**Supplementary Information**

Y-shaped potential third-order nonlinear optical material - 3-(2-amino-2-oxoethyl)-5-methyl hexanoic acid: An analysis of structural, spectroscopic and docking studies

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**Fig. S8** Pictorial representation of HOMO-LUMO plots of AOEMHA.

**Fig. S9** Atomic absorption and emission spectra of AOEMHA are computed at TD-DFT/B3LYP/6-311++G(d) level of theory.

**Fig. S10** Representative of MEP surface of AOEMHA.

**Fig. S11** Two dimensional graphical embodiments of Electron Localization Function (ELF) of AOEMHA.

**Fig. S12** Two dimensional graphical embodiments of Localized Orbital Locator (LOL) of AOEMHA.

**Fig. S13** Groups acid (A), amide (B) and isopropyl (C) of AOEMHA compound.

**Table S1.** Topological analysis performed via QTAIM for the crystal structures of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid, all data are in a.u..

**Table S2.** Geometrical parameters of the 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid.

**Table S3.** Calculated scaled wave numbers, observed IR and Raman bands and assignment of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid.

**Table S4.** Second-order perturbation theory analysis of Fock matrix in NBO basis corresponding to the intramolecular bonds of the title compound.

**Table S5.** NBO results showing the formation of Lewis and non-Lewis orbitals.

**Table S6.** Partial Charges in isolated and embedded molecule

**Table S7.** Comparison of linear refractive index for 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid crystal with experimental results for others organic crystals.

**Table S8.** Molecular docking values of AOEMHA with target proteins (a) 4BDU, (b) 4DBS, (c) 4DBW, (d) 4FAL and (e) 4FAM.

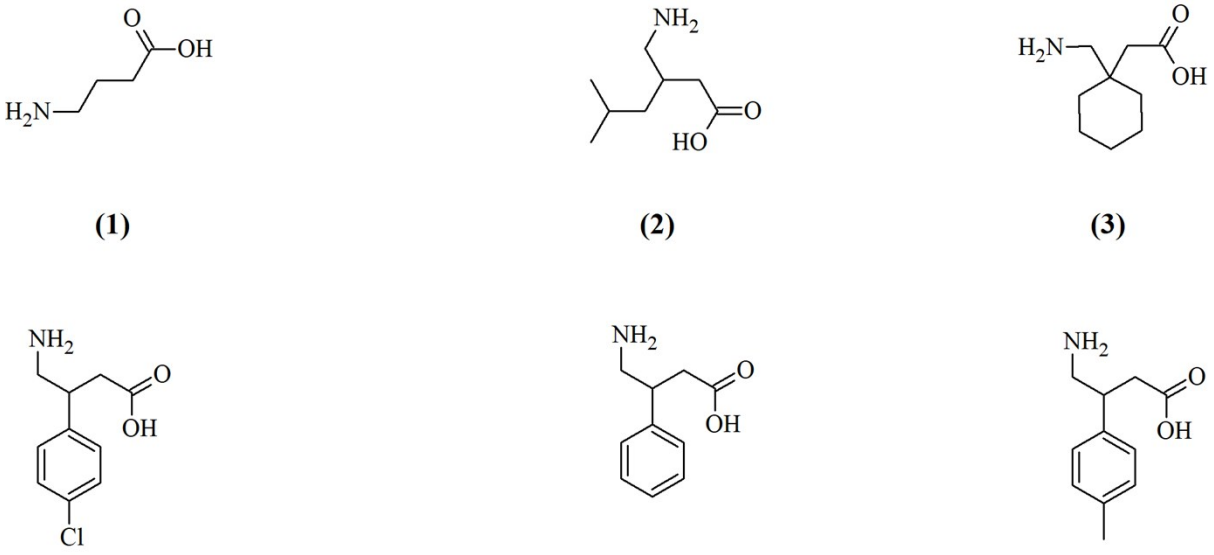



**Fig. S1** Some potent biologically active drug moieties.

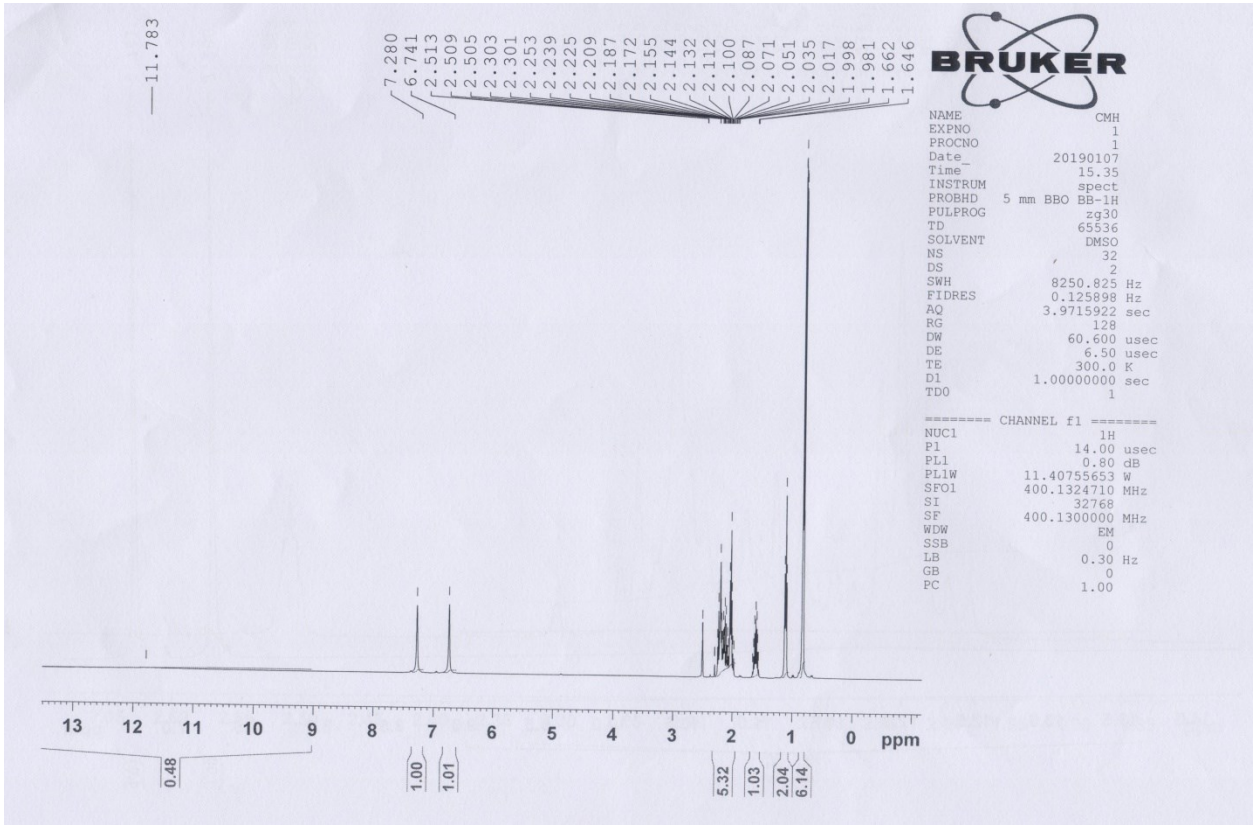



**Fig. S2** $^{1}$H-NMR spectrum of AOEMHA.

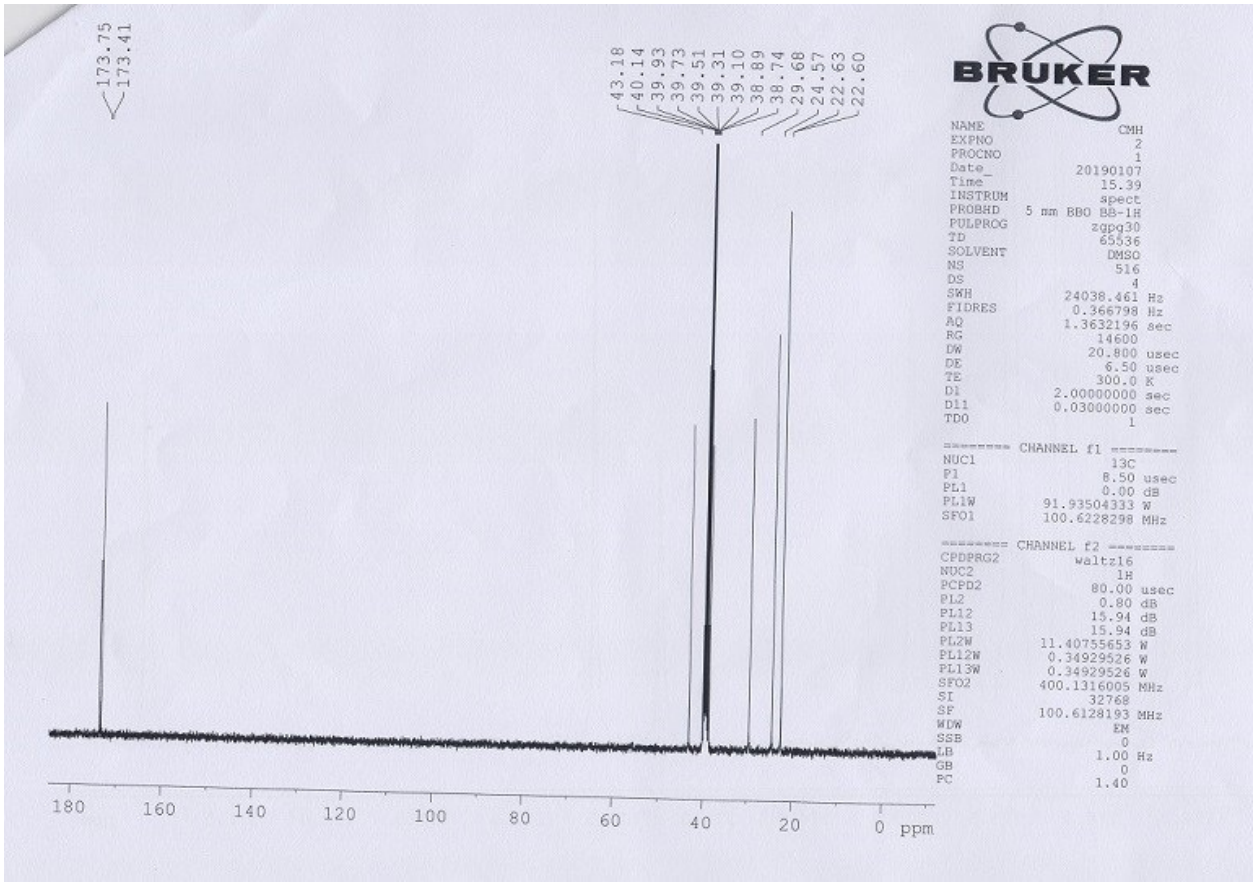
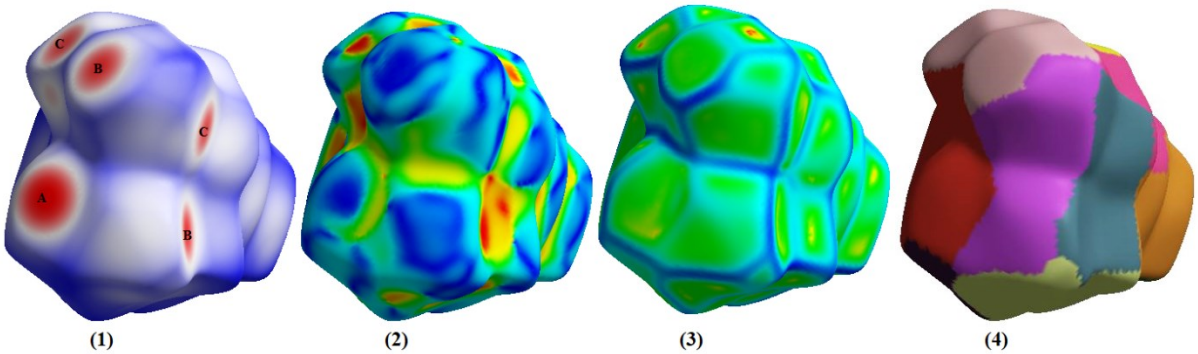
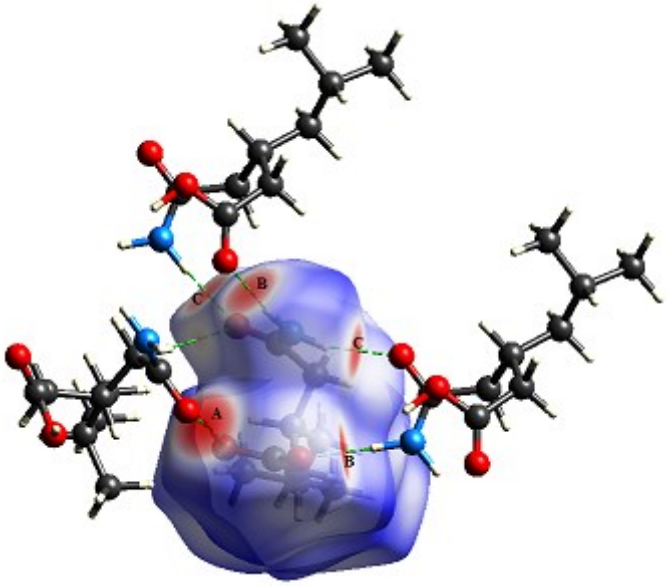


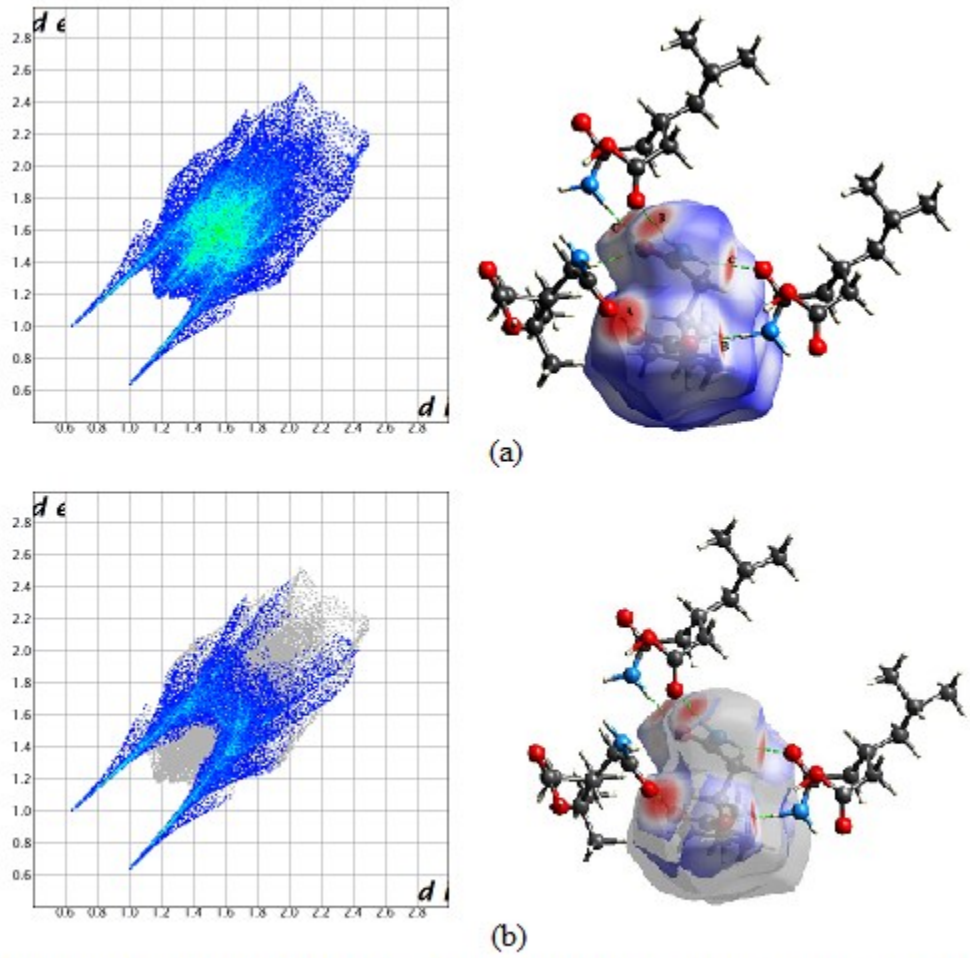

**Fig. S3** $^{13}$C-NMR spectrum of AOEMHA.




(A) Pictorial representation of Hirshfeld surfaces of AOEMHA $d_{norm}$ (1), *shape index* (2), *curvedness* (3) and *fragment path* (4).




(B) View of O2-H3---O1, N5-H6---O4 and N5-H7---O1 interactions on $d_{norm}$ surface.




(c) Finger print analysis (a) Total interaction 100% (b) O---H/H---O interaction 33.3%.

(C) 2D Finger print plots of AOEMHA along with percentage of interactions.

**Fig. S4** 3D Hirshfeld surface and 2D Finger print analysis of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid.

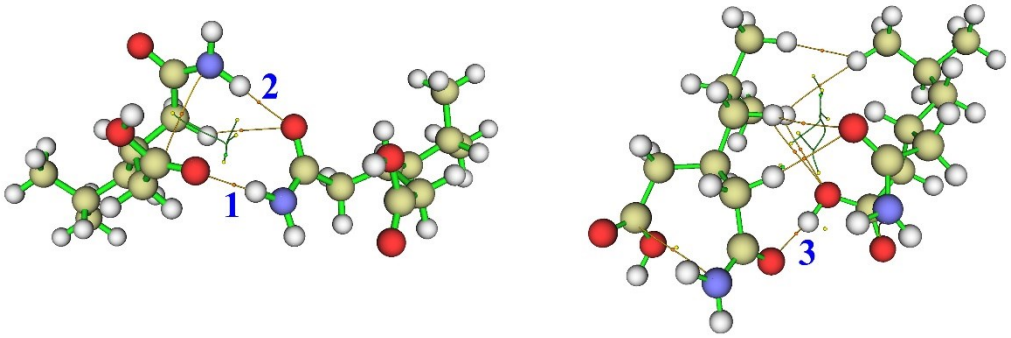



**Fig. S5** Representation of bond critical points (BCP) for the crystal structures of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid indicating the bond paths analyzed in Table S1.

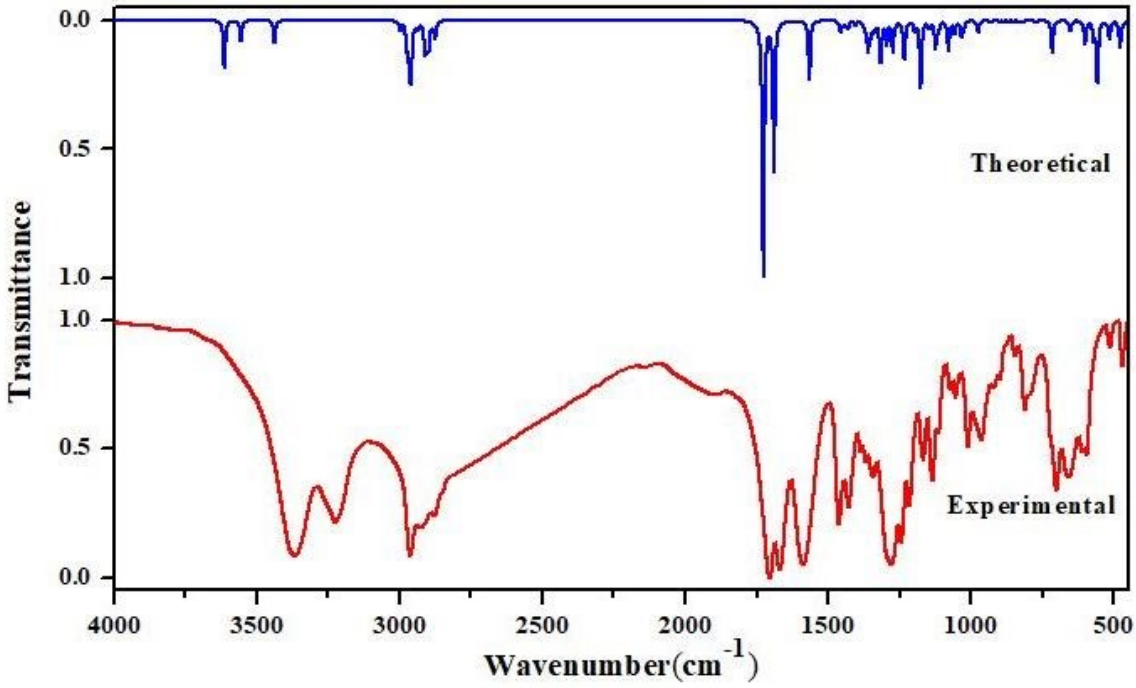



**Fig. S6** Infrared spectrum of AOEMHA using (a) DFT/B3LYP/6-311++G (d,p) and (b) experimental data.

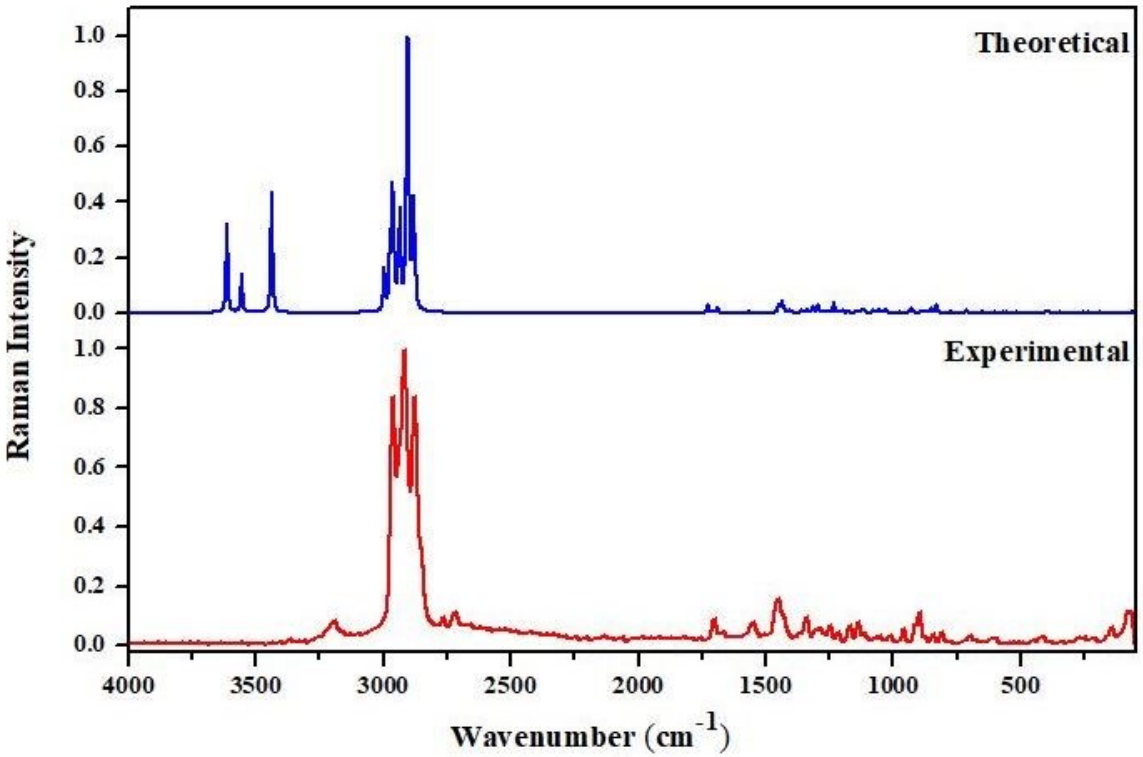



**Fig. S7** Raman spectrum of AOEMHA using (a) DFT/B3LYP/6-311++G (d,p) and (b) experimental data.

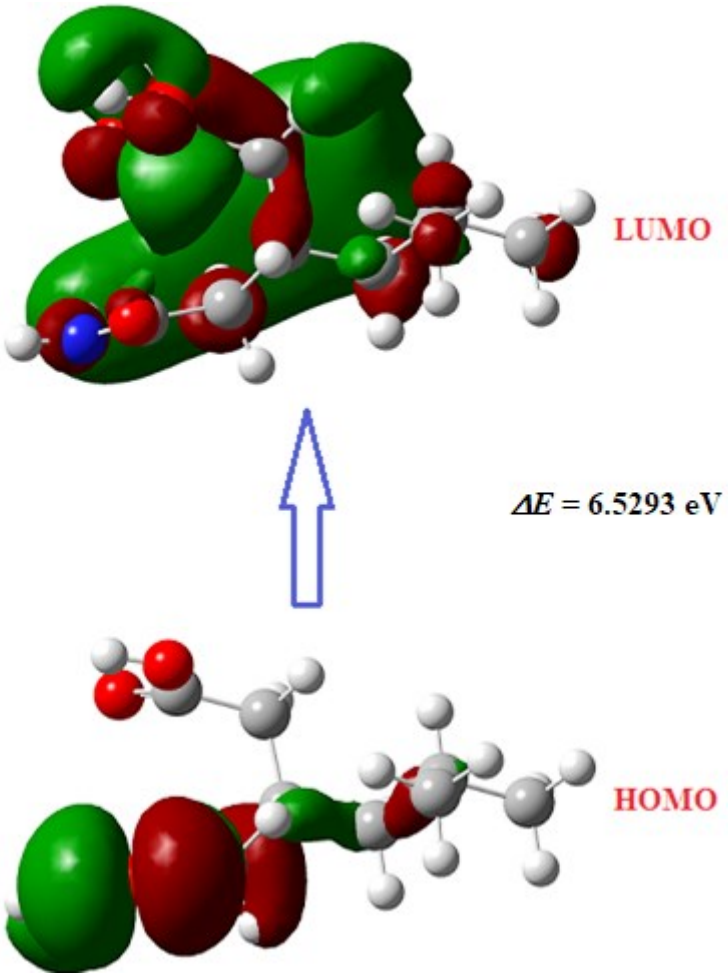



**Fig. S8** Pictorial representation of HOMO-LUMO plots of AOEMHA.

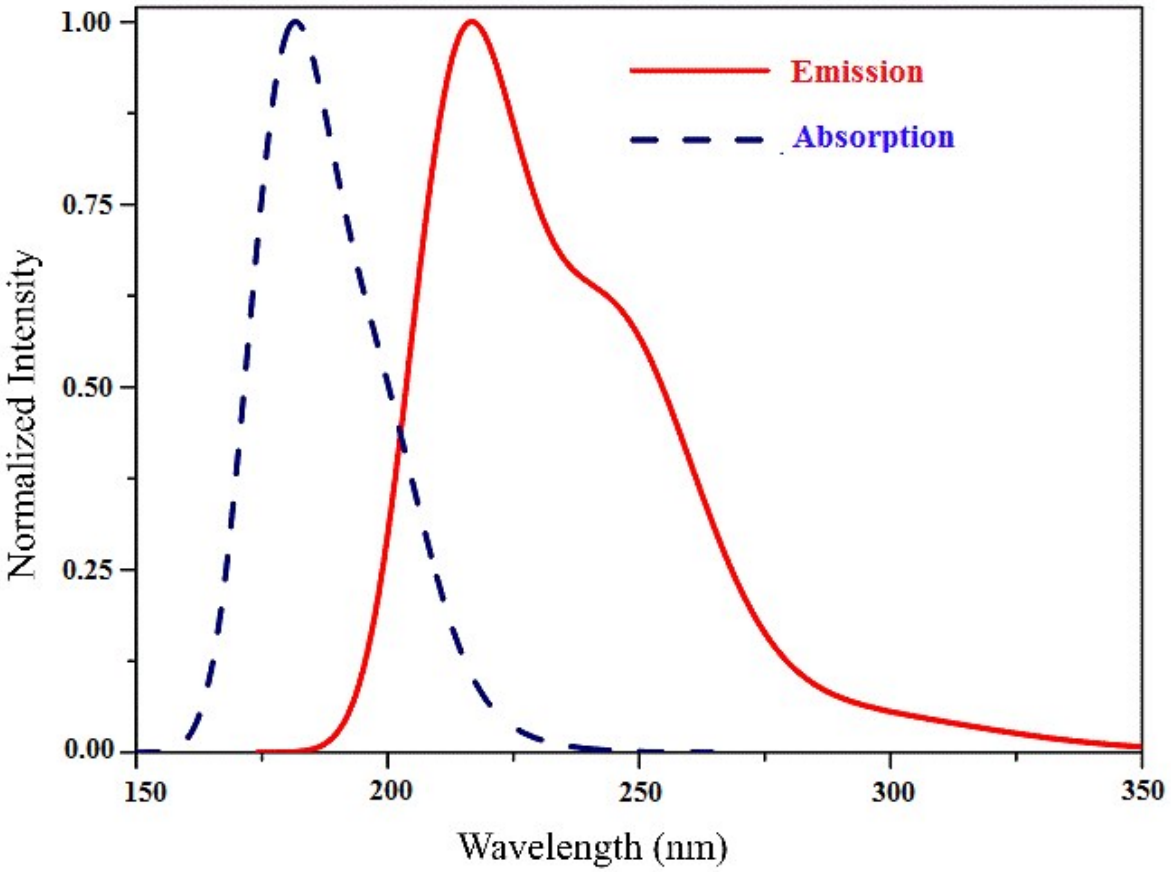



**Fig. S9** Atomic absorption and emission spectra were computed at TD-DFT/B3LYP/6-311++G(d) level of theory.

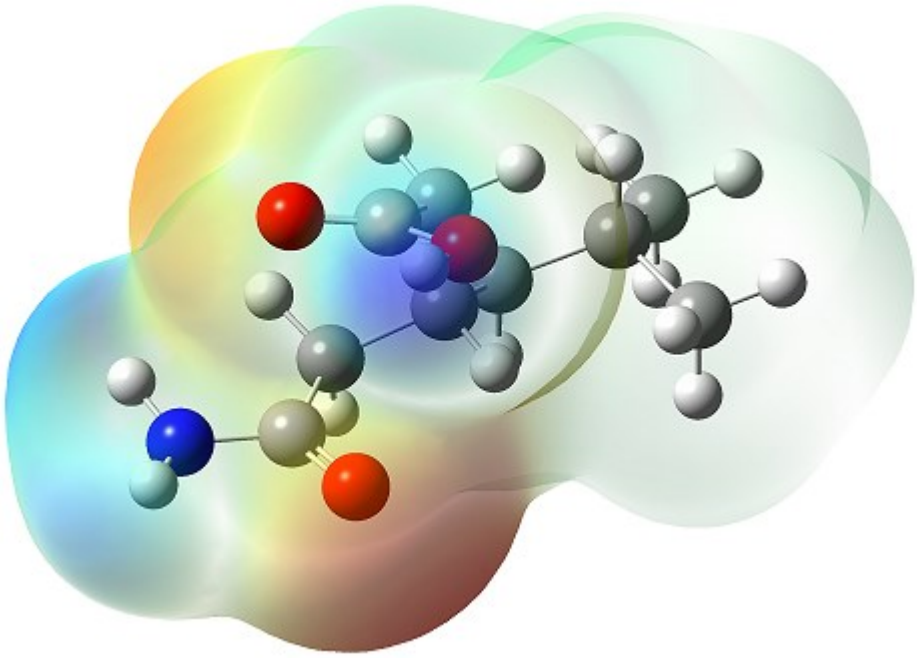


**Fig. S10** Representative of MEP surface of AOEMHA.

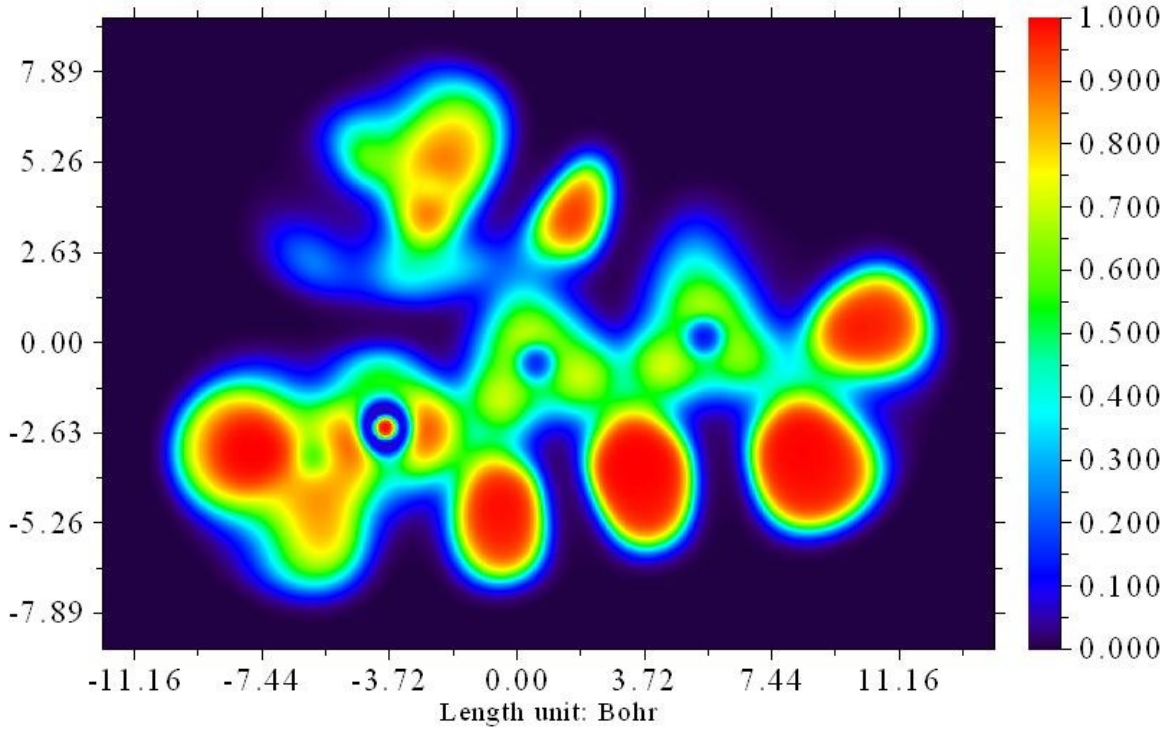



**Fig. S11** Two dimensional graphical embodiments of Electron Localization Function (ELF) of AOEMHA.

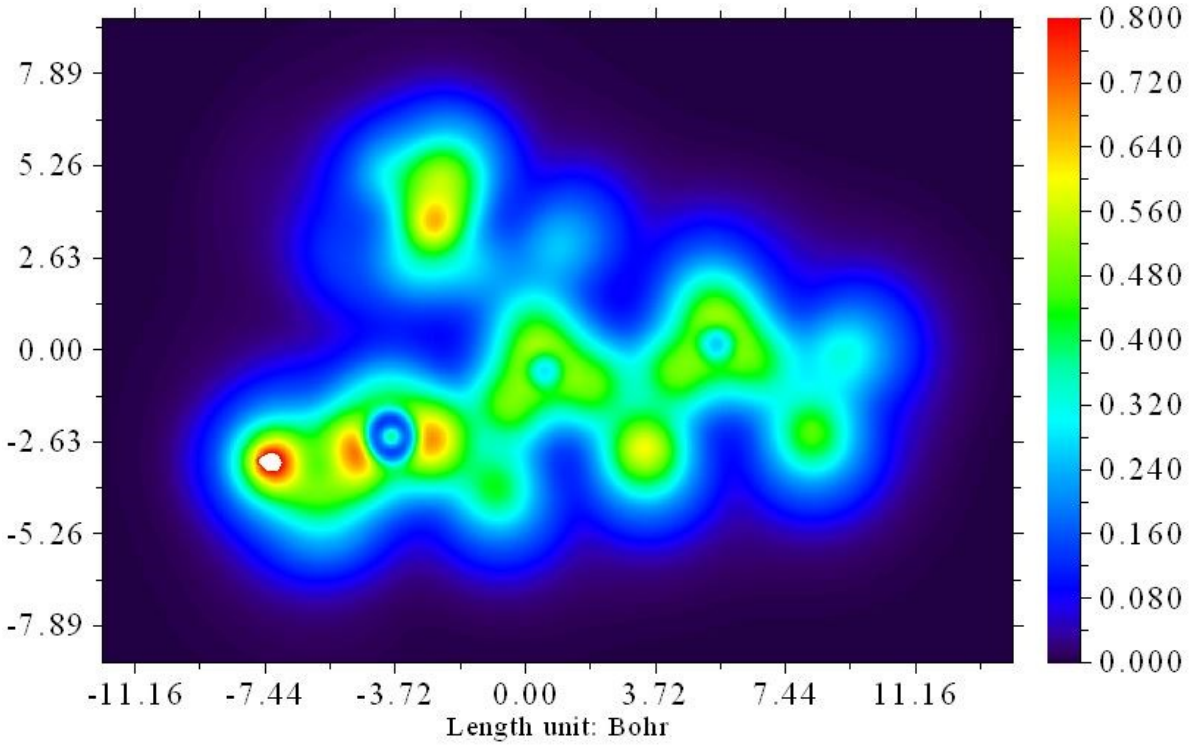



**Fig. S12** Two dimensional graphical embodiments of Localized Orbital Locator (LOL) of AOEMHA.

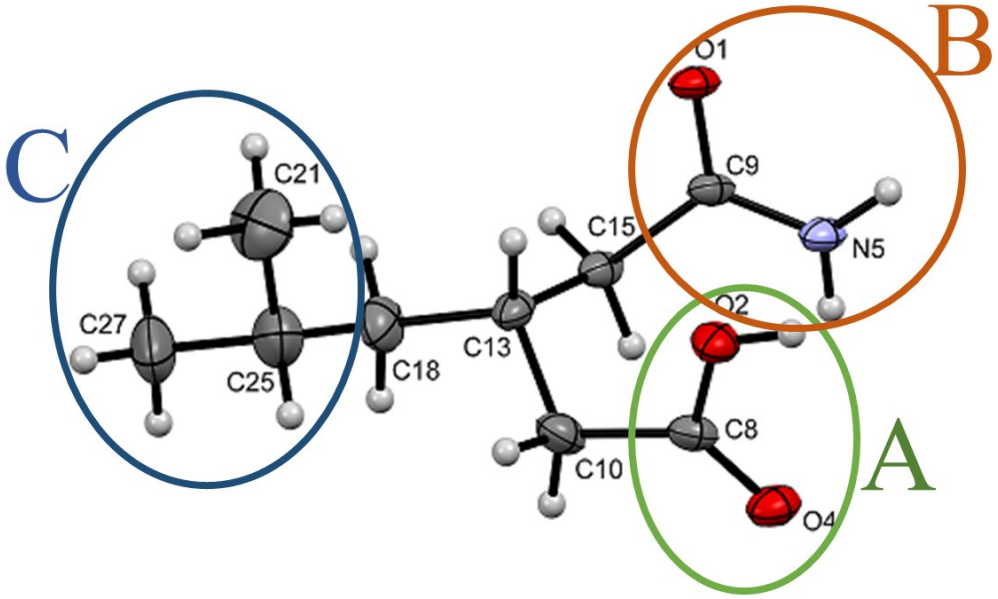



**Fig. S13** Groups acid (A), amide(B)and  isopropyl (C) of AOEMHA compound.

**Table S1**

Topological analysis performed via QTAIM for the crystal structures of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid, all data are in a.u..

| BCP | $\rho(r_{bcp})$ | $\nabla^2\rho(r_{bcp})$ | $V(r_{bcp})$ | $G(r_{bcp})$ | $H(r_{bcp})$ | Interactions |
|---|---|---|---|---|---|---|
| 1 | 0.0251 | 0.0929 | -0.0187 | 0.0209 | 0.0023 | N5-H6···O4 |
| 2 | 0.0211 | 0.0779 | -0.0146 | 0.0170 | 0.0024 | N5-H7···O1 |
| 3 | 0.0505 | 0.1411 | -0.0487 | 0.0420 | -0.0067 | O2-H3···O1 |

**Table S2**

Geometrical parameters of the 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid.

| Bond lengths (Å) DFT /XRD | | | |
|---|---|---|---|
| O1-C9 | 1.259/1.219 (6) | C18-C25 | 1.541/1.463(13) |
| C8-O2 | 1.351/1.313(7) | C21-C25 | 1.535/1.508(14) |
| C8-O4 | 1.209 /1.204(8) | C8-C10 | 1.508/1.494(10) |
| N5-C9 | 1.368/1.303(9) | C9-C15 | 1.528/1.502(8) |
| C13-C18 | 1.543/1.514(10) | C10-C13 | 1.551/1.539(10) |
| C13-C15 | 1.540/1.539(11) | | |
| Bond angles (º) DFT /XRD | | | |
| O4-C8-O2 | 122.4/122.6(7) | C25-C18-C13 | 117.4/118.4(8) |
| O4-C8-C10 | 125.3/123.9(6) | C18-C25-C21 | 112.3/114.7(8) |
| O2-C8-C10 | 112.2/113.5(6) | C18-C25-C27 | 109.8/107.5(11) |
| O1-C9-N5 | 122.2/122.3(5) | C9-C15-C13 | 114.1/114.9(5) |
| O1-C9-C15 | 122.2/120.2(6) | C21-C25-C27 | 110.6/107.2(10) |
| N5-C9-C15 | 115.3/117.5(5) | C18-C13-C15 | 109.8/108.8(6) |
| C8-C10-C13 | 113.5/116.7(5) | C10-C13-C15 | 112.0/111.3(5) |
| C18-C13-C10 | 110.4/112.4(6) | | |
| Dihedral angle (º) DFT /XRD | | | |
| O4-C8-C10-C13 | -88.9/-119.1(7) | C18-C13-C15-C9 | 154.0/150.2(5) |
| O2-C8-C10-C13 | 90.5/58.9(8) | C10-C13-C15-C9 | -82.7/-85.4(6) |
| C8-C10-C13-C18 | -179.0/176.3(6) | C10-C13-C18-C25 | 60.5/68.4(10) |
| C8-C10-C13-C15 | 58.0/53.9(8) | C15-C13-C18-C25 | -175.3/-167.9(7) |
| O1-C9-C15-C13 | -31.7/-60.4(7) | C13-C18-C25-C21 | 58.7/60.8(13) |
| N5-C9-C15-C13 | 153.0/119.6(6) | C13-C18-C25-C27 | -177.6/179.9(8) |

**Table S3**

Calculated scaled wave numbers, observed IR and Raman bands and assignment of 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid.

| B3LYP/6-311G++(d.p) | | | ν(IR) | ν(Raman) | Assignments [a] |
|---|---|---|---|---|---|
| ν ($cm^{-1}$) | IR intensity | Raman activity | ($cm^{-1}$) | ($cm^{-1}$) | |
| 3612 | 70.901 | 116.0642 | 3440 | - | νO(2)-H(3) (100) |
| 3554 | 31.8096 | 52.1058 | 3366 | 3366 | νN(5)-H2(6,7) (100) |
| 3437 | 33.8974 | 158.4244 | 3219 | 3215 | νN(5)-H2(6,7) (100) |
| 2995 | 12.4581 | 53.9274 | - | - | νC(10)-H2(11,12) (97) |
| 2972 | 33.12 | 54.4869 | - | - | νC(21)-H3(22,23,24) (91) |
| 2964 | 53.6399 | 123.5973 | 2960 | 2961 | νC(27)-H3(28,29,30) (83) |
| 2959 | 60.0862 | 73.8392 | - | 2959 | νC(21)-H3(22,23,24) (48)<br>νC(27)-H3(28,29,30) (40) |
| 2956 | 19.9134 | 4.7642 | 2955 | 2955 | νC(21)-H3(22,23,24) (10)<br>νC(15)-H2(16,17) (11)<br>νC(13)-H(14) (58) |
| 2953 | 5.7175 | 20.5157 | - | 2949 | νC(21)-H3(22,23,24) (24)<br>νC(27)-H3(28,29,30) (64) |
| 2940 | 4.2926 | 33.837 | - | 2938 | νC(15)-H2(16,17) (80)<br>νC(13)-H(14) (11) |
| 2933 | 9.3423 | 116.375 | 2930 | - | νC(10)-H2(12,11) (81)<br>νC(13)-H(14) (13) |
| 2910 | 38.3656 | 58.1247 | 2916 | - | νC(18)-H2(19,20) (71) |
| 2902 | 17.817 | 274.6999 | 2901 | - | νC(21)-H3(22,23,24) (75) |
| 2896 | 34.1761 | 40.1875 | - | - | νC(21)-H3(22,23,24) (11)<br>νC(27)-H3(28,29,30) (78) |
| 2881 | 8.4607 | 123.5375 | 2879 | - | νC(25)-H(26) (84) |
| 2873 | 24.3515 | 67.7387 | 2874 | 2875 | νC(18)-H2(19,20) (97) |
| 1725 | 390.0101 | 9.646 | 1702 | 1701 | νC(8)=O(4) (82) |
| 1688 | 226.8163 | 9.1042 | 1667 | 1668 | νC(9)=O(1) (79) |
| 1564 | 89.1245 | 2.7225 | - | 1551 | δN(5)-H2(6,7) (83) |
| 1454 | 15.181 | 0.3587 | 1460 | - | δC(21)-H3(22,23,24) (49)<br>δC(27)-H3(28,29,30) (26) |
| 1447 | 5.5011 | 11.444 | - | 1449 | δC(21)-H3(22,23,24) (19)<br>δC(27)-H3(28,29,30) (38) |
| 1437 | 3.5032 | 0.3825 | - | 1435 | δC(27)-H3(28,29,30) (29)<br>δC(21)-H3(22,23,24) (21)<br>δC(18)-H2(19,20) (15) |
| 1434 | 1.8608 | 14.832 | 1431 | 1432 | δC(27)-H3(28,29,30) (46)<br>δC(21)-H3(22,23,24) (27) |
| 1428 | 11.2586 | 2.2754 | 1426 | 1427 | δC(10)-H2(11,12) (64)<br>δC(18)-H2(19,20) (10) |
| 1424 | 0.4432 | 3.2615 | - | - | δC(18)-H2(19,20) (44) |
| 1403 | 5.7633 | 3.666 | - | 1405 | δC(15)-H2(16,17) (82) |
| 1369 | 10.7188 | 0.1412 | 1368 | 1367 | δC(21)-H3(22,23,24) (46)<br>δC(27)-H3(28,29,30) (37) |
| 1340 | 13.73 | 0.36103 | 1341 | 1339 | δC(21)-H3(22,23,24) (37) |

| | | | | | |
|---|---|---|---|---|---|
| | | | | | δC(27)-H3(28,29,30) (47)<br>δC(25)-H(26) (22) |
| 1315 | 48.5725 | 2.8269 | 1312 | 1311 | δC(10)-H2(11,12) (10)<br>δO(2)-H(3) (14) |
| | | | | | νC(8)-O(2) (11) |
| 1272 | 46.0338 | 4.5367 | 1243 | 1245 | δC(9)-N(5) (12) |
| 1174 | 103.2899 | 1.3971 | 1169 | 1170 | δO(2)-H(3) (18)<br>δC(15)-H2(16,17) (21) |
| | | | | | δC(21)-H3(22,23,24) (15) |
| 1144 | 10.0084 | 2.7744 | 1136 | 1137 | δC(27)-H3(28,29,30) (12) |
| | | | | | νC(25)-C(18) (11) |
| 1122 | 39.8068 | 3.6323 | - | - | νC(8)-O(2) (11)<br>δC(15)-H2(16,17) (14) |
| 1112 | 13.9083 | 3.9656 | 1112 | 1112 | δC(27)-H3(28,29,30) (12) |
| 1056 | 17.6148 | 6.2216 | 1054 | 1053 | δN(5)-H2(6,7) (33)<br>νC(9)-N(5) (21) |
| 973 | 16.929 | 1.6342 | 974 | 977 | νC(18)-C(13) (13) |
| | | | | | δC(21)-H3(22,23,24) (11) |
| 929 | 1.3727 | 3.6284 | 927 | 931 | δC(27)-H3(28,29,30) (29) |
| | | | | | νC(21)-C(25) (15) |
| 926 | 1.9159 | 4.1986 | 921 | - | νC(27)-C(25) (24)<br>νC(25)-C(28) (29) |
| 896 | 1.3223 | 0.5884 | 895 | 896 | δC(21)-H3(22,23,24) (24)<br>δC(27)-H3(28,29,30) (17) |
| 886 | 1.6389 | 2.0727 | 883 | - | νC(8)-C(10) (15)<br>νC(15)-C(13) (13) |
| | | | | | νC(8)-O(2) (10) |
| 865 | 2.0423 | 3.1983 | - | - | νC(8)-C(10) (17)<br>νC(10)-C(13) (20) |
| | | | | | δC(15)-H2(16,17) (16) |
| 851 | 1.3855 | 6.0553 | 848 | - | νC(8)-O(2) (13) |
| 816 | 3.2241 | 0.4641 | 812 | 810 | δC(18)-H2(19,20) (12)<br>νC(9)-C(15) (11) |
| | | | | | νC(21)-C(25) (27) |
| 771 | 3.5548 | 1.9663 | - | 770 | νC(25)-C(27) (10)<br>νC(25)-C(18) (15) |
| | | | | | δC(18)-H2 (19,20) (10) |
| 713 | 48.7772 | 4.6316 | 718 | 717 | δC(8)-O(2) (38)<br>νC(10)-C(13) (15) |
| 651 | 14.4062 | 2.784 | 653 | 650 | δC(5)-N(9) (17)<br>δC(9)=O(1) (17) |
| 598 | 34.5304 | 1.2808 | 595 | 597 | δC(8)=O(4) (26)<br>τO(2)-H(3) (32) |
| 568 | 24.294 | 1.2541 | - | 565 | δC(8)=O(4) (10)<br>τH(6)-N(5)-H(7) (17) |
| 555 | 93.4842 | 1.1898 | - | 553 | δC(8)=O(4) (21)<br>τO(2)-H(3) (46) |
| 513 | 27.1171 | 0.8682 | 512 | 512 | δC(9)=O(1) (18)<br>δC(25)-C(18)-C(13) (13) |
| 385 | 27.4428 | 1.403 | - | 382 | δC(9)-N(5) (10) |

| | | | | | |
|---|---|---|---|---|---|
| | | | | | δC(18)-C(25)-C(21) (12)<br>δC(27)-C(25)-C(21) (29) |
| 345 | 0.3553 | 1.4913 | - | 344 | δC(9)-N(5) (14)<br>δC(8)-O(2) (10) |
| 254 | 0.1882 | 1.7422 | - | 252 | δC(10)-C(15)-C(18)-C(13) (32)<br>δC(21)-H3(22,23,24) (10)<br>δC(15)-C(13)-C(18) (16) |
| 236 | 0.7314 | 1.3663 | - | - | δC(21)-H3(22,23,24) (14)<br>δC(27)-H3 (28,29,30) (64)<br>δC(21)-C(25)-C(27) (21) |
| 218 | 0.1036 | 0.0129 | - | 216 | δC(21)-H3(22,23,24) (14)<br>δC(27)-H3(28,29,30) (64) |
| 42 | 7.6319 | 0.9935 | - | - | τN(5)-C(9) (60) |

[a]ν-stretching; δ-in-plane deformation and out-of-plane deformation; τ-torsion; potential energy distribution is given in brackets (%) in the assignment column.

**Table S4**

Second-order perturbation theory analysis of Fock matrix in NBO basis corresponding to the intramolecular bonds of the title compound.

| Donor(i) | Type | ED/e | Acceptor(j) | Type | ED/e | E(2)[a] | E(j)-E(i)[b] | F(i,j)[c] |
|---|---|---|---|---|---|---|---|---|
| O1-C9 | σ | 1.99423 | N5-C9 | σ* | 0.06693 | 0.80 | 1.45 | 0.031 |
| | | | C9-C15 | σ* | 0.06616 | 1.03 | 1.37 | 0.034 |
| O1-C9 | π | 1.98752 | O1-C9 | π* | 0.23724 | 1.03 | 0.51 | 0.022 |
| O4-C8 | σ | 1.99619 | C8-C10 | σ* | 0.05680 | 1.50 | 1.48 | 0.043 |
| O4-C8 | π | 1.99013 | O1-C9 | π* | 0.23724 | 0.51 | 0.47 | 0.051 |
| - | | - | O4-C8 | π* | 0.21238 | 0.77 | 0.40 | 0.016 |
| N5-C9 | σ | 1.99480 | O1-C9 | σ* | 0.04383 | 0.71 | 1.39 | 0.028 |
| - | | - | C13-C15 | σ* | 0.01739 | 0.77 | 1.21 | 0.027 |
| C8-C10 | σ | 1.97926 | O4-C8 | σ* | 0.02304 | 1.14 | 1.26 | 0.034 |
| - | | - | C10-C13 | σ* | 0.02160 | 0.74 | 1.02 | 0.025 |
| - | | - | C13-C18 | σ* | 0.01806 | 1.78 | 1.04 | 0.039 |
| C9-C15 | σ | 1.97941 | O1-C9 | σ* | 0.04383 | 0.74 | 1.18 | 0.027 |
| | | | C13-C15 | σ* | 0.01739 | 0.68 | 1.01 | 0.023 |
| LPO1 | σ | 1.97714 | N5-C9 | σ* | 0.06693 | 1.57 | 1.13 | 0.038 |
| - | | - | C9-C15 | σ* | 0.06616 | 2.34 | 1.05 | 0.045 |
| LPO1 | π | 1.86742 | N5-C9 | σ* | 0.06693 | 24.75 | 0.70 | 0.120 |
| | | | C9-C15 | σ* | 0.06616 | 19.40 | 0.62 | 0.100 |
| LPO2 | σ | 1.97696 | O4-C8 | σ* | 0.02304 | 7.04 | 1.24 | 0.083 |
| LPO2 | π | 1.81759 | O4-C8 | π * | 0.21238 | 45.37 | 0.34 | 0.112 |
| LPO4 | σ | 1.97713 | O2-C8 | σ* | 0.09936 | 1.38 | 1.05 | 0.035 |
| - | - | - | C8-C10 | σ* | 0.05680 | 2.69 | 1.69 | 0.049 |
| LPO4 | π | 1.85504 | O2-C8 | σ* | 0.09936 | 32.95 | 0.62 | 0.129 |
| - | | - | C8-C10 | σ* | 0.05680 | 16.77 | 0.66 | 0.096 |
| LPN5 | σ | 1.76508 | O1-C9 | σ* | 0.23724 | 3.43 | 0.84 | 0.050 |
| - | | - | O1-C9 | π * | 0.01084 | 35.29 | 0.37 | 0.101 |

**Table S5**

NBO results showing the formation of Lewis and non-Lewis orbitals.

| Bond(A-B) | ED/e[a] | EDA% | EDB% | NBO | s% | p% |
|---|---|---|---|---|---|---|
| σO1-C9 | 1.99423 | 65.32 | 34.68 | 0.8082(sp1.70)O+ | 37.04 | 62.84 |
| - | -0.99528 | - | - | 0.5889(sp2.36)C | 29.71 | 70.11 |
| πO1-C9 | 1.98752 | 70.17 | 29.83 | 0.8377(sp23.39)O+ | 4.09 | 95.79 |
| - | -0.43597 | - | - | 0.5461(sp33.92)C | 2.85 | 96.70 |
| σO4-C8 | 1.99619 | 65.21 | 34.79 | 0.8076(sp1.43)O+ | 41.05 | 58.82 |
| - | -1.09905 | - | - | 0.5898(sp1.95)C | 33.86 | 65.98 |
| πO4-C8 | 1.99013 | 70.56 | 29.44 | 0.8400(sp1.00)O+ | 0.01 | 99.87 |
| - | -0.39615 | - | - | 0.5426(sp99.99)C | 0.01 | 99.47 |
| σN5-C9 | 1.99480 | 61.52 | 38.48 | 0.7844(sp1.60)N+ | 38.49 | 61.45 |
| - | -0.84039 | - | - | 0.6203(sp2.18)C | 31.44 | 68.46 |
| σC8-C10 | 1.97926 | 49.01 | 50.99 | 0.7001(sp1.55)C+ | 39.15 | 60.82 |
| - | -0.65949 | - | - | 0.7141(sp2.94)C | 25.37 | 74.56 |
| σC9-C15 | 1.97941 | 48.51 | 51.49 | 0.6965(sp1.78)C+ | 35.93 | 64.04 |
| - | -0.63444 | - | - | 0.7176(sp2.85)C | 25.94 | 74.00 |
| n1O1 | 1.97714 | - | - | sp0.70 | 58.88 | 41.11 |
| - | -0.68206 | - | - | - | - | - |
| n2O1 | 1.86742 | - | - | sp99.99 | 0.03 | 99.90 |
| - | -0.25214 | - | - | - | - | - |
| n1O2 | 1.97696 | - | - | sp1.22 | 45.05 | 54.91 |
| - | -0.63366 | - | - | - | - | - |
| n2O2 | 1.81759 | - | - | sp99.99 | 0.04 | 99.90 |
| - | -0.34337 | - | - | - | - | - |
| n1O4 | 1.97713 | - | - | sp0.70 | 58.97 | 41.01 |
| - | -0.71064 | - | - | - | - | - |
| n2O4 | 1.85504 | - | - | sp99.99 | 0.02 | 99.90 |
| - | -0.27818 | - | - | - | - | - |
| n1N5 | 1.76508 | - | - | sp17.93 | 5.28 | 94.70 |
| - | -0.28851 | - | - | - | - | - |

[a] ED/e is expressed in a.u.

**Table S6**

Partial Charges in isolated and embedded molecule

| | | Isolated | Enbedded | Δ% |
|---|---|---|---|---|
| 1 | O1 | -0.64216 | -0.86436 | 34.60239 |
| 2 | O2 | -0.65783 | -0.70026 | 6.45125 |
| 3 | H2 | 0.453281 | 0.533309 | 17.65527 |
| 4 | O4 | -0.60573 | -0.68518 | 13.11649 |
| 5 | N5 | -1.00406 | -0.91446 | 8.923734 |
| 6 | H1A | 0.438875 | 0.44947 | 2.414127 |
| 7 | H1B | 0.43395 | 0.453312 | 4.461804 |
| 8 | C8 | 0.797366 | 0.882077 | 10.62385 |
| 9 | C9 | 0.855179 | 0.982773 | 14.92015 |
| 10 | C10 | -0.18827 | -0.32223 | 71.15101 |
| 11 | H8A | 0.046685 | 0.075207 | 61.09457 |
| 12 | H8B | 0.01742 | 0.044151 | 153.4501 |
| 13 | C13 | 0.448429 | 0.480093 | 7.061096 |
| 14 | H1 | -0.08142 | -0.07813 | 4.047947 |
| 15 | C15 | -0.43193 | -0.61299 | 41.91899 |
| 16 | H6A | 0.074392 | 0.157918 | 112.2782 |
| 17 | H6B | 0.098332 | 0.152924 | 55.51804 |
| 18 | C18 | -0.23558 | -0.21247 | 9.810131 |
| 19 | H2A | 0.044388 | 0.055196 | 24.34892 |
| 20 | H2B | 0.036963 | 0.0518 | 40.14014 |
| 21 | C21 | -0.22882 | -0.22898 | 0.070361 |
| 22 | H5A | 0.035764 | 0.029397 | 17.80282 |
| 23 | H5B | 0.047476 | 0.04427 | 6.752886 |
| 24 | H5C | 0.047986 | 0.043446 | 9.461093 |
| 25 | C25 | 0.389423 | 0.378975 | 2.682944 |
| 26 | H3 | -0.08958 | -0.08463 | 5.529198 |
| 27 | C27 | -0.25239 | -0.24936 | 1.202098 |
| 28 | H4A | 0.06072 | 0.065769 | 8.315217 |
| 29 | H4B | 0.053721 | 0.04795 | 10.74254 |
| 30 | H4C | 0.037416 | 0.025002 | 33.17832 |
| | Group A | -0.0129 | 0.029946 | 332.0496 |
| | Group B | 0.081785 | 0.106735 | 30.50682 |
| | Group C | 0.101715 | 0.071844 | 29.36735 |

**Table S7**

Comparison of linear refractive index for 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid crystal with experimental results for others organic crystals.

| | $n$ |
|---|---|
| 3-(2-amino-2-oxoethyl)-5-methylhexanoic acid (Present work) | 1.455 |
| 1-(5-chlorothiophen-2-yl)-3-(2,3-dimethoxyphenyl)prop-2-en-1-one(CTDMP)[84,85] | 1.594 |
| (2E)-3[4(methylsulfanyl)phenyl]-1-(4-nitrophenyl)prop-2-en-1-one(4N4MSP)[9,85] | 1.360 |
| (2E)-1-(4-bromophenyl)-3-[4(methylsulfanyl)phenyl]prop-2-en-1-one(4Br4MSP)[9,85] | 1.363 |
| (2E)-1-[3-bromophenyl)-3(2E)-1-(3-bromophenyl)-3-[(4methylsulfanyl)phenyl]-prop-2-en-1-one(3Br4MSP)[9,85] | 1.365 |

**Table S8**

Molecular docking values of AOEMHA with target proteins (a) 4BDU, (b) 4DBS, (c) 4DBW, (d) 4FAL and (e) 4FAM.

| Protein (PDB ID) | Bond distance (Å) | Bonded residues | Estimated inhibition constant (μm) | Binding energy (kcal/mol) | Intermolecular energy (kcal/mol) | Reference RMSD (Å) |
|---|---|---|---|---|---|---|
| 4BDU | 2.5 | SER 271 | 236.05 | -4.95 | -7.04 | 47.401 |
| | 2.1 | ARG 276 | | | | |
| | 2.0 | LYS270 | | | | |
| | 1.8 | TYR272 | | | | |
| 4DBS | 1.7 | LYS270 | 927.65 | -4.14 | -6.23 | 30.006 |
| | 2.3 | ARG276 | | | | |
| | 2.1 | ARG276 | | | | |
| 4DBW | 2.4 | LYS270 | 339.39 | -4.73 | -6.82 | 30.052 |
| | 1.8 | LYS270 | | | | |
| | 2.4 | ARG276 | | | | |
| | 1.8 | ARG276 | | | | |
| | 2.2 | TYR272 | | | | |
| 4FAL | 2.4 | LYS270 | 484.06 | -4.52 | -6.61 | 3.191 |
| | 2.2 | SER271 | | | | |
| | 1.8 | LYS270 | | | | |
| | 2.0 | ARG276 | | | | |
| | 2.2 | ARG276 | | | | |
| | 2.4 | TYR272 | | | | |
| 4FAM | 1.8 | ARG276 | 377.69 | -4.67 | -6.76 | 15.296 |
| | 2.4 | TYR272 | | | | |
| | 2.0 | LYS270 | | | | |
| | 2.3 | LYS270 | | | | |
| | 2.3 | GLN222 | | | | |