(H-O-C-C)COOH(24)]
541	523	532	τ_i[(H-O-C-C)COOH(27)]
426	412	422	τ_i[(C-C-C-C)R1+R3(75)]
399	386	415	β [(C58-C57-N7)(19)]
392	379		β [(O-C-C)COOH(42)]
385	373		τ_o[(H-C-C-C)R2(23)]
285	275		β [(C-O-C)CH_3-O-R1(22)]
237	229		τ_i[(H-C-O-C)CH_3-O-R1(46)]
228	220		τ_i[(H-C-C-C)CH_3-R2(22)]
222	215		τ_i[(H-C-C-C)CH_3-R4+R4(19)]
152	147		τ_i[(H-C-C-C)CH_3-R4+R4(18)]
141	136		β [(C-C-C)R2+R4(20)]
106	102		τ_i[(C-C-C-C)R2(24)]
84	81		τ_i[(C-C-C-C)CH_3-O-R1(24)]
79	76		τ_i[(C-C-C-C)CH_3-O-R1(20)]
63	61		τ_i[(O-C-C-C)COOH(35)]
61	59		τ_i[(C-C-C-C)R1+R2+R3+R4(26)]
43	42		τ_i[(C57-C4-C8-N7)(27)]

115 ν: stretching; ν_s: symmetric stretching; ν_{as}: anti-symmetric stretching; β: bending in-plane; β_O: bending out-of-plane;

116 τ_i: torsion in plane; τ_o : torsion out-of-plane

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Table S-IV: Vibrational analysis of prominent modes of NTDOSA at the B3LYP/6-311++G (d, p) level

Calculated Freq., cm^{-1}	Scaled Freq., cm^{-1}	Exp. Freq., cm^{-1}	Assignment
3751	3627	3631	ν_{as}[(O-H)COOH(100)]
3637	3517	3312	ν_{s}[(O-H)COOH(99)]
3221	3115		ν_{s} [C-H)R1(91)]
3220	3114		ν_{as} [C-H)R1(92)]
3200	3094		ν_{s} [C-H)R1(82)]
3199	3093	3069	ν_{as} [C-H)R1(82)]
3148	3045		ν_{as} [C-H) CH_2 (90)]
3104	3002	3002	ν_{as} [C-H)R2(82)]
3099	2997		ν_{as} [C-H) CH_3-R4 (79)]
3096	2993		ν [C52-H54)(95)]
3091	2989		ν_{as} [C-H) CH_3-R4 (46)]
3090	2988		ν_{as} [C-H) CH_3-R2 (82)]
3087	2985		ν_{as} [C-H) CH_3-R4 (69)]
3086	2983		ν_{as} [C-H) CH_3-R2+R2 (77)]
3085	2983		ν_{as} [C-H) R4 (62)]
3082	2981		ν_{as} [C-H) CH_3-R2+R2 (26)]
3080	2979		ν [C-H)R3(90)]
3080	2978		ν_{as} [C-H) CH_3-R4 (87)]
3077	2975		ν_{as} [C-H) CH_3-R2 (83)]
3063	2962		ν [C-H)R4(71)]
3060	2959	2959	ν [C53-H56)(87)]
3041	2941		ν_{as} [C-H) R2 (78)]
3027	2927		ν_{s} [C-H) CH_3-R4 (79)]
3024	2924		ν_{s} [C-H) CH_3-R2 (29)]
3017	2918		ν_{s} [C-H) CH_3-R4 (70)]
3016	2916		ν_{s} [C-H) CH_3-R4 (70)]
3009	2909		ν_{s} [C-H) R2 (74)]
3006	2907		ν_{s} [C-H) R4 (74)]
2988	2889	2877	ν_{s} [C-H) R4 (73)]
1845	1784	1808	ν_{s} [O=C) COOH (84)]
1835	1775	1731	ν_{s} [O=C) COOH (82)]
1721	1665	1668	ν_{s} [O=C) R2+R4 (90)]
1716	1659		ν [O=C) R2 (68)]
1678	1623	1618	ν_{s} [C=C) R3 (67)]
1642	1588	1586	ν_{as} [C-C) R1(36)]
1633	1579	1576	ν_{as} [C-C) R1(28)]+ β [(H-C-C)R1(18)]
1624	1571	1556	ν_{as} [C=C) R3 (73)]
1569	1517	1510	ν_{as} [(O-N) NO_2 (77)]
1523	1472		β [(H-C-C)R1(63)]
1514	1464		β_O [(H-C-H)CH_3-R2(40)]
1513	1463	1461	β_O [(H-C-H)CH_3-R4(61)]
1508	1458		β_O [(H-C-H)CH_3-R4(57)]
1506	1457		β_O [(H-C-H)CH_3-R2(56)]
1499	1449		β_O [(H-C-H)CH_3-R4+R4(57)]
1498	1448		β_O [(H-C-H)CH_3-R2+R2(66)]
1490	1441	1440	β_O [(H-C-H)CH_3-R2+R2(51)]
1489	1440		β_O [(H-C-H)CH_3-R4(42)]
1482	1433	1434	β_O [(H-C-H)R4+CH_2(54)]
1481	1432		β_O [(H-C-H)CH_3-R2+R2(55)]

1477	1428		β_O [(H-C-H)R4+CH_2(66)]
1463	1414		β_O [(H-C-H)CH_3-R4+R4(71)]
1461	1413		β_O [(H-C-H)CH_3-R2+R2(61)]
1454	1406		ν_{as} [C-C) R1(19)]+ β [(H-C-C)R1(25)]
1436	1389		τ_i[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(21)]
1427	1380		β_O [(H-C-H)CH_3-R4(60)]
1423	1376		β_O [(H-C-H)CH_3-R2+R2(90)]
1405	1359	1360	β_O [(H-C-H)CH_3-R4(87)]
1402	1356		β_O [(H-C-H)CH_3-R2(42)]
1384	1338	1328	τ_i[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(16)]
1366	1321		ν_s [C-H) NO_2-R1 (66)]
1361	1316		β [(H-O-C)COOH(54)]
1355	1310		ν_s [C-C) R2+R4(16)]
1346	1302	1301	β [(H-C-C)R1(28)]+ β_O [(H-C-C)R2+CH_2(17)]
1343	1299		β [(H-C-C)R1(28)]
1319	1276		β [(H-O-C)COOH(16)]
1296	1253		β [(H-O-C)COOH(19)]
1265	1223		ν_{as} [(N-C) R3(19)]
1248	1207		ν_{as} [(N-C) R3(34)]
1233	1192		β_O [(H-C-C)COOH(34)]
1211	1171		β [(H-C-C)R1(51)]
1209	1169		β [(H-C-C)R1(16)]
1187	1148	1137	ν_{as} [O-C) COOH(19)]
1145	1107	1108	ν_{as} [O-C) COOH(24)]+ β [(H-O-C)COOH(17)]
1143	1105		β_O [(H-C-H)R2(23)]
1140	1102		β_O [(H-C-H)R4(23)]
1135	1097		β [(H-C-C)R1(46)]
1122	1085		ν_{as} [C-C) R2+R3(18)]
1118	1081	1031	ν [N-C) NO_2+R1(21)]
1036	1002		τ_i[{(H-C-C-C)(CH3-R2+R2)(16)]
1034	1000		τ_i[{(H-C-C-C)(CH3-R2)(21)]
1033	998	998	β [(C-C-C)R1(69)]
1014	981		β [(H-C-C)R1(65)]
997	964	934	τ_i[{(H-C-C-C)(R1)(57)]
952	921		ν_{as} [C-C) CH_3-R4+R4(24)]+ τ_i[{(H-C-C-C)(CH_3-R4)(17)]
950	919		τ_i[{(H-C-C-C)(CH_3-R4)(18)]
944	913	910	β [(H-C-C)R1+R2+R3(18)]
904	875	882	τ_i[{(H-C-C-C)(R2)(27)]
892	863		τ_i[{(H-C-C-C)(R1)(43)]
877	848	845	τ_i[{(H-C-C-C)(R1)(95)]
871	842		ν_{as} [(O-C) COOH(17)]
859	830		τ_i[{(H-C-C-C)(R1)(93)]
837	810	811	β [(O-N-C)NO_2(17)]
788	762	776	ν_{as} [(C-C) CH3-R2+R2(16)]
761	736		τ_o[{(O-C-C-C)(R1)+(O-C-O-C)COOH}(40)]
743	719	722	τ_o[(O-C-O-N)(NO_2-R1)(40)]
712	689		τ_o[(O-C-O-N)(NO_2-R1)(19)]
708	684	685	τ_o[(O-C-O-N)(NO_2-R1)(21)]
690	667	667	τ_i[(H-O-C-C)(COOH)(21)]
666	644		τ_i[(H-O-C-C)(COOH)(35)]

642	621		β [(O-N-O)COOH(17)]
640	618		β [(C-C-C)R1+R3(41)]
621	600		β [(O-N-O)COOH(18)]
594	574		β [(O-N-O)COOH(18)]+ τ_i[(H-O-C-C)(COOH)(20)]
576	557		β [(O-C-C)R2+R4(25)]
543	525	5532	τ_i[(H-O-C-C)(COOH)(30)]
539	521		β [(O-N-C)NO_2-R1(26)]
534	516		β [(O-N-C)NO_2-R1(19)]
517	500	459	β [(O-N-C)NO_2-R1(19)]
419	405	415	τ_i[(C-C-C-C)(R1)(53)]
398	385		β [(O-C-C)COOH(16)+(C53-C52-N7)(19)]
390	377		τ_o[(C-C-C-C)(CH_3-R4+R4)(40)]
389	377		τ_o[(C-C-C-C)(CH_3-R2+R2)(40)]
375	363		τ_o[(C-C-C-C)(CH_3-R2+R2)(30)]
272	263		τ_o[(N-C-C-C)(NO_2-R1+R1)(27)]
241	233		τ_i[(H-C-C-C)(CH3-R2+R2)(20)]+ τ_i[(H-C-C-C)(CH3-R4+R4)(16)]
230	222		τ_i[(H-C-C-C)(CH3-R2+R2)(23)]
224	216		τ_i[(H-C-C-C)(CH3-R4+R4)(43)]
175	169		β [(N-C-C)NO_2-R1(22)+(C-C-C)COOH+R1(18)]
106	103		τ_i[{(C-C-C-C)(R2)+(C53-C52-N7-C4)}(22)]
79	77		τ_i[{(C-C-C-C)(R2)+(C53-C52-N7-C4)}(19)]
65	63		τ_i[(O-N-C-C)(NO_2-R1)(30)]+ τ_i[(C-C-C-C)(R1+R2+R3-R4)(18)]
62	60		τ_i[(O-C-C-C)(COOH)(35)]
58	56		τ_i[(C-C-C-C)(R1+R2+R3-R4)(20)]
43	41		τ_o[(C52-C4-C8-N7)(34)]
41	40		τ_i[(C-C-C-C)(R1+R2+R3-R4)(19)]
32	33		τ_i[(O-N-C-C)(NO_2-R1)(29)]
31	30		τ_i[(O-C-C-C)(COOH)(24)]
25	25		τ_i[(O-C-C-C)(COOH)(18)]

ν: stretching; ν_s: symmetric stretching; ν_{as}: anti-symmetric stretching; β: bending in-plane; β_O: bending out-of-plane; τ_i: torsion in plane; τ_o : torsion out-of-plane

Tab. S-V: Experimental and calculated absorption wavelengths, *nm*, excitation energies, *eV*, absorbance values and oscillator strengths of MTDOSA

Excitation energy, *eV*	Wavelength, *nm*		Oscillator strength	Orbital transition
	TD-DFT/B3LYP/6-311++G(d,p)	Experimental		
5.5109	224.98	225.6	0.1984	HOMO-4→LUMO+4(5%) HOMO→LUMO+6(18%) HOMO→LUMO+7(50%) HOMO→LUMO+8(6%)
5.4198	228.76		0.0100	HOMO→LUMO+5(36%) HOMO→LUMO+6(29%)

				HOMO→LUMO+7(39%)
5.3300	232.61		0.0002	HOMO-4→LUMO+1(68%) HOMO-4→LUMO+2(13%)
				HOMO-2→LUMO+1(12%)
4.3627	284.19	288.2	0.0187	HOMO-1→LUMO+1(11%) HOMO →LUMO+1(70%)
				HOMO→LUMO+2(09%)
3.5586 eV	348.41		0.1312	HOMO-1 →LUMO(77%) HOMO →LUMO(20%)

Tab. S-VI: Experimental and calculated absorption wavelengths, *nm*, excitation energies, *eV*, absorbance values and oscillator strengths of NTDOSA

Excitation energy, *eV*	Wavelength, *nm*		Oscillator strength	Orbital transition
	TD-DFT/B3LYP/6-311++G(d,p)	Experimental		
4.0163	308.70	269.4	0.1391	HOMO-4→LUMO(70%) HOMO-3→LUMO(25%)
4.3298	286.35		0.1751	HOMO-5→LUMO(88%) HOMO→LUMO+2(7%)
4.4276	280.02		0.0109	HOMO-11→LUMO(34%) HOMO-10→LUMO(38%) HOMO-3→LUMO+1(15%) HOMO →LUMO+2(15%)
4.4376	279.39		0.0502	HOMO-11→LUMO(08%) HOMO-10 →LUMO(9%) HOMO-5→LUMO(7%) HOMO -3→LUMO+1(12%) HOMO →LUMO+2(57%)
4.6466	266.83		0.0110	HOMO-3 →LUMO+1(14%) HOMO→LUMO+3(67%) HOMO→LUMO+4(5%) HOMO→LUMO+5(09%)
4.6933	264.17		0.0067	HOMO→LUMO+3(8%) HOMO →LUMO+4(89%)
5.0769	244.21		0.0521	HOMO -4→LUMO+1(26%) HOMO-3 →LUMO+1(06%) HOMO -2→LUMO+2(46%) HOMO-2 →LUMO+3(06%) HOMO-1 →LUMO+1(5%)
5.2619	236.25		0.0717	HOMO-5→LUMO+1(25%) HOMO→LUMO+6(26%) HOMO→LUMO+7(35%)
5.2780	234.91	233.2	0.1370	HOMO-5→LUMO+1(32%) HOMO→LUMO+7(48%)

Table S-VII: Experimental and theoretical, ^{1}H and ^{13}C NMR isotropic chemical shifts (δ, in *ppm*) (with respect to TMS) MTDOSA with DFT (B3LYP/6-311++G(d,p)) method in DMSO.

Atom	δcal.	δexp.	Assignment
C1	56.5682	40.96	[C(R2)]
C2	42.6899	31.05	[C(R2)]
C3	45.5566	32.27	[C(R2)]
C4	167.2499	115.88	[C(R2,R3)]
C5	126.1185	113.57	[C(R2,R3)]
C6	205.9577	196.62	[C(R2)]
C8	162.6507	115.88	[C(R3,4)]
C9	127.596	113.57	[C(R3,4)]
C10	37.2998	50.86	[C(R3)]
C11	46.3124	32.27	[C(R4)]
C12	42.923	31.05	[C(R4)]
C13	56.0562	40.96	[C(R4)]
C14	205.9336	196.62	[C(R4)]
C17	146.5313	129.40	[C(R1)]
C18	138.1241	136.59	[C(R1)]
C19	123.7251	129.40	[C(R1)]
C20	167.5973	158.06	[C(R1)]
C21	114.6153	129.40	[C(R1)]
C22	136.3578	136.59	[C(R1)]
C23	33.6405	27.43	[C(CH_3-R2)]
C24	26.7414	27.43	[C(CH_3-R2)]
C25	33.8613	29.34	[C(CH_3-R4)]
C26	26.8242	29.34	[C(CH_3-R4)]
C28	57.4729	55.21	[C(CH_3-O-R1)]
C57	61.5561	93.52	[C(NR3)]
C58	48.0001	50.86	[C(CH_2)]
C62	177.5777	162.21	[C(COOH)]
C66	176.9226	162.21	[C(COOH)]
	Chemical shift for Hydrogen		
Atom	δcal.	δexp.	Assignment
H29	2.1596	2.44(2H, s)	[s, H(R2)]
H30	2.4513	2.44(2H, s)	[s, H(R2)]
H31	2.9517	2.16-2.12(2H, m)	[m, H(R2)]
H32	2.1395	2.16-2.12(2H, m)	[m, H(R2)]
H33	5.3505	4.78(br s)	[s, H(C-R1,R3)]
H34	2.6412	2.23-2.19(2H, m)	[m, H(R4)]
H35	1.8643	2.23-2.19(2H, m)	[m, H(R4)]
H36	2.1917	2.44(2H, s)	[s, H(R4)]
H37	2.0298	2.44(2H, s)	[s, H(R4)]
H38	7.8589	7.17(1H, *d*, *J* = 8.8 Hz)	[d, H(R1)]
H39	6.9039	6.73(1H, *d*, *J* = 8.4 Hz)	[d, H(R1)]
H40	6.8884	6.73 (1H, *d*, *J* = 8.4 Hz)	[d, H(R1)]
H41	8.1223	7.17 (1H, *d*, *J* = 8.8 Hz)	[d, H(R1)]
H42	1.1034	0.97 (3H, s)	[s, H(CH_3-R2)]
H43	1.1004	0.97 (3H, s)	[s, H(CH_3-R2)]
H44	1.1731	0.97 (3H, s)	[s, H(CH_3-R2)]
H45	1.3565	0.97 (3H, s)	[s, H(CH_3-R2)]
H46	0.8171	0.97 (3H, s)	[s, H(CH_3-R2)]
H47	0.8885	0.97 (3H, s)	[s, H(CH_3-R2)]
H48	0.9945	1.08 (3H, s)	[s, H(CH_3-R4)]
H49	1.0912	1.08 (3H, s)	[s, H(CH_3-R4)]

H50	1.1789	1.08 (3H, s)	[s, H(CH_3-R4)]
H51	0.8115	1.08 (3H, s)	[s, H(CH_3-R4)]
H52	1.3637	1.08 (3H, s)	[s, H(CH_3-R4)]
H53	0.8535	1.08 (3H, s)	[s, H(CH_3-R4)]
H54	4.1108	3.71 (3H, s)	[s, H(CH_3-O-R1)]
H55	3.7625	3.71 (3H, s)	[s, H(CH_3-O-R1)]
H56	3.7903	3.71 (3H, s)	[s, H(CH_3-O-R1)]
H59	4.7417	4.78	[H(C-R3)]
H60	3.752	4.67	[H(CH_2)]
H61	2.8325	4.67	[H(CH_2)]
H65	9.7824		[H(COOH)]
H69	6.9706		[H(COOH)]

Table S-VIII: Experimental and theoretical, ^{1}H and ^{13}C NMR isotropic chemical shifts (δ, in *ppm*) (with respect to TMS) of NTDOSA with DFT (B3LYP/6-311++G(d,p)) method in DMSO

Atom	δcal.	δexp.	Assignment
		Corbon	
C1	55.8721	35.09	[C(R2)]
C2	42.4765	24.55	[C(R2)]
C3	45.4334	26.84	[C(R2)]
C4	168.7219	114.87	[C(R2,R3)]
C5	125.0398	113.54	[C(R2,R3)]
C6	205.9295	177.45	[C(R2)]
C8	164.4064	126.43	[C(R3,R4)]
C9	125.6429	107.62	[C(R3,R4)]
C10	39.3279	36.95	[C(R3)]
C11	46.4148	26.84	[C(R4)]
C12	42.9173	24.55	[C(R4)]
C13	55.6659	35.09	[C(R4)]
C14	206.2335	179.83	[C(R4)]
C17	164.7724	127.47	[C(R1)]
C18	138.2502	129.49	[C(R1)]
C19	130.0735	146.14	[C(R1)]
C20	156.7579	163.94	[C(R1)]
C21	131.4079	139.25	[C(R1)]
C22	136.0572	129.15	[C(R1)]
C23	33.4636	15.83	[C(CH_3-R2)]
C24	26.7644	15.83	[C(CH_3-R2)]
C25	33.1922	21.50	[C(CH_3-R4)]
C26	26.7744	21.50	[C(CH_3-R4)]
C52	61.8097	67.45	[C(NR3)]
C53	47.6303	30.94	[C(CH_2)]
C57	177.6375	173.11	[C(COOH)]
C61	176.4971	169.99	[C(COOH)]
		Hydrogen	
H27	2.2047	2.69-2.59 (2H, m)	[m, H(R2)]
H28	2.419	2.69-2.59 (2H, m)	[m, H(R2)]
H29	2.9088	2.69-2.59 (2H, m)	[m, H(R2)]
H30	2.1713	2.69-2.59 (2H, m)	[m, H(R2)]
H31	5.5051	4.51 (s)	[s, H(R3)]
H32	2.6342	2.69-2.59 (2H, m)	[m, H(R4)]

H33	1.9143	2.69-2.59 (2H, m)	[m, H(R4)]
H34	2.2446	2.69-2.59 (2H, m)	[m, H(R4)]
H35	2.1475	2.69-2.59 (2H, m)	[m, H(R4)]
H36	8.0988	6.76 (1H, *d*, *J* = 8.8 Hz)	[d, H(R1)]
H37	8.1757	7.07 (1H, *d*, *J* = 8.4 Hz)	[d, H(R1)]
H38	8.4868	7.07 (1H, *d*, *J* = 8.4 Hz)	[d, H(R1)]
H39	8.4312	6.76 (1H, *d*, *J* = 8.8 Hz)	[d, H(R1)]
H40	1.1063	1.83 (3H, s)	[s, H(CH_3-R2)]
H41	1.119	1.83 (3H, s)	[s, H(CH_3-R2)]
H42	1.2112	1.83 (3H, s)	[s, H(CH_3-R2)]
H43	1.3445	1.23 (3H, s)	[s, H(CH_3-R2)]
H44	0.8175	1.23 (3H, s)	[s, H(CH_3-R2)]
H45	0.895	1.23 (3H, s)	[s, H(CH_3-R2)]
H46	0.9771	2.25 (3H, s)	[s, H(CH_3-R4)]
H47	1.071	2.25 (3H, s)	[s, H(CH_3-R4)]
H48	1.1639	2.25 (3H, s)	[s, H(CH_3-R4)]
H49	0.8346	1.94 (3H, s)	[s, H(CH_3-R4)]
H50	1.3659	1.94 (3H, s)	[s, H(CH_3-R4)]
H51	0.8936	1.94 (3H, s)	[s, H(CH_3-R4)]
H54	4.7507	2.34-2.33 (1H, m)	[s, H(C-R3)]
H55	3.801	2.33-2.28 (2H, m)	[m, H(CH_2)]
H56	2.8027	2.33-2.28 (2H, m)	[m, H(CH_2)]
H60	9.8863		[H(COOH)]
H64	6.9745		[H(COOH)]

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