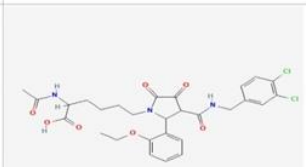
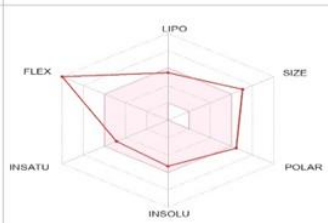
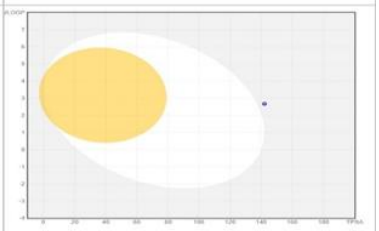
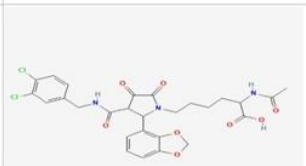
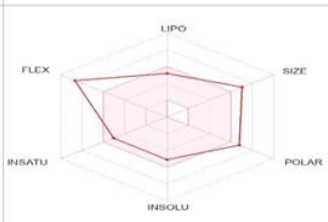
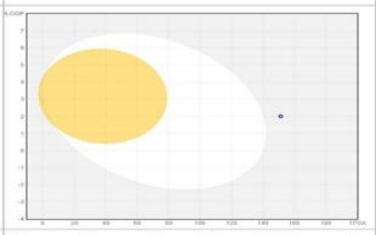
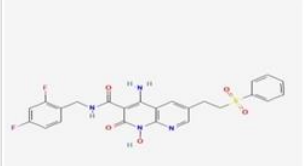
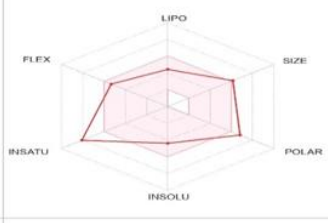
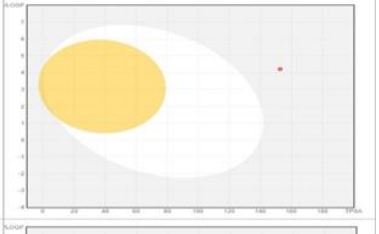
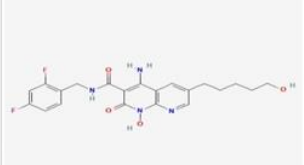
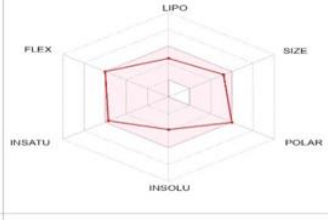
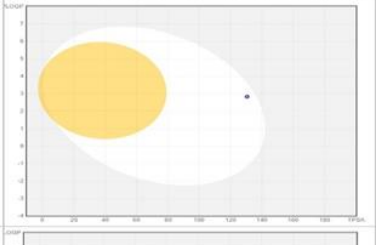
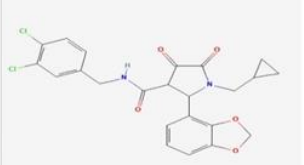
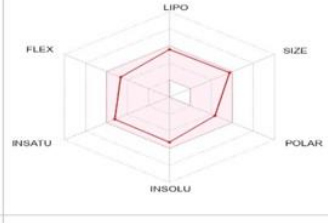
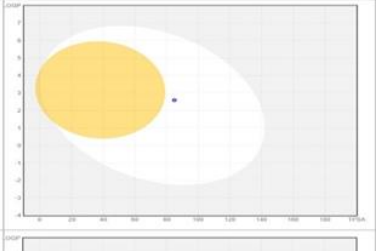
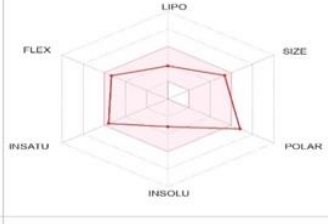
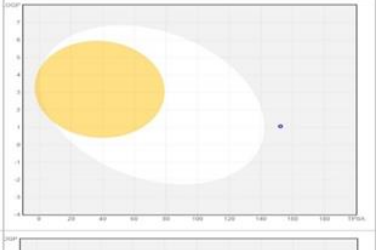
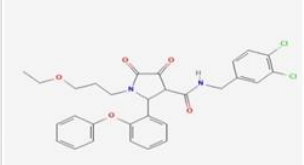
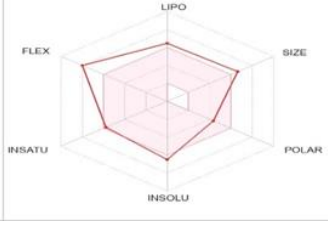
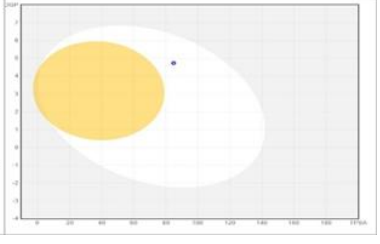
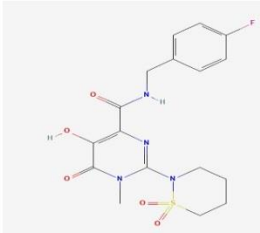
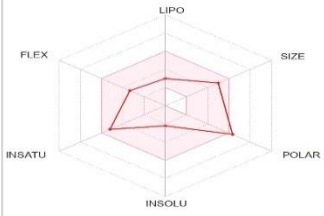
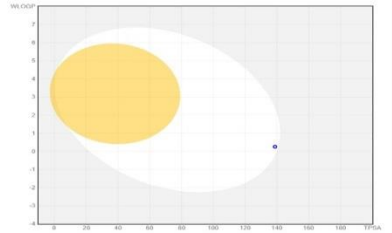
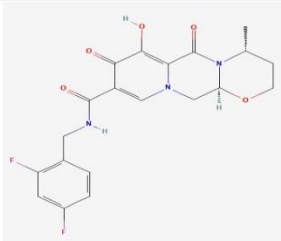
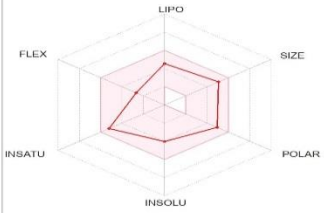
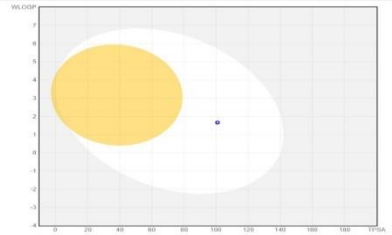
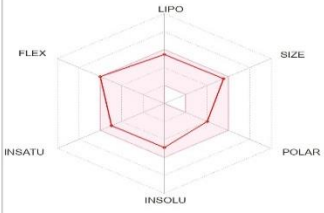
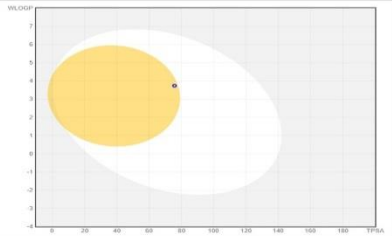
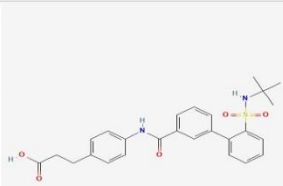
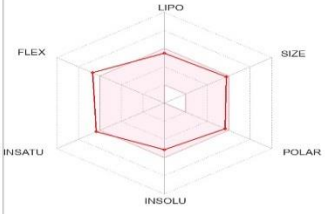
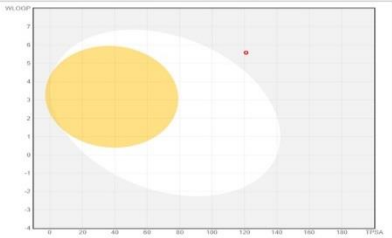
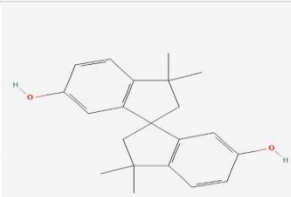
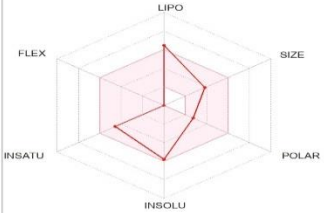
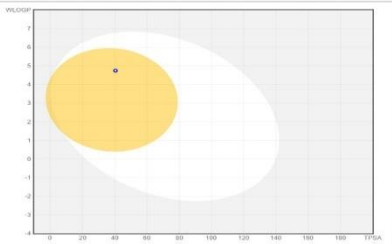
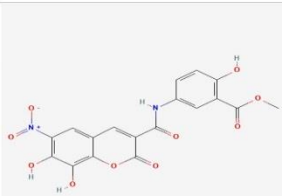
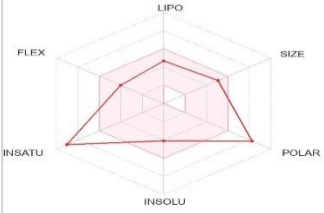
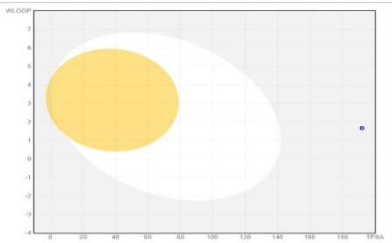
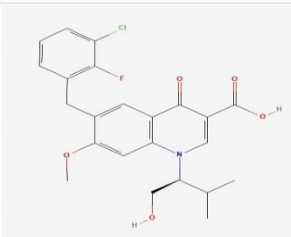
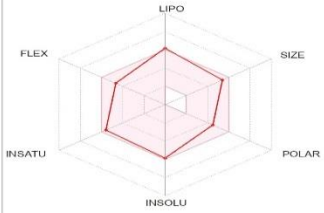
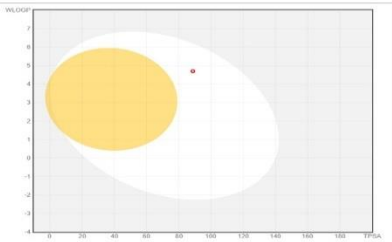
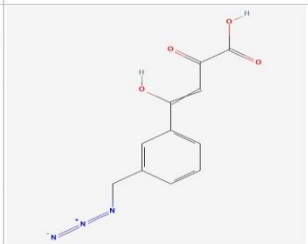
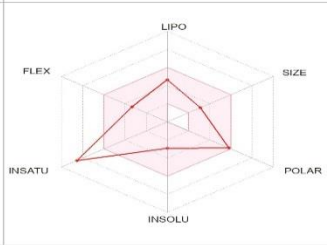
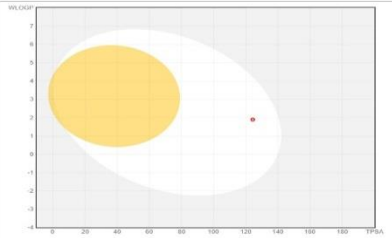
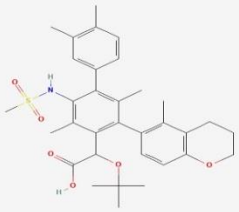
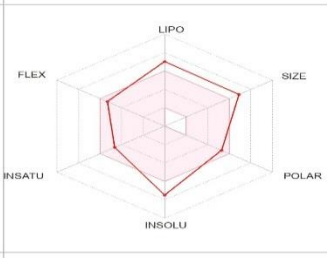
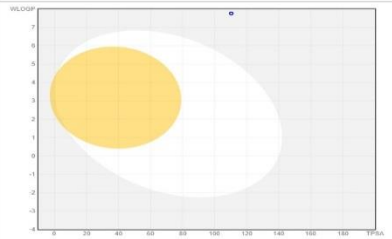
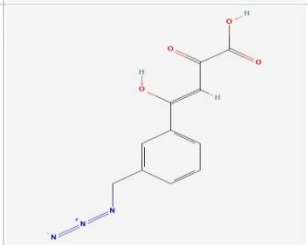
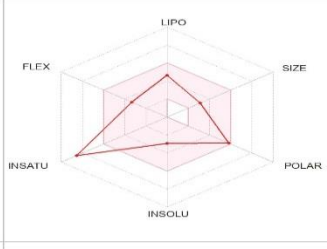
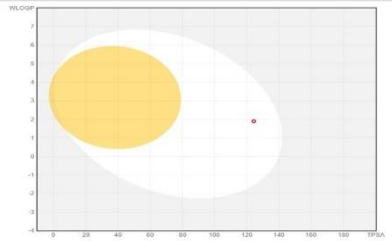
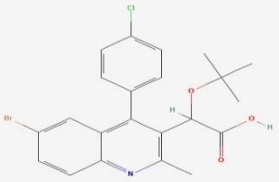
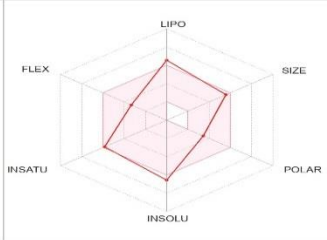
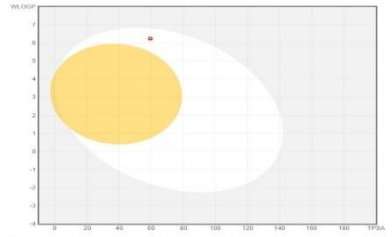
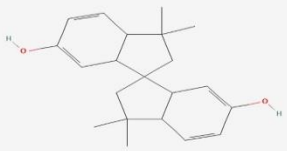
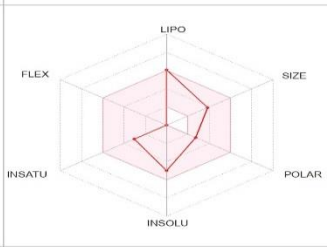
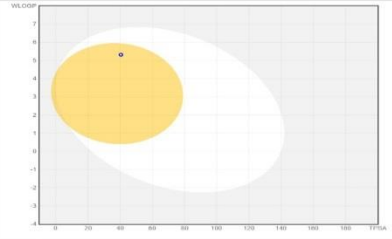
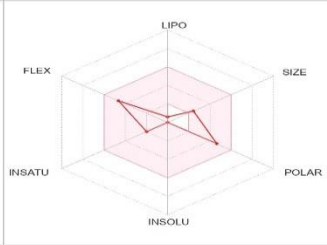
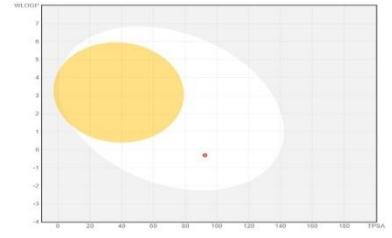
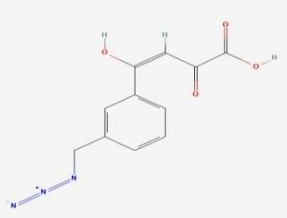
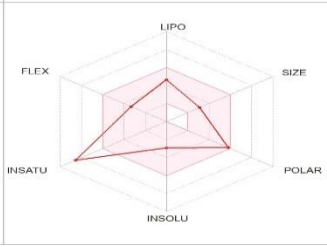
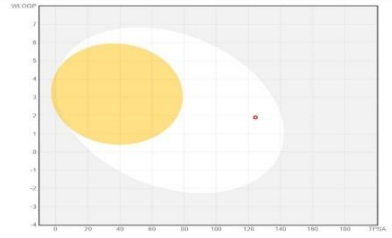
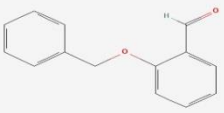
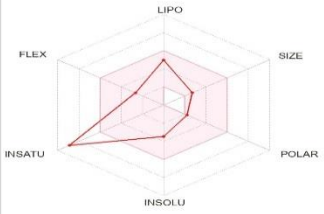
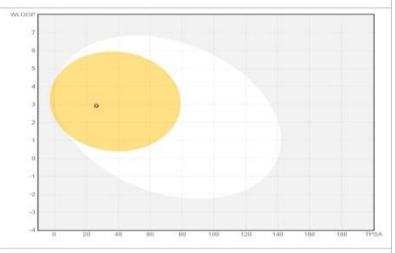
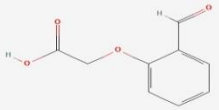
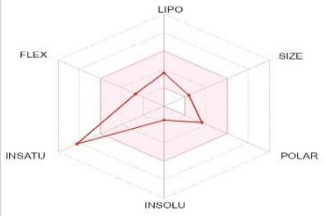
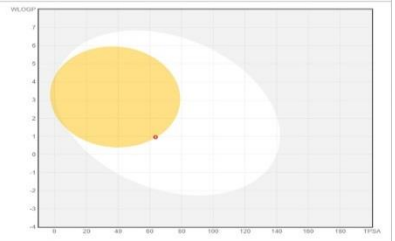
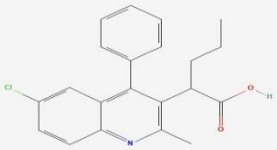
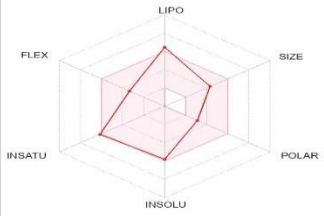
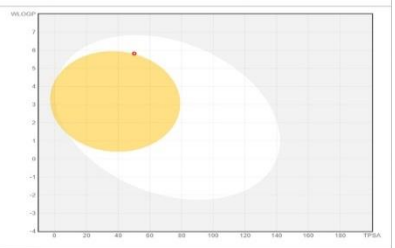
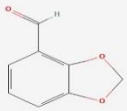
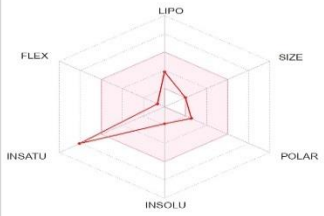
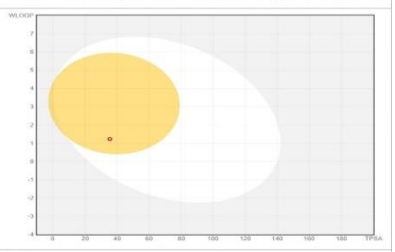
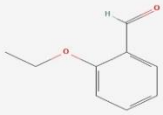
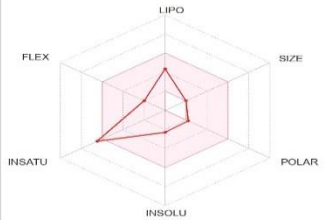
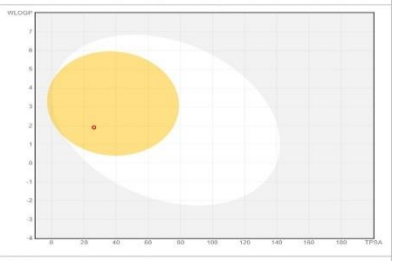
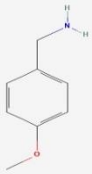
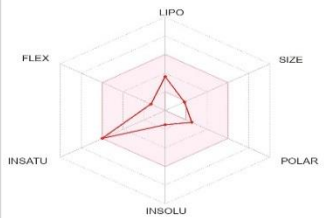
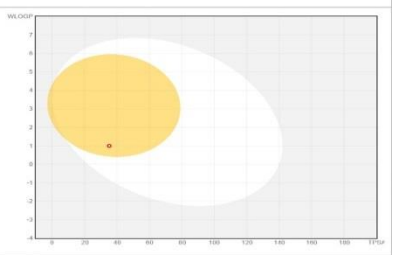
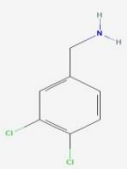
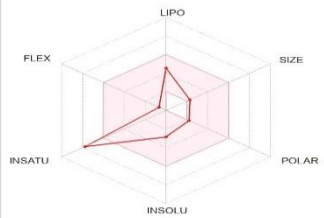
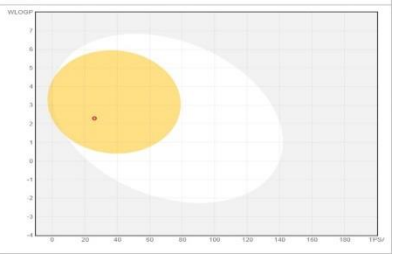
Supplementary File: Figure S1, Table S1, Table S2

CID Number	IUPAC Name	2D– Structure of studied compounds	Radar Scale of studied compounds	Egg Plot Scale of studied compounds
91899503	2-acetamido-6-[3-[(3,4-dichlorophenyl)methylcarbamoyl]-2-(2-ethoxyphenyl)-4,5-dioxopyrrolidin-1-yl]hexanoic acid			
91899501	2-acetamido-6-[2-(1,3-benzodioxol-4-yl)-3-[(3,4-dichlorophenyl)methylcarbamoyl]-4,5-dioxopyrrolidin-1-yl]hexanoic acid			
117696807	4-amino-6-[2-(benzenesulfonyl)ethyl]-N-[(2,4-difluorophenyl)methyl]-1-hydroxy-2-oxo-1,8-naphthyridine-3-carboxamide			
117697114	4-amino-N-[(2,4-difluorophenyl)methyl]-1-hydroxy-6-(5-hydroxypentyl)-2-oxo-1,8-naphthyridine-3-carboxamide			
91899500	2-(1,3-benzodioxol-4-yl)-1-(cyclopropylmethyl)-N-[(3,4-dichlorophenyl)methyl]-4,5-dioxopyrrolidine-3-carboxamide			
54671008	N-[2-[4-[(4-fluorophenyl)methylcarbamoyl]-5-hydroxy-1-methyl-6-oxopyrimidin-2-yl]propan-2-yl]-5-methyl-1,3,4-oxadiazole-2-carboxamide			
91899502	N-[(3,4-dichlorophenyl)methyl]-1-(3-ethoxypropyl)-4,5-dioxo-2-(2-phenoxyphenyl)pyrrolidine-3-carboxamide			

CID Number	IUPAC Name	2D– Structure of studied compounds	Radar Scale of studied compounds	Egg Plot Scale of studied compounds
54682040	2-(1,1-dioxothiazinan-2-yl)-N-[(4-fluorophenyl) methyl]-5-hydroxy-1-methyl-6-oxopyrimidine-4-carboxamide			
54726191	(3S,7R)-N-[(2,4-difluorophenyl) methyl]-11-hydroxy-7-methyl-9,12-dioxo-4-oxa-1,8-diazatricyclo [8.4.0.03,8] tetradeca-10,13-diene-13-carboxamide			
91899504	1-(cyclopropylmethyl)-N-[(4-methoxyphenyl) methyl]-4,5-dioxo-2-[2-(trifluoromethyl) phenyl] pyrrolidine-3-carboxamide			
135397695	3-[4-[[3-[2-(6,7,8-butyloulfamoyl) phenyl]benzoyl] amino]phenyl] propanoic acid			
74071	1,1,1',1'-tetramethyl-3,3'-spirobi[2,1]-indene]-5,5'-diol			
163321963	methyl 5-[(7,8-dihydroxy-6-nitro-2-oxochromene-3-carbonyl)amino]-2-hydroxybenzoate			
5277135	6-[(3-chloro-2-fluorophenyl) methyl]-1-[(2,S)-1-hydroxy-3-methylbutan-2-yl] -7-methoxy-4-oxoquinoline-3-carboxylic acid			

CID Number	IUPAC Name	2D– Structure of studied compounds	Radar Scale of studied compounds	Egg Plot Scale of studied compounds
511335	4-[3-(azidomethyl) phenyl]-4-hydroxy-2-oxobut 3 enoic acid			
86575523	2-[4-(3,4-dimethylphenyl)-3-(methanesulfonamido)-2,8-dimethyl-6-(5-methyl-3,4-dihydro-2*H*-chromen-6-yl) phenyl] 2-[(2-methylpropan-2-yl)oxy]acetic acid			
5496124	(*Z*)-4-[3-(azidomethyl) phenyl]-4-hydroxy 2 oxobut -3-enoic acid			
49770008	2-[6-bromo-4-(4-chlorophenyl)-2-methylquinolin-3-yl]-2-[(2-methylpropan-2-yl)oxy]acetic acid			
133081875	1,1,1',1'-tetramethyl-3,3'-spirobi[3*a*,7*a*-dihydro-2*H*-indene]-5,5'-diol			
23390002	(2*S*)-2-acetamido-6 aminohexanoic acid			
86767865	(*E*)-4-[3-(azidomethyl) phenyl]-4-hydroxy 2 oxobut -3-enoic acid			

CID Number	IUPAC Name	2D– Structure of studied compounds	Radar Scale of studied compounds	Egg Plot Scale of studied compounds
344784	2-phenylmethoxybenzaldehyde			
46533	2-(2-formylphenoxy) acetic acid			
24800940	2-(6-chloro-2-methyl-4-phenylquinolin-3-yl)pentanoic acid			
82264	1,3-benzodioxole-4-carbaldehyde			
11950	2-ethoxybenzaldehyde			
75452	(4-methoxyphenyl) methanamine			
1608	(3,4-dichlorophenyl) methanamine			

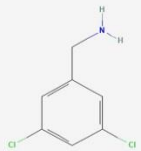
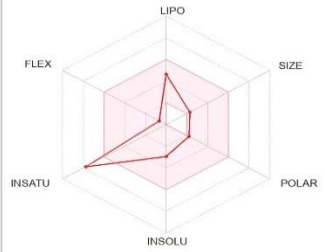
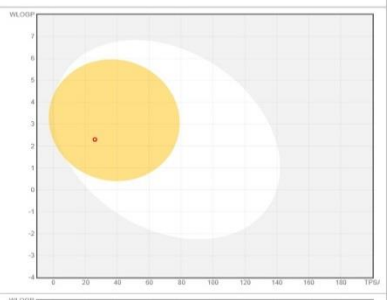
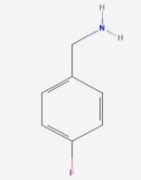
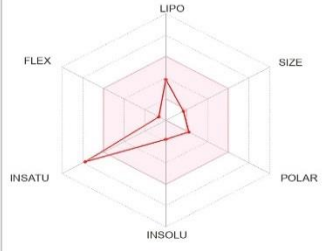
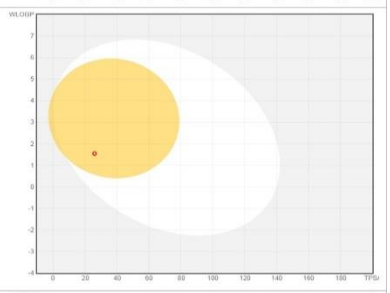
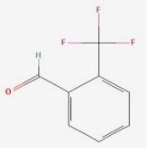
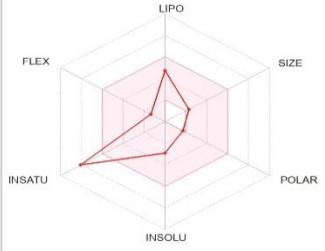
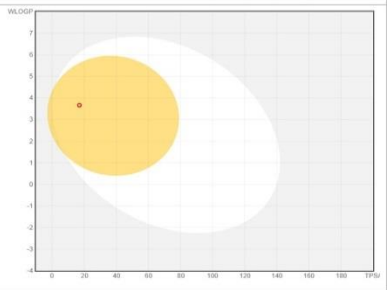
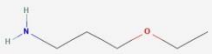
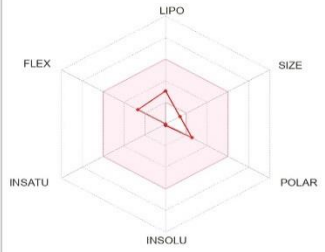
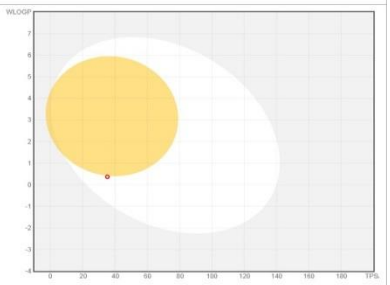
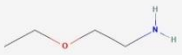
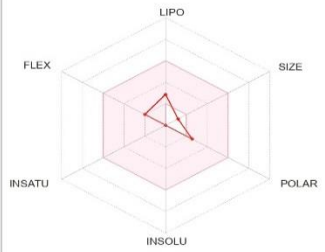
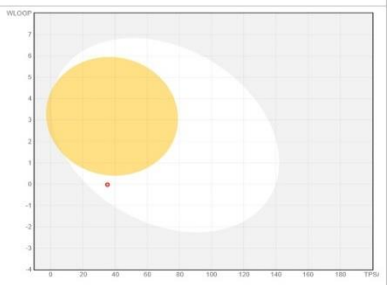
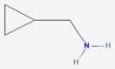
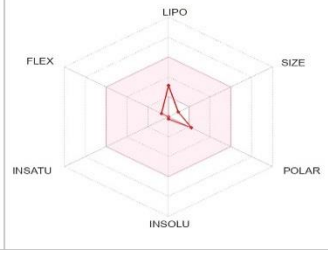
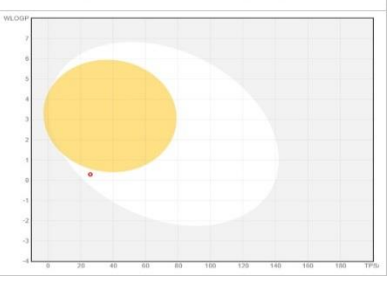
CID Number	IUPAC Name	2D– Structure of studied compounds	Radar Scale of studied compounds	Egg Plot Scale of studied compounds
457602	(3,5-dichlorophenyl) methanamine			
67326	(4-fluorophenyl) methanamine			
123067	2-(trifluoromethyl) benzaldehyde			
22720	3-ethoxypropan-1-amine			
66970	2-ethoxyethanamine			
75646	cyclopropylmethanamine			

Figure S1. The CID number, IUPAC name, and 2D structure of the studied compounds, along with a Bioavailability Radar scale of the compounds. The Bioavailability Radar scale allows for a quick assessment of a molecule's drug-likeness, with the optimal range for each property represented by the pink area. Additionally, the egg plot of the studied compounds is included. Yellow areas represent compounds that can passively cross the blood-brain barrier, white areas contain compounds that can be passively absorbed by the digestive system, and blue dots indicate compounds that can enter the central nervous system through P-glycoproteins. The red dots indicate compounds that can exit the central nervous system through P-glycoproteins.

Table S1. Molecular docking results of the studied compounds on the HIV Integrase Catalytic Core Model [PDB ID: 6WC8].

CID Number	IUPAC Name	Compounds Name	MolDock Score (kcal/mol)	Rerank Score (kcal/mol)	Torsions	H-Bond (kcal/mol)	Heavy Atoms	MW	(Ligand Efficiency) LE1 (MolDock Score/ Heavy Atoms)	Docking Score (kcal/mol)
91899503	2-acetamido-6-[3-[(3,4-dichlorophenyl)methylcarbamoyl]-2-(2-ethoxyphenyl)-4,5-dioxopyrrolidin-1-yl]hexanoic acid	BDBM93352	-202.382	-152.392	13	-8.79808	40	592.468	-5.05954	-205.926
91899501	2-acetamido-6-[2-(1,3-benzodioxol-4-yl)-3-[(3,4-dichlorophenyl)methylcarbamoyl]-4,5-dioxopyrrolidin-1-yl]hexanoic acid	BDBM93350	-165.881	-86.4989	11	-2.40898	40	592.425	-4.14701	-154.228
117696807	4-amino-6-[2-(benzenesulfonyl)ethyl]-N-[(2,4-difluorophenyl)methyl]-1-hydroxy-2-oxo-1,8-naphthyridine-3-carboxamide	SCHEMBL16236090	-165.001	-94.8155	7	-2.00291	36	514.501	-4.58337	-177.932
117697114	4-amino-*N*-[(2,4-difluorophenyl)methyl]-1-hydroxy-6-(5-hydroxypentyl)-2-oxo-1,8-naphthyridine-3-carboxamide	CHEMBL4101122	-154.038	-90.8332	8	-4.48405	31	432.421	-4.96896	-159.233
91899500	2-(1,3-benzodioxol-4-yl)-1-(cyclopropylmethyl)-*N*-[(3,4-dichlorophenyl)methyl]-4,5-dioxopyrrolidine-3-carboxamide	BDBM93349	-150.432	-29.6595	6	-4.49333	32	475.321	-4.701	-160.361
54671008	N-[2-[4-[(4-fluorophenyl)methylcarbamoyl]-5-hydroxy-1-methyl-6-oxopyrimidin-2-yl]propan-2-yl]-5-methyl-1,3,4-oxadiazole-2-carboxamide	Raltegravir	-143.925	-76.8294	6	-6.72736	32	444.416	-4.49766	-143.74
91899502	N-[(3,4-dichlorophenyl)methyl]-1-(3-ethoxypropyl)-4,5-dioxo-2-(2-phenoxyphenyl)pyrrolidine-3-carboxamide	BDBM93351	-139.653	-80.513	11	0	38	555.449	-3.67507	-137.876
54682040	2-(1,1-dioxothiazinan-2-yl)-N-[(4-fluorophenyl)methyl]-5-hydroxy-1-methyl-6-oxopyrimidine-4-carboxamide	BMS-707035	-132.628	-106.663	4	-10.1548	28	410.42	-4.73672	-140.496

54726191	(3S,7R)-N-[(2,4-difluorophenyl)methyl]-11-hydroxy-7-methyl-9,12-dioxo-4-oxa-1,8-diazatricyclo[8.4.0.03,8]tetradeca-10,13-diene-13-carboxamide	Dolutegravir	-129.509	-101.146	3	-2.9078	30	419.379	-4.31696	-133.135
91899504	1-(cyclopropylmethyl)-*N*-[(4-methoxyphenyl)methyl]-4,5-dioxo-2-[2-(trifluoromethyl)phenyl]pyrrolidine-3-carboxamide	BDBM93353	-123.078	-89.2792	8	-0.961646	33	460.446	-3.72963	-123.821
135397695	3-[4-[[3-[2-(*tert*-butylsulfamoyl)phenyl]benzoyl]amino]phenyl]propanoic acid	starbld0037140	-122.566	-92.112	9	-12.3021	34	480.576	-3.60487	-123.275
74071	1,1,1',1'-tetramethyl-3,3'-spirobi[2*H*-indene]-5,5'-diol	SPIROBIINDANE	-121.379	-78.4514	0	-0.995663	23	308.414	-5.27734	-122.147
163321963	methyl 5-[(7,8-dihydroxy-6-nitro-2-oxochromene-3-carbonyl)amino]-2-hydroxybenzoate	CHEMBL4867922	-120.832	-80.2688	5	-7.45396	30	416.295	-4.02773	-133.49
5277135	6-[(3-chloro-2-fluorophenyl)methyl]-1-[(2*S*)-1-hydroxy-3-methylbutan-2-yl]-7-methoxy-4-oxoquinoline-3-carboxylic acid	Elvitegravir	-116.093	-85.3028	7	-5.10043	31	447.884	-3.74493	-123.789
511335	4-[3-(azidomethyl)phenyl]-4-hydroxy-2-oxobut-3-enoic acid	HIV-1 Integrase Inhibitor	-113.793	-88.5071	5	-8.11758	18	247.207	-6.32182	-114.321
86575523	2-[4-(3,4-dimethylphenyl)-3-(methanesulfonamido)-2,5-dimethyl-6-(5-methyl-3,4-dihydro-2*H*-chromen-6-yl)phenyl]-2-[(2-methylpropan-2-yl)oxy]acetic acid	Integrase-LEDGF/p75?allosteric?inhibitor?1	-112.391	2.92283	8	-6.17703	41	579.747	-2.74125	-109.976
5496124	(*Z*)-4-[3-(azidomethyl)phenyl]-4-hydroxy-2-oxobut-3-enoic acid	CHEMBL564495	-109.54	-85.181	5	-4.45793	18	247.207	-6.08554	-115.041
49770008	2-[6-bromo-4-(4-chlorophenyl)-2-methylquinolin-3-yl]-2-[(2-methylpropan-2-yl)oxy]acetic acid	BIB-II; ALLINI-2	-107.329	-32.8324	5	-3.7718	28	462.764	-3.83316	-104.587
133081875	1,1,1',1'-tetramethyl-3,3'-spirobi[3*a*,7*a*-dihydro-2*H*-indene]-5,5'-diol	Spiro Biindane Bisphenol	-105.654	-71.8638	0	-5	23	312.446	-4.59365	-107.215
23390002	(2*R*)-2-acetamido-6-aminohexanoic acid	Ac-D-Lys-OH	-104.779	-81.8777	6	-4.41419	13	188.224	-8.05994	-111.836

86767865	(*E*)-4-[3-(azidomethyl)phenyl]-4-hydroxy-2-oxobut-3-enoic acid	NCGC00390769-01	-103.199	-69.3491	5	-10.4285	18	247.207	-5.7333	-113.446
344784	2-phenylmethoxybenzaldehyde	2-(Benzyloxy)benzaldehyde	-101.743	-73.8898	4	0	16	212.244	-6.35895	-98.8839
46533	2-(2-formylphenoxy)acetic acid	2-Formylphenoxyacetic acid	-93.6054	-76.1677	4	-2.3028	13	180.157	-7.20042	-94.4918
24800940	2-(6-chloro-2-methyl-4-phenylquinolin-3-yl)pentanoic acid	LEDGIN6	-90.3829	-60.5756	5	-4.62866	25	353.842	-3.61532	-90.382
82264	1,3-benzodioxole-4-carbaldehyde	1,3-benzodioxole-4-carbaldehyde	-76.6749	-64.6696	1	-4.31831	11	150.131	-6.97044	-76.2294
11950	2-ethoxybenzaldehyde	2-ETHOXYBENZALDEHYDE	-73.7016	-63.1541	3	0	11	150.174	-6.70014	-72.4053
75452	(4-methoxyphenyl)methanamine	4-Methoxybenzylamine	-71.8712	-62.2071	2	-2.5	10	137.179	-7.18712	-71.5274
1608	(3,4-dichlorophenyl)methanamine	3,4-Dichlorobenzylamine	-69.8571	-57.3917	1	0	10	176.043	-6.98571	-68.6723
457602	(3,5-dichlorophenyl)methanamine	3,5-Dichlorobenzylamine	-69.7305	-54.0165	1	0	10	176.043	-6.97305	-68.1287
67326	(4-fluorophenyl)methanamine	4-Fluorobenzylamine	-67.2611	-56.9754	1	0	9	125.144	-7.47346	-65.9761
123067	2-(trifluoromethyl)benzaldehyde	2-(Trifluoromethyl)benzaldehyde	-67.0042	-59.9321	2	-2.5	12	174.12	-5.58369	-65.0221
22720	3-ethoxypropan-1-amine	3-Ethoxypropylamine	-63.2725	-52.0592	4	-5.32568	7	103.163	-9.03893	-63.6614
66970	2-ethoxyethanamine	2-Ethoxyethylamine	-56.9274	-44.2091	3	-1.87098	6	89.1362	-9.48789	-59.1666

75646	cyclopropylmethanamine	Cyclopropylmethylamine	-47.2857	-38.5696	1	-0.767793	5	71.121	-9.45714	-50.7085

Table S2. Physicochemical Properties of Studied Compounds.

CID Number	Formula	MW	Heavy atoms	Aromatic heavy atoms	Fraction Csp3	Rotatable bonds	H-bond acceptors	H-bond donors	MR (molecular refractivity)	TPSA	iLOGP	XLOGP3	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Class
91899503	C28H31Cl2N3O7	592.47	40	12	0.39	15	7	3	152.58	142.11	2.5	4.04	-5.29	0.0030400	Moderately soluble
91899501	C27H27Cl2N3O8	592.42	40	12	0.37	13	8	3	147.34	151.34	2.36	3.52	-5.09	0.0047600	Moderately soluble
117696807	C24H20F2N4O5S	514.5	36	22	0.12	8	8	3	127.74	152.76	2.22	2.25	-4.37	0.0219000	Moderately soluble
117697114	C21H22F2N4O4	432.42	31	16	0.29	9	7	4	110.71	130.47	2.83	2.44	-3.85	0.0616000	Soluble
91899500	C23H20Cl2N2O5	475.32	32	12	0.35	7	5	1	121.23	84.94	2.94	4.25	-5.28	0.0024900	Moderately soluble

54671008	C20H21FN6O5	444.42	32	17	0.3	8	9	3	109.03	152.24	2.71	1.1	-3.15	0.3120000	Soluble
91899502	C29H28Cl2N2O5	555.45	38	18	0.28	12	5	1	149.68	84.94	3.53	5.79	-6.49	0.0001800	Poorly soluble
54682040	C17H19FN4O5S	410.42	28	12	0.35	5	8	3	102.18	138.77	1.19	-0.27	-2.2	2.5800000	Soluble
54726191	C20H19F2N3O5	419.38	30	12	0.35	4	7	2	104.48	100.87	2.1	2.44	-4.01	0.0410000	Moderately soluble
91899504	C24H23F3N2O4	460.45	33	12	0.38	9	7	1	116.64	75.71	2.9	4.03	-4.91	0.0056800	Moderately soluble
135397695	C26H28N2O5S	480.58	34	18	0.23	10	6	3	132.8	120.95	2.81	4.09	-5.13	0.0035800	Moderately soluble
74071	C21H24O2	308.41	23	12	0.43	0	2	2	94.14	40.46	2.99	5.83	-5.81	0.0004760	Moderately soluble
163321963	C18H12N2O10	416.3	30	16	0.06	6	10	4	102.87	192.12	1.48	2.67	-4.1	0.0329000	Moderately soluble

5277135	C23H23ClFNO5	447.88	31	16	0.3	7	6	2	117.73	88.76	2.65	5.32	-5.89	0.0005790	Moderately soluble
511335	C11H9N3O4	247.21	18	6	0.09	5	7	2	59.48	124.35	1.59	2.61	-2.93	0.2880000	Soluble
86575523	C33H41NO6S	579.75	41	18	0.42	8	6	2	166.46	110.31	3.99	6.76	-7.49	0.0000188	Poorly soluble
5496124	C11H9N3O4	247.21	18	6	0.09	5	7	2	59.48	124.35	1.59	2.61	-2.93	0.2880000	Soluble
49770008	C22H21BrClNO3	462.76	28	16	0.27	5	4	1	116.75	59.42	4.81	5.97	-6.56	0.0001270	Poorly soluble
133081875	C21H28O2	312.45	23	0	0.62	0	2	2	95.07	40.46	2.89	5.13	-5.01	0.0030600	Moderately soluble
23390002	C8H16N2O3	188.22	13	0	0.75	7	4	3	48.05	92.42	1.2	-4.45	2.26	34100.0000000	Highly soluble
86767865	C11H9N3O4	247.21	18	6	0.09	5	7	2	59.48	124.35	1.33	2.61	-2.93	0.2880000	Soluble

344784	C14H12O2	212.24	16	12	0.07	4	2	0	62.81	26.3	2.39	3.21	-3.47	0.0720000	Soluble
46533	C9H8O4	180.16	13	6	0.11	4	4	1	44.9	63.6	1.13	0.81	-1.54	5.1400000	Very soluble
24800940	C21H20ClNO2	353.84	25	16	0.24	5	3	1	103.12	50.19	3.11	5.78	-5.82	0.0005370	Moderately soluble
82264	C8H6O3	150.13	11	6	0.12	1	3	0	37.89	35.53	1.7	1.2	-1.86	2.0500000	Very soluble
11950	C9H10O2	150.17	11	6	0.22	3	2	0	43.13	26.3	2.03	2.09	-2.29	0.7640000	Soluble
75452	C8H11NO	137.18	10	6	0.25	2	2	1	40.61	35.25	1.7	0.84	-1.53	4.0300000	Very soluble
1608	C7H7Cl2N	176.04	10	6	0.14	1	1	1	44.14	26.02	1.92	2.48	-2.87	0.2360000	Soluble
457602	C7H7Cl2N	176.04	10	6	0.14	1	1	1	44.14	26.02	1.99	2.64	-2.97	0.1870000	Soluble

67326	C7H8FN	125.14	9	6	0.14	1	2	1	34.07	26.02	1.56	1.2	-1.8	1.9900000	Very soluble
123067	C8H5F3O	174.12	12	6	0.12	2	4	0	36.83	17.07	1.67	2.78	-2.91	0.2150000	Soluble
22720	C5H13NO	103.16	7	0	1	4	2	1	29.94	35.25	1.7	-0.14	-0.13	76.9000000	Very soluble
66970	C4H11NO	89.14	6	0	1	3	2	1	25.13	35.25	1.58	-0.5	0.12	118.0000000	Highly soluble
75646	C4H9N	71.12	5	0	1	1	1	1	21.94	26.02	1.36	0.03	-0.23	41.5000000	Very soluble