Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. *85* (1) S35–S56 (2020) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Spectroscopic (FTIR, UV–Vis and NMR), theoretical investigation and molecular docking of substituted 1,8-dioxodecahydroacridine derivatives

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J. Serb. Chem. Soc. *85* (1) (2020) 53–66

CHARACTERIZATION DATA OF THE SYNTHESIZED COMPOUNDS **4a** AND **4b**

*2-(9-(4-Methoxyphenyl)-3,3,6,6-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydroacridin-10(1*H*)-yl)succinic acid (**4a**)*. White solid: yield 86 %; mp 255 °C; R_f (50 % ethyl acetate/petroleum ether) 0.69; IR (KBr), ν_{max} / cm^{-1}: 3312 (COOH), 3069, 3002, 2959, 2877, 2834, 2359, 1710(COOH), 1668 (CO), 1606, 1510, 1461, 1360, 1301, 1260, 1233, 1194, 1163, 1137, 1108, 1031, 998, 934, 845, 776, 685, 637, 567, 532, 422; ^{1}H-NMR (400 MHz, $CDCl_3$), δ / ppm: 7.17 (2H, *d, J* = 8.8 Hz, Ar-H), 6.73 (2H, *d*, *J* = 8.4 Hz, Ar-H), 4.78 (2H, *s*, CH and NC**H**(COOH)), 4.67 (2H, *br s*, CH_2), 3.71 (3H, *s*, Ar-OCH_3), 2.44 (4H, *s*, 2×CH_2), 2.23–2.19 (2H, *m*, CH_2), 2.16–2.12 (2H, *m*, CH_2), 1.08 (6H, *s*, 2×CH_3), 0.97 (6H, *br s*, 2×CH_3); ^{13}C-NMR (100 MHz, $CDCl_3$), δ / ppm: 196.62 (2×CO), 162.21 (2×COOH), 158.06 (2C), 136.59 (2C), 129.40 (3C), 115.88 (2C), 113.57 (2C), 93.52 (N–C), 55.21 (Ar–O**C**H_3), 50.86 (CH_2), 40.96 (2×CO**C**H_2), 32.27 (2×CH_2), 31.05 (2C), 29.34 (2×CH_3), 27.43 (2×CH_3). Elemental analysis: Calcd. (%) for $C_{28}H_{33}NO_7$: C, 67.86; H, 6.71; N, 2.83; found: C, 67.94; H, 6.70; N, 2.80.

*2-(3,3,6,6-Tetramethyl-9-(4-nitrophenyl)-1,8-dioxo-2,3,4,5,6,7,8,9-octahydroacridin-10(1*H*)-yl)succinic acid (**4b**)*. White solid: yield 74 %; mp 215 °C, R_f (50 % ethyl acetate/petroleum ether) 0.65; IR (KBr), ν_{max} / cm^{-1}: 3382 (COOH), 3117, 2956, 2866, 2360, 1731 (COOH), 1722 (COOH), 1665 (CO), 1593, 1474, 1386, 1299, 1194, 1114, 1017, 910, 858, 788, 750, 678, 660, 573, 523, 461; ^{1}H--NMR (400 MHz, DMSO-d_6), δ / ppm: 7.07 (2H, *d*, *J* = 8.4 Hz, Ar-H), 6.76 (2H,

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d, *J* = 8.8 Hz, Ar-H), 4.51 (1H, *s*, CH), 2.69–2.59 (8H, *m*, 4×CH_2), 2.34–2.33 (1H, *m*, CH), 2.33–2.28 (2H, *m*, CH_2), 2.25 (3H, *s*, CH_3), 1.94 (3H, *s*, CH_3), 1.83 (3H, *s*, CH_3), 1.23 (3H, *s*, CH_3); ^{13}C-NMR (100 MHz, DMSO--d_6): δ / ppm: 179.83 (*C*O), 177.45 (CO), 173.11 (COOH), 169.99 (COOH), 163.94, 146.14, 139.25, 129.49, 129.15, 127.47, 126.43, 114.87, 113.54, 107.62, 67.45 (N–C), 36.95 (CH), 35.09 (2×CO**C**H_2), 30.94 (**C**H_2(COOH)), 26.84 (2×CH_2), 24.55 (2C), 21.50 (2×CH_3), 15.83 (2×CH_3). Elemental analysis: Calcd. (%) for $C_{27}H_{30}N_2O_8$: C, 63.52; H, 5.92; N, 5.49; found: C, 63.58; H, 5.90; N, 5.51.

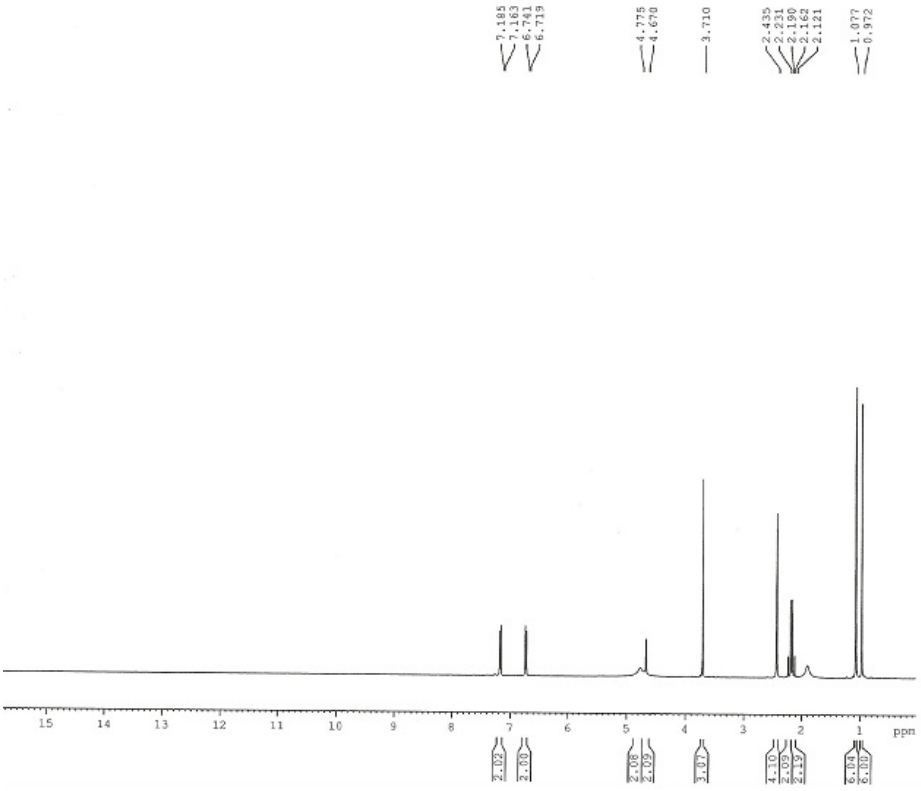

Fig. S-1. Experimental ^{1}H-NMR plot of MTDOSA.

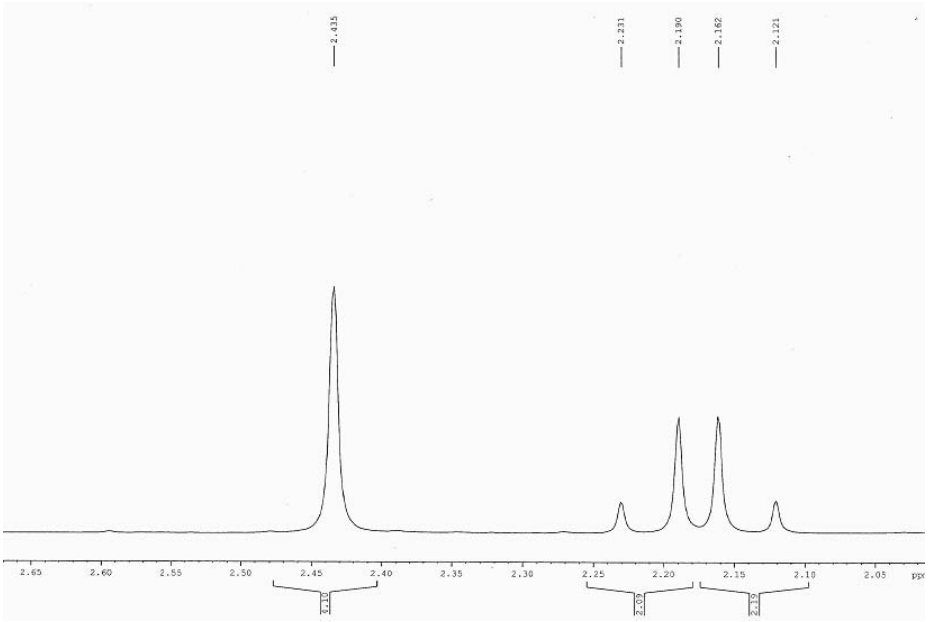

Fig. S-2. Experimental ^{1}H-NMR plot of MTDOSA (extended scale-I).

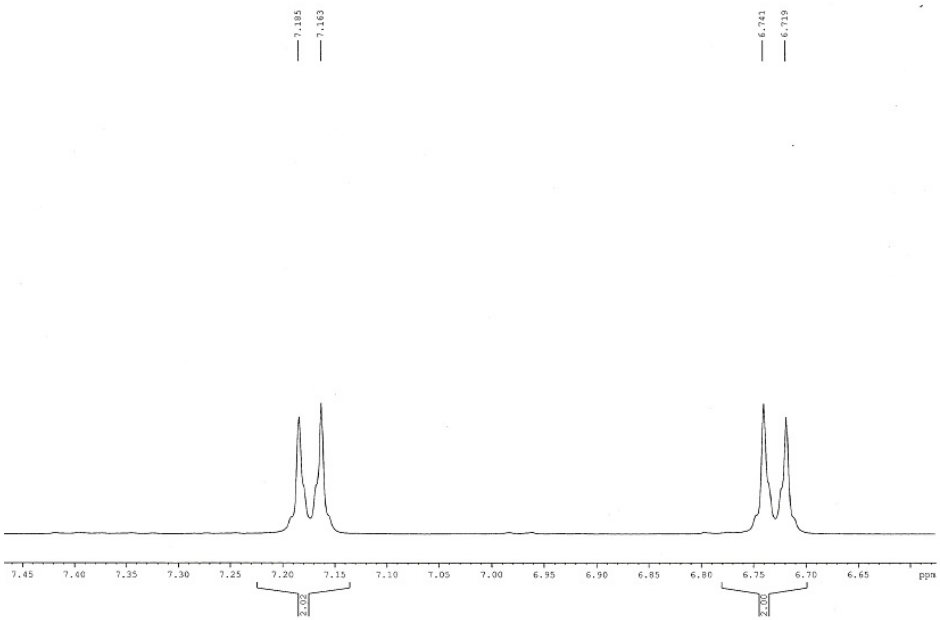

Fig. S-3. Experimental ^{1}H-NMR plot of MTDOSA (extended scale-II).

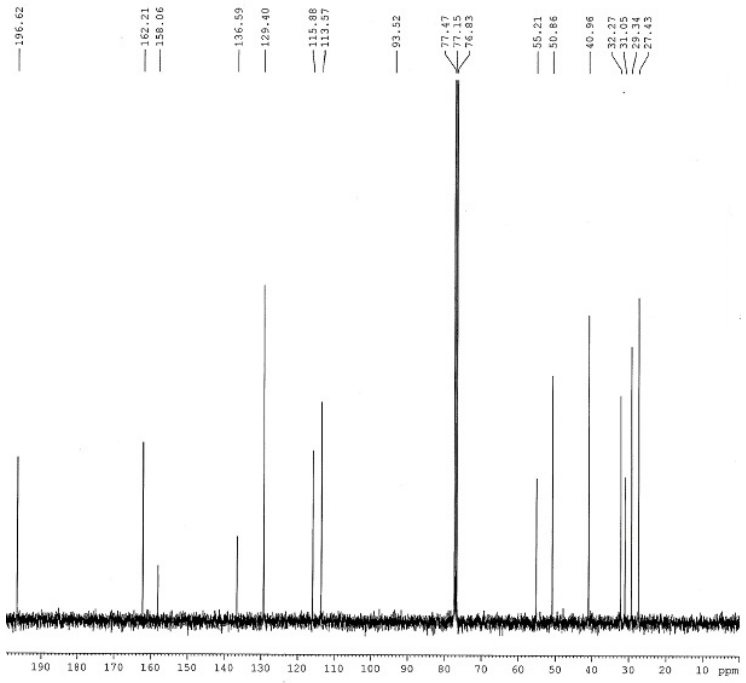

Fig. S-4. Experimental ^{13}C-NMR Plot of MTDOSA.

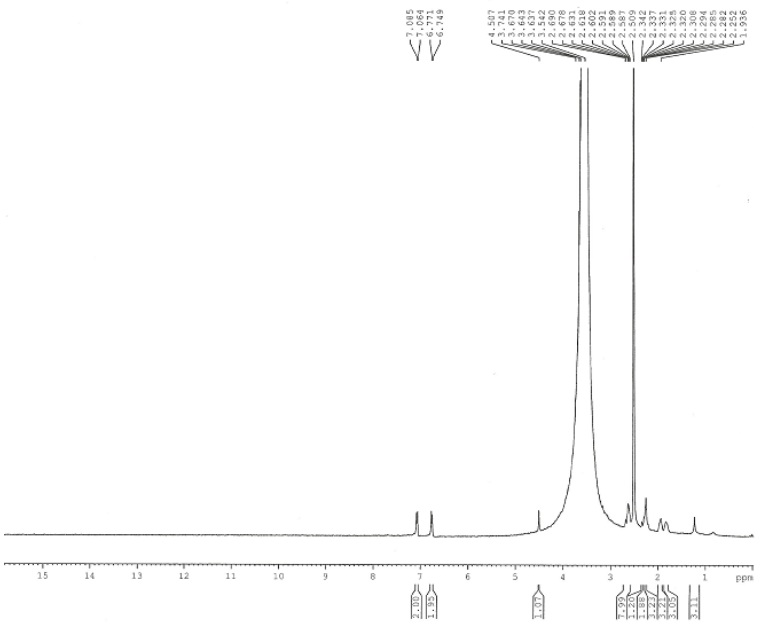

Fig. S-5. Experimental ^{1}H-NMR plot of NTDOSA.

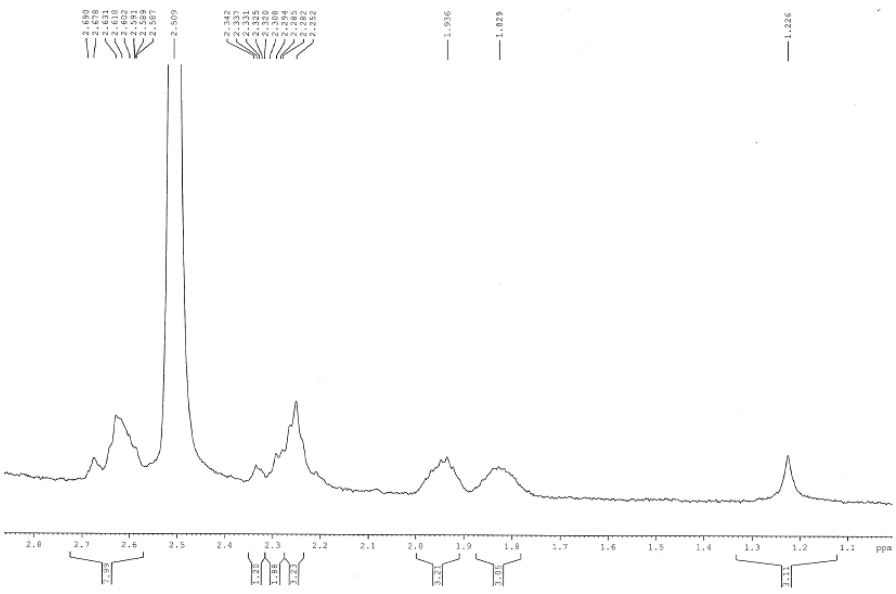

Fig. S-6. Experimental ^{1}H-NMR plot of NTDOSA (extended scale-I).

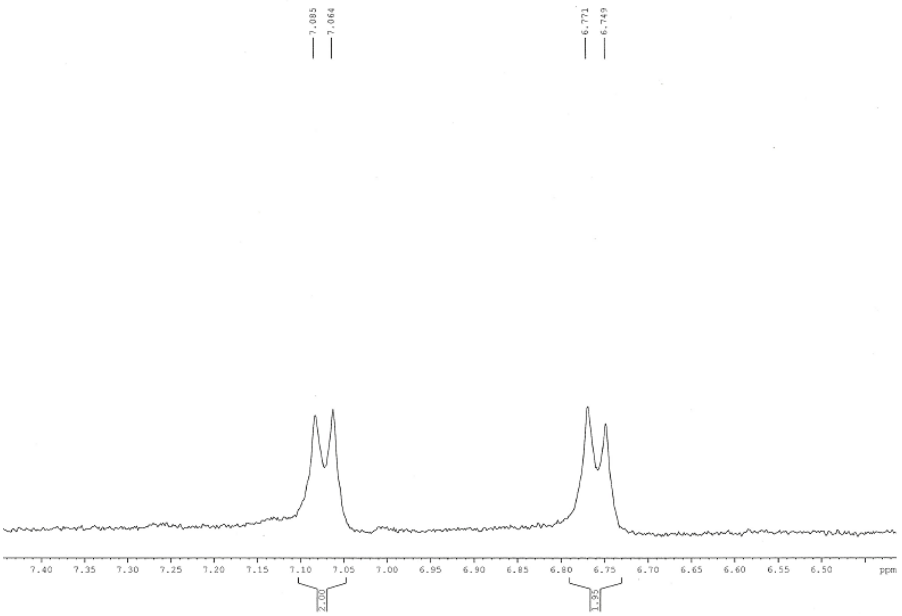

Fig. S-7. Experimental ^{1}H-NMR plot of NTDOSA (extended scale-II).

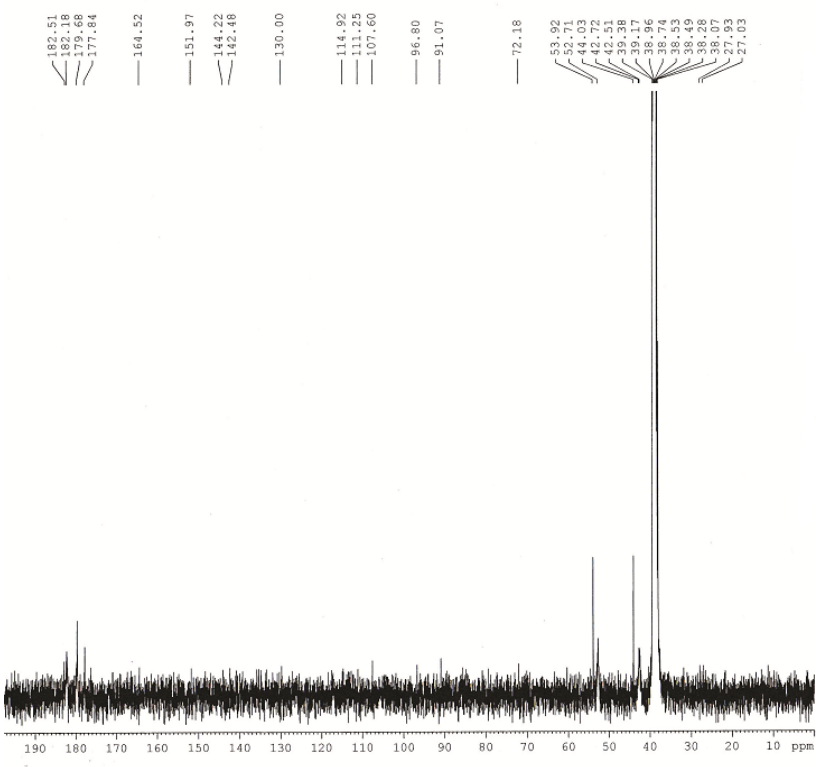

Fig. S-8. Experimental ^{13}C-NMR Plot of NTDOSA.

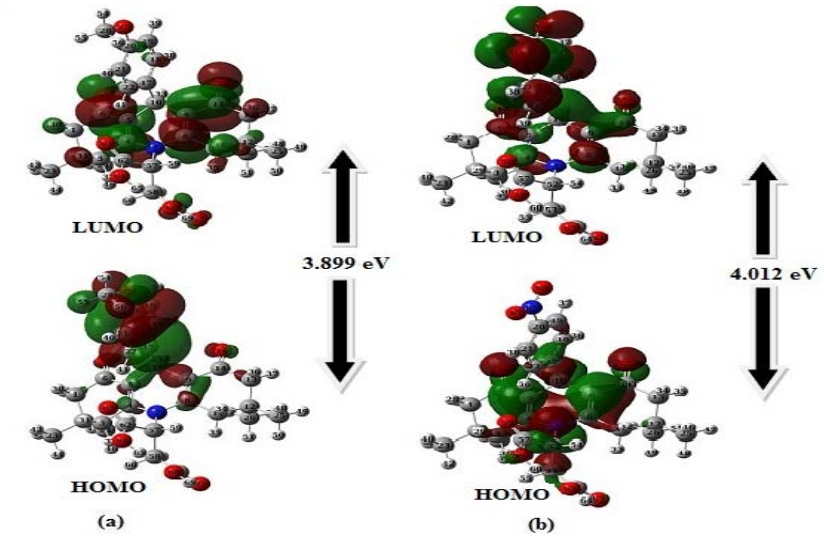

Fig. S-9. HOMO, LUMO plots of MTDOSA (a) and NTDOSA (b) molecules.

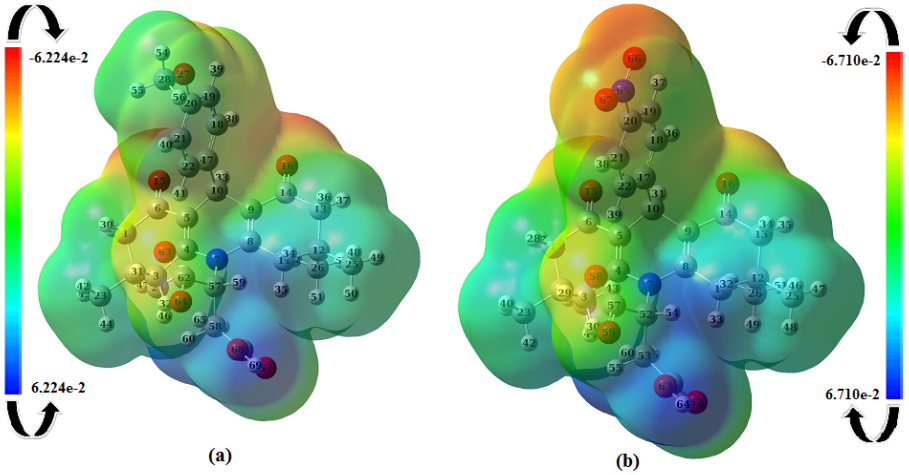

Fig. S-10. MESP Surface forMTDOSA (a) and NTDOSA (b) calculated at B3LYP/6-311++G (d,p).

TABLE S-I. Optimized geometric parameter for MTDOSA

Parameter	DFT/B3LYP6311++G(d,p) Bond length, Å	Parameter	DFT/B3LYP6311++G(d,p) Dihedral angle, °
C1-C2	1.537	C6-C1-C2-C3	53.25
C1-C6	1.518	C6-C1-C2-C23	171.72
C2-C3	1.546	C6-C1-C2-C24	-67.97
C3-C4	1.515	C2-C1-C6-C5	-33.75
C4-C5	1.355	C2-C1-C6-O15	147.79
C4-N7	1.416	C1-C2-C3-C4	-59.60
C5-C6	1.476	C23-C2-C3-C4	-168.84
C5-C10	1.511	C24-C2-C3-C4	71.36
C6-O15	1.220	C2-C3-C4-C5	26.53
N7-C8	1.415	C2-C3-C4-N7	-151.00
N7-C57	1.461	C3-C4-C5-C6	-3.83
C8-C9	1.354	C3-C4-C5-C10	176.63
C8-C11	1.516	N7-C4-C5-C6	173.66
C9-C10	1.515	N7-C4-C5-C10	-5.87
C9-C14	1.475	C3-C4-CN7-C8	159.64
C10-C17	1.534	C3-C4-N7-C57	-23.90
C11-C12	1.547	C5-C4-N7-C8	-17.94
C12-C13	1.536	C3-C4-N7-C57	158.50
C12-C25	1.537	C4-C5-C6-C1	7.42
C12-C26	1.541	C4-C5-C6-O15	-174.13
C13-C14	1.519	C10-C5-C6-C1	-173.01
C14-O16	1.221	C10-C5-C6-O15	4.43
C17-C18	1.402	C4-C5-C10-C9	26.43
C17-C22	1.393	C4-C5-C10-C17	-99.03

Parameter	DFT/B3LYP6311++G(d,p)	Parameter	DFT/B3LYP6311++G(d,p)
	Bond length, Å		Dihedral angle, °
C18-C19	1.386	C6-C5-C10-C9	-153.12
C19-C20	1.399	C6-C5-C10-C17	81.41
C20-C21	1.395	C4-N7-C8-C9	17.88
C20-O27	1.369	C4-N7-C8-C11	-159.18
C21-C22	1.398	C57-N7-C8-C9	-158.71
O27-C28	1.418	C57-N7-C8-C11	24.21
C57-C58	1.576	C4-N7-C57-C58	79.23
C57-C62	1.551	C4-N7-C57-C62	-52.58
C58-C66	1.511	C8-N7-C57-C58	-104.31
C62-O63	1.197	C8-N7-C57-C62	123.87
C62-O64	1.346	N7-C8-C9-C10	6.00
O64-H65	0.973	N7-C8-C9-C14	-173.13
C66-O67	1.198	C11-C8-C9-C10	-177.07
C66-O68	1.372	C11-C8-C9-C14	3.79
O68-H69	0.97	N7-C8-C11-C12	151.92
	Bond Angle, °	C9-C8-C11-C12	-25.08
C2-C1-C6	113.48	C8-C9-C10-C5	-26.41
C1-C2-C3	107.84	C8-C9-C10-C17	99.90
C1-C2-C23	109.97	C14-C9-C10-C5	152.75
C1-C2-C24	110.42	C14-C9-C10-C17	-80.94
C3-C2-C23	108.77	C8-C9-C14-C13	-8.69
C3-C2-C24	110.83	C8-C9-C14-O16	172.84
C23-C2-C24	108.98	C10-C9-C14-C13	172.14
C2-C3-C4	114.11	C10-C9-C14-O16	-6.32
C3-C4-C5	121.87	C5-C10-C17-C18	-149.36
C3-C4-N7	118.33	C5-C10-C17-C22	41.44
C5-C4-N7	119.74	C9-C10-C17-C18	96.70
C4-C5-C6	120.89	C9-C10-C17-C22	-82.49
C4-C5-C10	122.20	C8-C11-C12-C13	48.17
C6-C5-C10	116.90	C8-C11-C12-C25	167.80
C1-C6-C5	117.96	C8-C11-C12-C26	-72.65
C1-C6-O15	120.76	C11-C12-C13-C14	-53.15
C5-C6-O15	121.27	C25-C12-C13-C14	-172.02
C4-N7-C8	118.69	C26-C12-C13-C14	67.63
C4-N7-C57	122.68	C12-C13-C14-C9	34.93
C8-N7-C57	118.52	C12-C13-C14-O16	-146.59
N7-C8-C9	120.31	C10-C17-C18-C19	-179.00
N7-C8-C11	117.41	C22-C17-C18-C19	-0.21
C9-C8-C11	122.22	C10-C17-C22-C21	179.05
C8-C9-C10	121.61	C18-C17-C22-C21	-0.15
C8-C9-C14	120.79	C17-C18-C19-C20	-0.14
C10-C9-C14	117.58	C18-C19-C20-C21	0.01
C5-C10-C9	109.09	C18-C19-C20-O27	-179.77
C5-C10-C17	113.38	C19-C20-C21-C22	0.07

Parameter	DFT/B3LYP6311++G(d,p)	Parameter	DFT/B3LYP6311++G(d,p)
	Bond length, Å		Dihedral angle, °
C9-C10-C17	111.93	O27-C20-C21-C22	179.81
C8-C11-C12	114.22	C19-C20-O27-C28	178.73
C11-C12-C13	108.10	C21-C20-O27-C28	-1.02
C11-C12-C25	108.90	C20-C21-C22-C17	0.02
C11-C12-C26	110.34	N7-C57-C58-C66	129.19
C13-C12-C25	110.11	C62-C57-C58-C66	-99.43
C13-C12-C26	110.41	N7-C57-C62-O63	-1.65
C25-C12-C26	108.96	N7-C57-C62-O64	-179.67
C12-C13-C14	113.47	C58-C57-C62-O63	-133.63
C9-C14-C13	117.88	C58-C57-C62-O64	48.34
C9-C14-O16	121.44	C57-C58-C66-O67	-124.96
C13-C14-O16	120.66	C57-C58-C66-O68	55.32
C10-C17-C18	119.85	C21-C20-O27-C28	-1.02
C10-C17-C22	122.16	C20-C21-C22-C17	0.02
C18-C17-C22	117.98	N7-C57-C58-C66	129.19
C17-C18-C19	121.23	C62-C57-C58-C66	-99.43
C18-C19-C20	120.17	N7-C57-C62-O63	-1.65
C19-C20-C21	119.46	N7-C57-C62-O64	-179.67
C19-C20-O27	115.94	C58-C57-C62-O63	-133.63
C21-C20-O27	124.61	C58-C57-C62-O64	48.34
C20-C21-C22	119.67	C57-C58-C66-O67	-124.96
C17-C22-C21	121.49		
C20-O27-C28	118.42		
N7-C57-C58	114.08		
C58-C57-C62	113.74		
C57-C58-C66	114.52		
C57-C62-O63	124.04		
C57-C62-O64	115.14		
O63-C62-O64	120.79		
C58-C66-O67	126.75		
C58-C66-O68	111.28		
O67-C66-O68	121.96		

TABLE S-II. Optimized geometric parameters for NTDOSA

Parameter	DFT/B3LYP6311++G(d,p) Bond length, Å	Parameter	DFT/B3LYP6311++G(d,p) Dihedral angle, °
C1-C2	1.538	C6-C1-C2-C3	52.83
C1-C6	1.517	C6-C1-C2-C23	171.23
C2-C3	1.548	C6-C1-C2-C24	-68.48
C2-C23	1.538	C2-C1-C6-C5	-32.48
C2-C24	1.541	C2-C1-C6-O15	159.65
C3-C4	1.514	C1-C2-C3-C4	-49.73
C4-C5	1.355	C23-C2-C3-C4	-169.93
C4-N7	1.415	C24-C2-C3-C4	71.35
C5-C6	1.476	C2-C3-C4-C5	26.26
C5-C10	1.510	C2-C3-C4-N7	-151.12
C6-O15	1.221	C3-C4-C5-C6	-2.74
N7-C8	1.4132	C3-C4-C5-C10	177.47
N7-C52	1.4637	N7-C4-C5-C6	174.61
C8-C9	1.355	N7-C4-C5-C10	-5.16
C8-C11	1.516	C3-C4-N7-C8	159.78
C9-C10	1.515	C3-C4-N7-C52	-24.86
C9-C14	1.475	C5-C4-N7-C8	-17.68
C10-C17	1.534	C5-C4-N7-C52	157.69
C11-C12	1.547	C4-C5-C6-C1	5.82
C12-C13	1.573	C4-C5-C6-O15	-176.03
C12-C25	1.537	C10-C5-C6-C1	-174.38
C12-C26	1.542	C10-C5-C6-O15	3.75
C13-C14	1.517	C4-C5-C10-C9	24.95
C14-O16	1.221	C4-C5-C10-C17	-100.29
C17-C18	1.400	C6-C5-C10-C9	-154.83
C17-C22	1.400	C6-C5-C10-C17	79.91
C18-C19	1.389	C4-N7-C8-C9	17.54
C19-C20	1.391	C4-N7-C8-C11	-159.31
C20-C21	1.391	C52-N7-C8-C9	-157.99
C20-N65	1.475	C52-N7-C8-C11	25.14
C21-C22	1.390	C4-N7-C52-C53	79.63
C52-C53	1.574	C4-N7-C52-C57	-52.35
C52-C57	1.552	C8-N7-C52-C53	-105.01
C53-C61	1.511	C8-N7-C52-C57	123.01
C57-O58	1.198	N7-C8-C9-C10	5.38
C57-O59	1.344	N7-C8-C9-C14	-173.33
C61-O62	1.198	C11-C8-C9-C10	-177.89
C61-O63	1.371	C11-C8-C9-C14	3.38
N65-O66	1.226	N7-C8-C11-C12	151.56
N65-O67	1.227	C9-C8-C11-C12	-25.25

Parameter	DFT/B3LYP6311++G(d,p) Bond angle, °	Parameter	DFT/B3LYP6311++G(d,p) Dihedral angle, °
C2-C1-C6	113.55	C8-C9-C10-C5	-24.99
C1-C2-C3	107.96	C8-C9-C10-C17	101.23
C1-C2-C23	109.92	C14-C9-C10-C5	153.77
C1-C2-C24	110.48	C14-C9-C10-C17	-79.99
C3-C2-C23	108.67	C8-C9-C14-C13	-7.80
C3-C2-C24	110.45	C8-C9-C14-C16	173.90
C23-C2-C24	108.97	C10-C9-C14-C13	173.41
C2-C3-C4	113.11	C10-C9-C14-O16	-4.87
C3-C4-C5	121.67	C5-C10-C17-C18	-138.92
C3-C4-N7	118.40	C5-C10-C17-C22	41.97
C5-C4-N7	119.87	C9-C10-C17-C18	97.10
C4-C5-C6	121.13	C9-C10-C17-C22	-81.99
C4-C5-C10	122.31	C8-C11-C12-C13	48.43
C6-C5-C10	116.55	C8-C11-C12-C25	168.02
C1-C6-C5	118.04	C8-C11-C12-C26	-72.36
C1-C6-O15	121.98	C11-C12-C13-C14	-52.92
C5-C6-O15	120.94	C25-C12-C13-C14	-171.74
C4-N7-C8	118.74	C26-C12-C13-C14	67.84
C4-N7-C52	122.51	C12-C13-C14-C9	34.15
C8-N7-C52	118.58	C12-C13-C14-O16	-147.55
N7-C8-C9	120.46	C10-C17-C18-C19	-178.81
N7-C8-C11	117.42	C10-C17-C22-C21	178.78
C9-C8-C11	122.02	C18-C17-C22-C21	-0.32
C8-C9-C10	121.68	C17-C18-C19-C20	0.012
C8-C9-C14	120.94	C18-C19-C20-C21	-0.29
C10-C9-C14	117.35	C18-C19-C20-N65	179.90
C5-C10-C9	109.29	C19-C20-C21-C22	0.28
C5-C10-C17	113.35	N65-C20-C21-C22	-179.91
C9-C10-C17	111.66	C19-C20-N65-O66	0.01
C8-C11-C12	114.23	C19-C20-N65-O67	-179.85
C11-C12-C13	108.11	C21-C20-N65-O66	-179.80
C11-C12-C25	108.88	C21-C20-N65-O67	0.33
C11-C12-C26	110.34	C20-C21-C22-C17	-0.02
C13-C12-C25	110.08	N7-C52-C53-C61	130.24
C13-C12-C26	110.38	C57-C52-C53-C61	-98.68
C25-C12-C26	109.02	N7-C52-C57-O58	-3.19
C12-C13-C14	113.53	N7-C52-C57-O59	178.86
C9-C14-C13	117.95	C53-C52-C57-O58	-135.10
C9-C14-O16	121.18	C53-C52-C57-O59	46.95
C13-C14-O16	120.83	C52-C53-C61-O62	-122.93
C10-C17-C18	119.58	C52-C53-C61-O63	57.14
C10-C17-C22	121.48	N65-C20-C21-C22	-179.91
C18-C17-C22	118.92	C19-C20-N65-O66	0.01
C17-C18-C19	120.94	C19-C20-N65-O67	-179.85

Parameter	DFT/B3LYP6311++G(d,p) Bond angle, °	Parameter	DFT/B3LYP6311++G(d,p) Dihedral angle, °
C18-C19-C20	118.77	C21-C20-N65-O66	-179.80
C19-C20-C21	121.68	C21-C20-N65-O67	0.33
C19-C20-N65	119.20	C20-C21-C22-C17	-0.02
C21-C20-N65	119.11	N7-C52-C53-C61	130.24
C20-C21-C22	118.81	C57-C52-C53-C61	-98.68
C17-C22-C21	120.86	N7-C52-C57-O58	-3.19
N7-C52-C53	114.06	N7-C52-C57-O59	178.86
N7-C52-C57	112.32	C53-C52-C57-O58	-135.10
C53-C52-C57	114.21	C53-C52-C57-O59	46.95
H54-C52-C57	102.47		
C52-C53-C61	114.29		
C52-C57-O58	125.45		
C52-C57-O59	115.45		
O58-C57-O59	120.92		
C57-O59-H60	113.01		
C53-C61-O62	126.68		
C53-C61-O63	111.22		
O62-C61-O63	122.09		
C61-O63-H64	109.16		
C20-N65-O66	117.88		
C20-N65-O67	117.85		
O66-C65-O67	124.27		

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

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)}]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

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

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

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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)]

Frequency, cm^{-1}			Assignment
Cal.	Scaled	Exp. FTIR	
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

TABLE S-V. Experimental and calculated absorption wavelengths, excitation energies, 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%)

TABLE S-VI. Experimental and calculated absorption wavelengths, excitation energies, 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 (with respect to TMS) MTDOSA with DFT (B3LYP/6-311++G(d,p)) method in DMSO

Atom	$\delta_{cal.}$ / ppm	$\delta_{exp.}$/ ppm	Assignment
		Carbon	
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,R4)]
C9	127.596	113.57	[C(R3,R4)]
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)]
		Hydrogen	
Atom	$\delta_{cal.}$ / ppm	$\delta_{exp.}$ / ppm	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(with respect to TMS) of NTDOSAwith DFT (B3LYP/6-311++G(d,p)) method in DMSO

Atom	$\delta_{cal.}$ / ppm	$\delta_{exp.}$/ ppm	Assignment
		Corbon	
C1	55.8721	53.92	[C(R2)]
C2	42.4765	39.38	[C(R2)]
C3	45.4334	42.72	[C(R2)]
C4	168.7219	164.52	[C(R2,R3)]
C5	125.0398	91.07	[C(R2,R3)]
C6	205.9295	182.18	[C(R2)]
C8	164.4064	151.97	[C(R3,R4)]
C9	125.6429	96.80	[C(R3,R4)]
C10	39.3279	39.17	[C(R3)]
C11	46.4148	42.72	[C(R4)]
C12	42.9173	42.51	[C(R4)]
C13	55.6659	52.71	[C(R4)]
C14	206.2335	182.51	[C(R4)]
C17	164.7724	144.22	[C(R1)]
C18	138.2502	130.00	[C(R1)]
C19	130.0735	107.60	[C(R1)]
C20	156.7579	142.48	[C(R1)]
C21	131.4079	111.25	[C(R1)]
C22	136.0572	114.92	[C(R1)]
C23	33.4636	38.28	[C(CH_3-R2)]
C24	26.7644	27.03	[C(CH_3-R2)]
C25	33.1922	38.07	[C(CH_3-R4)]
C26	26.7744	27.93	[C(CH_3-R4)]
C52	61.8097	72.18	[C(NR3)]
C53	47.6303	44.03	[C(CH_2)]
C57	177.6375	179.68	[C(COOH)]
C61	176.4971	177.84	[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)]

Atom	$\delta_{cal.}$ / ppm	$\delta_{exp.}$/ ppm	Assignment
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)]