Supplementary Information (SI) for New Journal of Chemistry.
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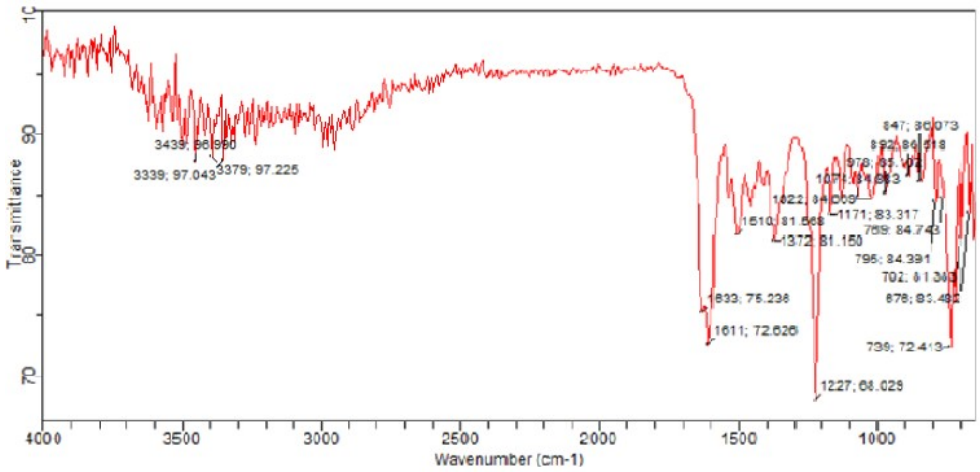
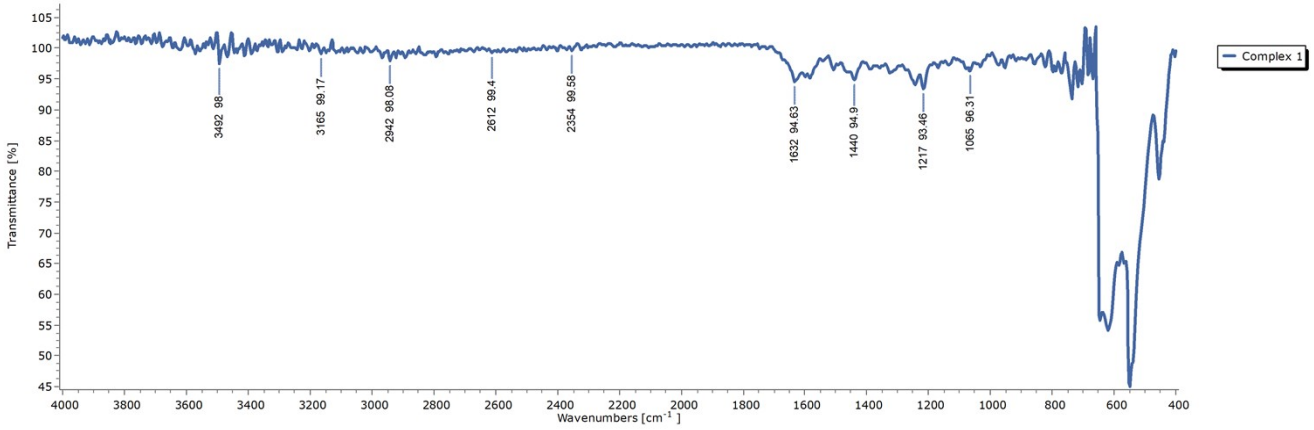
Synthesis, characterization, crystal structure, molecular docking of *o*-vanillin and L-valine Derived molecules: DFT study and antiproliferative activity against PANC-1 Cancer cell line

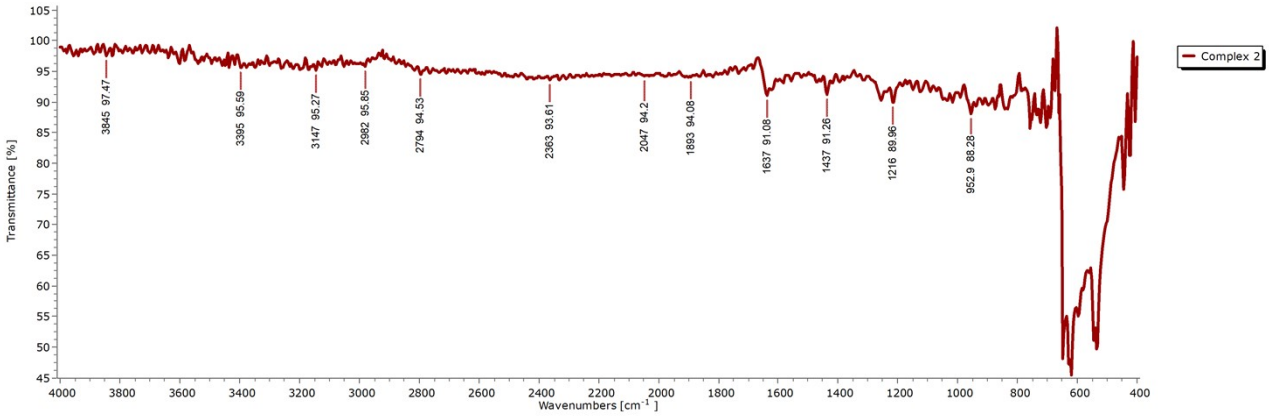
Supplementary Information



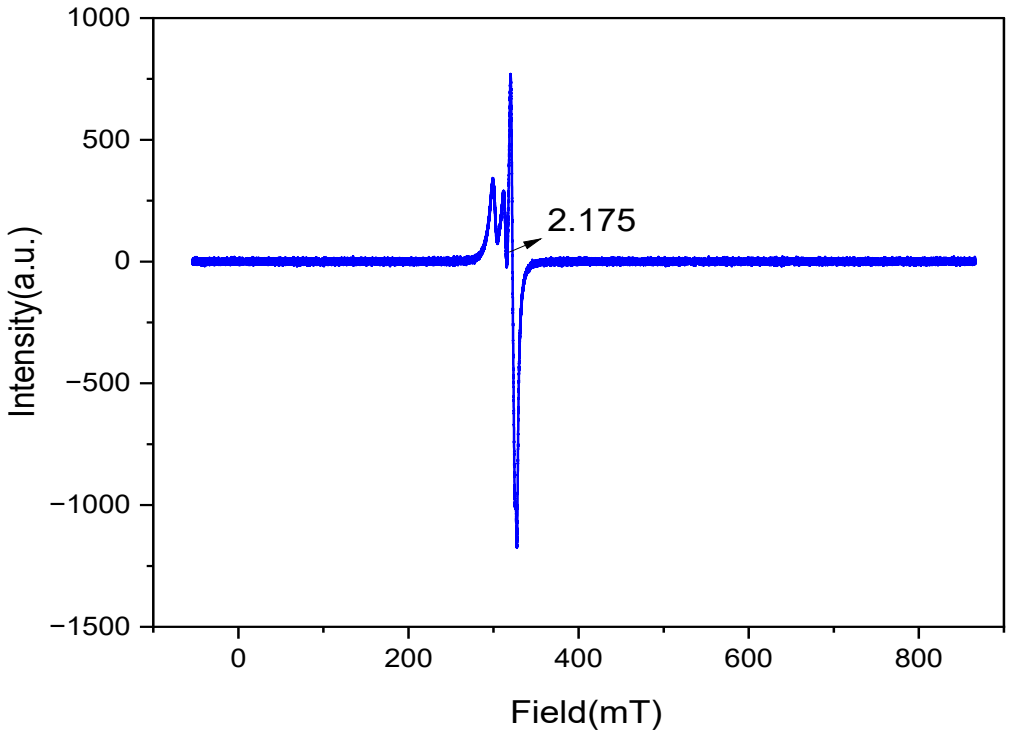
FigureS1: IR Spectra of Ligand (H_2L)



FigureS2: FTIR spectrum of Cu(II) complex1



FigureS3: FTIR spectra of L_2-Cu- Bipyridine complex (complex2)



FigureS4: EPR spectrum of Cu (II) complex1

Table S1. Crystallographic table and structure refinement parameters for **1**.

Compound	**1**
Empirical formula	$C_{23}H_{23}CuN_3O_4$
Formula weight /g mol^{-1}	468.98

Temperature / K	296
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a/ Å	8.9536(2)
b/ Å	10.3106(2)
c/ Å	23.2792(4)
α,β,γ/ °	90
Volume/ Å^3	2149.07(7)
Z	4
d_{cal}/ g cm^{-3}	1.449
μ/ mm^{-1}	1.051
F(000)	972
θ range for data collection/°	1.750 to 26.429
Index ranges	$-11 \leq h \leq 11$, $-12 \leq k \leq 12$, $-29 \leq l \leq 29$
Completeness	0.999
Reflections collected	98276
Independent reflections	4411 [R_{int} = 0.0236, R_{sigma} = 0.0116]
Data/restraints/parameters	4411/0/292
Goodness-of-fit on F^2	1.041
Final R indices [$I \geq 2\sigma(I)$]	R_1 = 0.0208, wR_2 = 0.0578
Final R indices [all data]	R_1 = 0.0229, wR_2 = 0.0589
Largest diff. peak/hole/e Å^3	0.18/-0.22
CCDC number	2240174

Table S2: Selected bond length/bond angle of complex1 obtained from optimized geometry

Bond angle (^{0})/Bond length (Å) Complex 1	Theoretical values
O(1)–Cu(1)–O(2)	98.78
O(2)–Cu(1)–O(3)	82.19
O(3)–Cu(1)–O(4)	88.00
O(4)–Cu(1)–O(1)	92.16
N(1)–Cu(1)–N(2)	169.08
N(1)–Cu(1)–O(1)	82.18
N(1)–Cu(1)–O(2)	98.82
N(1)–Cu(1)–O(3)	90.28
N(1)–Cu(1)–O(4)	88.00
N(2)–Cu(1)–O(1)	89.14
N(2)–Cu(1)–O(2)	98.23
N(2)–Cu(1)–O(3)	83.06
N(2)–Cu(1)–O(4)	89.27
Cu-O(1)(pheno)	2.09
Cu-O(2)(Phen)	2.04
Cu-O(1)(carbox)	2.01
Cu-O(2)(carbox)	2.02
Cu-N1(imine)	2.00
Cu-N2(imine)	2.01

Table S3: Details of Binding mode/interaction and energy of both the molecules with receptor Epidermal Growth Factor Receptor (EGFR) and Tyrosine Kinase(TRK)

Test molecule	R Receptor	Binding energy (Kcal/mol)	Hydrogen bonding		Hydrophobic		Salt bridge/WATER BRIDGE		π- π stacking	II-cation	Inhibition constant
			Residue	Bond length (Å)	Residue	Bond length (Å)	Residue	Bond length			

Ligand	EGFR Kinase (pdb id 1m17)	-6.37	THR766	2.57	LEU694 VAL702 ASP831	3.03 2.98 2.91	--	--	--		25.96nM
Complex 1		-10.87	Glu738 THR766 THR830 ASP831	3.88 2.89 3.57 3.70	LEU694 PHE699 VAL702 ALA719	3.04 2.97 3.05 2.89	ASP831	4.64	PHE699 LEU768 MET769 LEU794		469nM
Complex 2		-11.97	LYS721 MET769 ASP831	2.36 4.02 3.87	LEU694 PHE699 LEU820 ASP831	3.11 3.67 2.91 3.89	-	-	LYS721 LEU820 PHE699		534nM
Ligand	Tyrosine Kinase (pdb id 1t46)	-7.34	Glu640 THR670	2.86 2.98	GLU640 LEU644 VAL654	3.77-3.92			PHE811	Lys623 HIS790	31.67nM
Complex 1		-11.10	THR670 CYS673 ASP810	2.98 2.80 3.08	VAL603 LYS623 GLU640 LEU644 VAL654	3.99-4.12	LYS623 ASP810	3.50 5.50	PHE811	Lys623 HIS790	532nM
Complex 2		-11.97	Glu640 THR670 CYS673 ASP810	2.86 2.98 2.80 3.08	LEU595 VAL603 LYS623 GLU640 LEU644 VAL654	3.77-3.92	LYS623 ASP810	3.21 5.23	PHE811	Lys623 HIS790	578nM