**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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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) 13C 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) 13C 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, *Å* | 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 | νas[O-H)(99)] |
| 3644 | 3523 | 3312 | νs[O-H)(99)] |
| 3203 | 3097 | 3069 | νas [C-H)R1(94)] |
| 3195 | 3090 |  | νas [C-H)R1(98)] |
| 3188 | 3083 |  | νs [C-H)R1(89)] |
| 3180 | 3075 |  | νas [C-H)R1(98)] |
| 3148 | 3045 |  | νas [C-H) CH2 (98)] |
| 3127 | 3024 |  | νas [C-H) CH3-O (91)] |
| 3104 | 3002 | 3002 | νas [C-H)R2 (91)] |
| 3099 | 2997 |  | νas [C-H)CH3-R4 (76)] |
| 3098 | 2996 |  | νas [C-H)CH3-R2(64)] |
| 3097 | 2995 |  | ν[C57-H59 (94)] |
| 3090 | 2988 |  | νs [C-H)CH3-R4 (54)] |
| 3089 | 2987 |  | νas [C-H)CH3-R2(83)] |
| 3085 | 2983 |  | νas [C-H)CH3-R4(68)] |
| 3083 | 2981 |  | ν[C-H)R2 (54)] |
| 3083 | 2981 |  | νas [C-H){R2(44)+CH3-R2(26)}] |
| 3081 | 2979 |  | νas [(C-H){R2+R3+CH3-R2}(70)] |
| 3080 | 2979 |  | νas [(C-H){R2+R3+CH3-R2}(70)] |
| 3077 | 2976 |  | νas [C-H)CH3-R4(89)] |
| 3075 | 2974 |  | νas [C-H)CH3-R2(84)] |
| 3061 | 2960 | 2959 | νas [C-H)R4 (69)] |
| 3058 | 2957 |  | νs [C-H)CH2 (87)] |
| 3055 | 2954 |  | νas [C-H)CH3-O-R1(100)] |
| 3043 | 2943 |  | νs [C-H)R2 (79)] |
| 3026 | 2926 |  | νs [C-H)CH3-R4 (87)] |
| 3023 | 2923 |  | νs [C-H)CH3-R2 (31)] |
| 3016 | 2916 |  | νs [C-H)CH3-R4 (71)] |
| 3015 | 2915 |  | νas [C-H)CH3-R2(78)] |
| 3007 | 2908 |  | νs [C-H)R2 (73)] |
| 3004 | 2905 |  | νs [C-H)R24(76)] |
| 2999 | 2900 |  | νs [C-H)CH3-O-R1(91)] |
| 2985 | 2886 | 2877 | νs [C-H)R4 (72)] |
| 1846 | 1785 | 1808 | νs [(O=C)COOH(74)] |
| 1836 | 1776 | 1731 | νs [(O=C)COOH(82)] |
| 1722 | 1665 | 1668 | νs [(O=C)R2+R4(89)] |
| 1716 | 1660 |  | ν[(O=C)R4(64)] |
| 1678 | 1622 | 1618 | νs [(C=C)R3(68)] |
| 1648 | 1593 | 1600 | νas [C-C)R1(62)]+ β [(H-C-C)R1(19)] |
| 1627 | 1573 | 1575 | νas [(C=C)R3(71)] |
| 1616 | 1563 | 1556 | νas [C-C)R1(43)] |
| 1540 | 1489 | 1510 | β [(H-C-C)R1(48)] |
| 1514 | 1464 |  | βO [(H-C-H)CH3-R2(48)] |
| 1513 | 1463 | 1461 | βO [(H-C-H)CH3-R4(59)] |
| 1507 | 1457 |  | βO [(H-C-H)CH3-R4(55)] |
| 1506 | 1456 |  | βO [(H-C-H)CH3-R2(51)] |
| 1505 | 1456 |  | βO [(H-C-H)CH3-0-R1(72)] |
| 1500 | 1450 |  | βO [(H-C-H)CH3-R2+R2(39)] |
| 1498 | 1449 |  | βO [(H-C-H)CH3-R4+R4(52)] |
| 1491 | 1442 |  | βO [(H-C-H)CH3-O-R1(73)] |
| 1490 | 1441 |  | βO [(H-C-H)CH3-R2+R2(54)] |
| 1489 | 1440 | 1440 | βO [(H-C-H)CH3-R4(34)] |
| 1483 | 1434 | 1434 | βO [(H-C-H)CH3-R2+R2(56)] |
| 1481 | 1433 |  | βO [(H-C-H)R4+CH2(43)] |
| 1475 | 1427 |  | βO [(H-C-H)R4+CH2(64)] |
| 1474 | 1426 |  | βO [(H-C-H)CH3-O-R1(84)] |
| 1463 | 1415 |  | βO [(H-C-H)CH3-R4+R4(73)] |
| 1461 | 1413 |  | βO [(H-C-H)CH3-R2+R2(61)] |
| 1455 | 1407 |  | β [(H-C-C)R1(30)] |
| 1439 | 1391 |  | τi[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(22)] |
| 1424 | 1377 |  | βO [(H-C-H)CH3-R4(42)] |
| 1423 | 1376 |  | βO [(H-C-H)CH3-R1+R1(74)] |
| 1403 | 1356 | 1360 | βO [(H-C-H)CH3-R4(79)] |
| 1402 | 1357 |  | βO [(H-C-H)CH3-R1(22)] |
| 1385 | 1339 | 1328 | τi[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(18)] |
| 1361 | 1316 |  | β [(H-O-C)COOH(63)] |
| 1352 | 1308 |  | νs [C6-C5+C14-C9) (20)] |
| 1346 | 1301 | 1301 | βO [(H-C-H)CH2-R4(23)] |
| 1340 | 1295 |  | νs [(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 |  | νas [(N-C)R3 (17)] |
| 1249 | 1208 |  | ν[N7-C57) (20)] |
| 1235 | 1195 | 1194 | βO [(H-C-C)CH2(34)] |
| 1204 | 1164 | 1163 | β [(H-C-C)R1(58)] |
| 1201 | 1161 |  | τi[(H-C-O-C)CH3-O-R1(48)] |
| 1183 | 1143 |  | ν[(O-C) COOH(17)] |
| 1168 | 1130 | 1137 | βO [(H-C-H)CH3-O-R1(19)]+ τi[(H-C-O-C)CH3-O-R1(54)] |
| 1146 | 1108 | 1106 | ν[(O-C) COOH(26)]+ β [(H-O-C)COOH(19)] |
| 1142 | 1104 |  | βO [(H-C-C)R2(21)] |
| 1139 | 1101 |  | βO [(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 |  | τi[(H-C-C-C)CH3-R4+R4(21)] |
| 1034 | 999 | 998 | τi[(H-C-C-C)CH3-R2(21)] |
| 1027 | 993 |  | β [(H-C-C)R1(19)]+ β [(C-C-C)R1(60)] |
| 985 | 953 |  | τi[(H-C-C-C)R1(86)] |
| 968 | 936 | 934 | τi[(H-C-C-C)R1(51)] |
| 948 | 917 |  | τi[(H-C-C-C)CH3-R1(20)] |
| 944 | 913 | 910 | β [(C-C-N)R1+R2+R3(20)] |
| 905 | 875 | 882 | τi[(H-C-C-C)R2(26)] |
| 864 | 836 | 845 | τi[(H-C-C-C)R1(24)] |
| 826 | 799 | 806 | τi[(H-C-C-C)R1(66)] |
| 784 | 758 | 776 | ν[O27-C20) (18)] |
| 760 | 735 | 722 | τo [(O-C-O-C)COOH(41)] |
| 688 | 665 | 685 | τi[(H-O-C-C)COOH(20)] |
| 666 | 644 | 651 | τi[(H-O-C-C)COOH(38)] |
| 644 | 623 | 637 | τo [{(O15-C1-C5-C6)(R2+(O-C-O-C)(COOH)}(18)] |
| 642 | 621 | 606 | β [(O-C-O)COOH(20)] |
| 597 | 577 | 567 | τi[(H-O-C-C)COOH(24)] |
| 541 | 523 | 532 | τi[(H-O-C-C)COOH(27)] |
| 426 | 412 | 422 | τi[(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 |  | τo[(H-C-C-C)R2(23)] |
| 285 | 275 |  | β [(C-O-C)CH3-O-R1(22)] |
| 237 | 229 |  | τi[(H-C-O-C)CH3-O-R1(46)] |
| 228 | 220 |  | τi[(H-C-C-C)CH3-R2(22)] |
| 222 | 215 |  | τi[(H-C-C-C)CH3-R4+R4(19)] |
| 152 | 147 |  | τi[(H-C-C-C)CH3-R4+R4(18)] |
| 141 | 136 |  | β [(C-C-C)R2+R4(20)] |
| 106 | 102 |  | τi[(C-C-C-C)R2(24)] |
| 84 | 81 |  | τi[(C-C-C-C)CH3-O-R1(24)] |
| 79 | 76 |  | τi[(C-C-C-C)CH3-O-R1(20)] |
| 63 | 61 |  | τi[(O-C-C-C)COOH(35)] |
| 61 | 59 |  | τi[(C-C-C-C)R1+R2+R3+R4(26)] |
| 43 | 42 |  | τi[(C57-C4-C8-N7)(27)] |

ν: stretching; νs: symmetric stretching; νas: anti-symmetric stretching; β: bending in-plane; βO: bending out-of-plane; τi: torsion in plane; τo : torsion out-of-plane

**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 | νas[(O-H)COOH(100)] |
| 3637 | 3517 | 3312 | νs[(O-H)COOH(99)] |
| 3221 | 3115 |  | νs [C-H)R1(91)] |
| 3220 | 3114 |  | νas [C-H)R1(92)] |
| 3200 | 3094 |  | νs [C-H)R1(82)] |
| 3199 | 3093 | 3069 | νas [C-H)R1(82)] |
| 3148 | 3045 |  | νas [C-H) CH2 (90)] |
| 3104 | 3002 | 3002 | νas [C-H)R2(82)] |
| 3099 | 2997 |  | νas [C-H) CH3-R4 (79)] |
| 3096 | 2993 |  | ν[C52-H54)(95)] |
| 3091 | 2989 |  | νas [C-H) CH3-R4 (46)] |
| 3090 | 2988 |  | νas [C-H) CH3-R2 (82)] |
| 3087 | 2985 |  | νas [C-H) CH3-R4 (69)] |
| 3086 | 2983 |  | νas [C-H) CH3-R2+R2 (77)] |
| 3085 | 2983 |  | νas [C-H) R4 (62)] |
| 3082 | 2981 |  | νas [C-H) CH3-R2+R2 (26)] |
| 3080 | 2979 |  | ν[C-H)R3(90)] |
| 3080 | 2978 |  | νas [C-H) CH3-R4 (87)] |
| 3077 | 2975 |  | νas [C-H) CH3-R2 (83)] |
| 3063 | 2962 |  | ν[C-H)R4(71)] |
| 3060 | 2959 | 2959 | ν[C53-H56)(87)] |
| 3041 | 2941 |  | νas [C-H) R2 (78)] |
| 3027 | 2927 |  | νs [C-H) CH3-R4 (79)] |
| 3024 | 2924 |  | νs [C-H) CH3-R2 (29)] |
| 3017 | 2918 |  | νs [C-H) CH3-R4 (70)] |
| 3016 | 2916 |  | νs [C-H) CH3-R4 (70)] |
| 3009 | 2909 |  | νs [C-H) R2 (74)] |
| 3006 | 2907 |  | νs [C-H) R4 (74)] |
| 2988 | 2889 | 2877 | νs [C-H) R4 (73)] |
| 1845 | 1784 | 1808 | νs [O=C) COOH (84)] |
| 1835 | 1775 | 1731 | νs [O=C) COOH (82)] |
| 1721 | 1665 | 1668 | νs [O=C) R2+R4 (90)] |
| 1716 | 1659 |  | ν[O=C) R2 (68)] |
| 1678 | 1623 | 1618 | νs [C=C) R3 (67)] |
| 1642 | 1588 | 1586 | νas [C-C) R1(36)] |
| 1633 | 1579 | 1576 | νas [C-C) R1(28)]+ β [(H-C-C)R1(18)] |
| 1624 | 1571 | 1556 | νas [C=C) R3 (73)] |
| 1569 | 1517 | 1510 | νas [(O-N) NO2 (77)] |
| 1523 | 1472 |  | β [(H-C-C)R1(63)] |
| 1514 | 1464 |  | βO [(H-C-H)CH3-R2(40)] |
| 1513 | 1463 | 1461 | βO [(H-C-H)CH3-R4(61)] |
| 1508 | 1458 |  | βO [(H-C-H)CH3-R4(57)] |
| 1506 | 1457 |  | βO [(H-C-H)CH3-R2(56)] |
| 1499 | 1449 |  | βO [(H-C-H)CH3-R4+R4(57)] |
| 1498 | 1448 |  | βO [(H-C-H)CH3-R2+R2(66)] |
| 1490 | 1441 | 1440 | βO [(H-C-H)CH3-R2+R2(51)] |
| 1489 | 1440 |  | βO [(H-C-H)CH3-R4(42)] |
| 1482 | 1433 | 1434 | βO [(H-C-H)R4+CH2(54)] |
| 1481 | 1432 |  | βO [(H-C-H)CH3-R2+R2(55)] |
| 1477 | 1428 |  | βO [(H-C-H)R4+CH2(66)] |
| 1463 | 1414 |  | βO [(H-C-H)CH3-R4+R4(71)] |
| 1461 | 1413 |  | βO [(H-C-H)CH3-R2+R2(61)] |
| 1454 | 1406 |  | νas [C-C) R1(19)]+ β [(H-C-C)R1(25)] |
| 1436 | 1389 |  | τi[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(21)] |
| 1427 | 1380 |  | βO [(H-C-H)CH3-R4(60)] |
| 1423 | 1376 |  | βO [(H-C-H)CH3-R2+R2(90)] |
| 1405 | 1359 | 1360 | βO [(H-C-H)CH3-R4(87)] |
| 1402 | 1356 |  | βO [(H-C-H)CH3-R2(42)] |
| 1384 | 1338 | 1328 | τi[{(H-C-C-N)(R3+R4)+(H-C-C-O)(COOH)}(16)] |
| 1366 | 1321 |  | νs [C-H) NO2-R1 (66)] |
| 1361 | 1316 |  | β [(H-O-C)COOH(54)] |
| 1355 | 1310 |  | νs [C-C) R2+R4(16)] |
| 1346 | 1302 | 1301 | β [(H-C-C)R1(28)]+ βO [(H-C-C)R2+CH2(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 |  | νas [(N-C) R3(19)] |
| 1248 | 1207 |  | νas [(N-C) R3(34)] |
| 1233 | 1192 |  | βO [(H-C-C)COOH(34)] |
| 1211 | 1171 |  | β [(H-C-C)R1(51)] |
| 1209 | 1169 |  | β [(H-C-C)R1(16)] |
| 1187 | 1148 | 1137 | νas [O-C) COOH(19)] |
| 1145 | 1107 | 1108 | νas [O-C) COOH(24)]+ β [(H-O-C)COOH(17)] |
| 1143 | 1105 |  | βO [(H-C-H)R2(23)] |
| 1140 | 1102 |  | βO [(H-C-H)R4(23)] |
| 1135 | 1097 |  | β [(H-C-C)R1(46)] |
| 1122 | 1085 |  | νas [C-C) R2+R3(18)] |
| 1118 | 1081 | 1031 | ν[N-C) NO2+R1(21)] |
| 1036 | 1002 |  | τi[{(H-C-C-C)(CH3-R2+R2)(16)] |
| 1034 | 1000 |  | τi[{(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 | τi[{(H-C-C-C)(R1)(57)] |
| 952 | 921 |  | νas [C-C) CH3-R4+R4(24)]+ τi[{(H-C-C-C)(CH3-R4)(17)] |
| 950 | 919 |  | τi[{(H-C-C-C)(CH3-R4)(18)] |
| 944 | 913 | 910 | β [(H-C-C)R1+R2+R3(18)] |
| 904 | 875 | 882 | τi[{(H-C-C-C)(R2)(27)] |
| 892 | 863 |  | τi[{(H-C-C-C)(R1)(43)] |
| 877 | 848 | 845 | τi[{(H-C-C-C)(R1)(95)] |
| 871 | 842 |  | νas [(O-C) COOH(17)] |
| 859 | 830 |  | τi[{(H-C-C-C)(R1)(93)] |
| 837 | 810 | 811 | β [(O-N-C)NO2(17)] |
| 788 | 762 | 776 | νas [(C-C) CH3-R2+R2(16)] |
| 761 | 736 |  | τo[{(O-C-C-C)(R1)+(O-C-O-C)COOH}(40)] |
| 743 | 719 | 722 | τo[(O-C-O-N)(NO2-R1)(40)] |
| 712 | 689 |  | τo[(O-C-O-N)(NO2-R1)(19)] |
| 708 | 684 | 685 | τo[(O-C-O-N)(NO2-R1)(21)] |
| 690 | 667 | 667 | τi[(H-O-C-C)(COOH)(21)] |
| 666 | 644 |  | τi[(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)]+ τi[(H-O-C-C)(COOH)(20)] |
| 576 | 557 |  | β [(O-C-C)R2+R4(25)] |
| 543 | 525 | 5532 | τi[(H-O-C-C)(COOH)(30)] |
| 539 | 521 |  | β [(O-N-C)NO2-R1(26)] |
| 534 | 516 |  | β [(O-N-C)NO2-R1(19)] |
| 517 | 500 | 459 | β [(O-N-C)NO2-R1(19)] |
| 419 | 405 | 415 | τi[(C-C-C-C)(R1)(53)] |
| 398 | 385 |  | β [(O-C-C)COOH(16)+(C53-C52-N7)(19)] |
| 390 | 377 |  | τo[(C-C-C-C)(CH3-R4+R4)(40)] |
| 389 | 377 |  | τo[(C-C-C-C)(CH3-R2+R2)(40)] |
| 375 | 363 |  | τo[(C-C-C-C)(CH3-R2+R2)(30)] |
| 272 | 263 |  | τo[(N-C-C-C)(NO2-R1+R1)(27)] |
| 241 | 233 |  | τi[(H-C-C-C)(CH3-R2+R2)(20)]+ τi[(H-C-C-C)(CH3-R4+R4)(16)] |
| 230 | 222 |  | τi[(H-C-C-C)(CH3-R2+R2)(23)] |
| 224 | 216 |  | τi[(H-C-C-C)(CH3-R4+R4)(43)] |
| 175 | 169 |  | β [(N-C-C)NO2-R1(22)+(C-C-C)COOH+R1(18)] |
| 106 | 103 |  | τi[{(C-C-C-C)(R2)+(C53-C52-N7-C4)}(22)] |
| 79 | 77 |  | τi[{(C-C-C-C)(R2)+(C53-C52-N7-C4)}(19)] |
| 65 | 63 |  | τi[(O-N-C-C)(NO2-R1)(30)]+ τi[(C-C-C-C)(R1+R2+R3-R4)(18)] |
| 62 | 60 |  | τi[(O-C-C-C)(COOH)(35)] |
| 58 | 56 |  | τi[(C-C-C-C)(R1+R2+R3-R4)(20)] |
| 43 | 41 |  | τo[(C52-C4-C8-N7)(34)] |
| 41 | 40 |  | τi[(C-C-C-C)(R1+R2+R3-R4)(19)] |
| 32 | 33 |  | τi[(O-N-C-C)(NO2-R1)(29)] |
| 31 | 30 |  | τi[(O-C-C-C)(COOH)(24)] |
| 25 | 25 |  | τi[(O-C-C-C)(COOH)(18)] |

ν: stretching; νs: symmetric stretching; νas: anti-symmetric stretching; β: bending in-plane; βO: bending out-of-plane; τi: torsion in plane; τo : 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, 1H and 13C NMR isotropic chemical shifts (*δ*, in *ppm*) (with respect to TMS) MTDOSA with DFT (B3LYP/6-311++G(d,p)) method in DMSO.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | *δ*cal. | *δ*exp. | 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(CH3-R2)] |
| C24 | 26.7414 | 27.43 | [ C(CH3-R2)] |
| C25 | 33.8613 | 29.34 | [ C(CH3-R4)] |
| C26 | 26.8242 | 29.34 | [ C(CH3-R4)] |
| C28 | 57.4729 | 55.21 | [ C(CH3-O-R1)] |
| C57 | 61.5561 | 93.52 | [ C(NR3)] |
| C58 | 48.0001 | 50.86 | [ C(CH2)] |
| C62 | 177.5777 | 162.21 | [ C(COOH)] |
| C66 | 176.9226 | 162.21 | [ C(COOH)] |
| Chemical shift for Hydrogen |
| Atom | *δ*cal. | *δ*exp. | 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(CH3-R2)] |
| H43 | 1.1004 | 0.97 (3H, s) | [s, H(CH3-R2)] |
| H44 | 1.1731 | 0.97 (3H, s) | [s, H(CH3-R2)] |
| H45 | 1.3565 | 0.97 (3H, s) | [s, H(CH3-R2)] |
| H46 | 0.8171 | 0.97 (3H, s) | [s, H(CH3-R2)] |
| H47 | 0.8885 | 0.97 (3H, s) | [s, H(CH3-R2)] |
| H48 | 0.9945 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H49 | 1.0912 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H50 | 1.1789 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H51 | 0.8115 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H52 | 1.3637 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H53 | 0.8535 | 1.08 (3H, s) | [s, H(CH3-R4)] |
| H54 | 4.1108 | 3.71 (3H, s) | [s, H(CH3-O-R1)] |
| H55 | 3.7625 | 3.71 (3H, s) | [s, H(CH3-O-R1)] |
| H56 | 3.7903 | 3.71 (3H, s) | [s, H(CH3-O-R1)] |
| H59 | 4.7417 | 4.78 | [ H(C-R3)] |
| H60 | 3.752 | 4.67 | [ H(CH2)] |
| H61 | 2.8325 | 4.67 | [ H(CH2)] |
| H65 | 9.7824 |  | [ H(COOH)] |
| H69 | 6.9706 |  | [ H(COOH)] |

**Table S-VIII:** Experimental and theoretical, 1H and 13C 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 | *δ*cal. | *δ*exp. | 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(CH3-R2)] |
| C24 | 26.7644 | 15.83 | [ C(CH3-R2)] |
| C25 | 33.1922 | 21.50 | [C(CH3-R4)] |
| C26 | 26.7744 | 21.50 | [C(CH3-R4)] |
| C52 | 61.8097 | 67.45 | [ C(NR3)] |
| C53 | 47.6303 | 30.94 | [ C(CH2)] |
| 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(CH3-R2)] |
| H41 | 1.119 | 1.83 (3H, s) | [s, H(CH3-R2)] |
| H42 | 1.2112 | 1.83 (3H, s) | [s, H(CH3-R2)] |
| H43 | 1.3445 | 1.23 (3H, s) | [s, H(CH3-R2)] |
| H44 | 0.8175 | 1.23 (3H, s) | [s, H(CH3-R2)] |
| H45 | 0.895 | 1.23 (3H, s) | [s, H(CH3-R2)] |
| H46 | 0.9771 | 2.25 (3H, s) | [s, H(CH3-R4)] |
| H47 | 1.071 | 2.25 (3H, s) | [s, H(CH3-R4)] |
| H48 | 1.1639 | 2.25 (3H, s) | [s, H(CH3-R4)] |
| H49 | 0.8346 | 1.94 (3H, s) | [s, H(CH3-R4)] |
| H50 | 1.3659 | 1.94 (3H, s) | [s, H(CH3-R4)] |
| H51 | 0.8936 | 1.94 (3H, s) | [s, H(CH3-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(CH2)] |
| H56 | 2.8027 | 2.33-2.28 (2H, m) | [m, H(CH2)] |
| H60 | 9.8863 |  | [ H(COOH)] |
| H64 | 6.9745 |  | [ H(COOH)] |