

Supporting Information

Org. Commun. 17:2 (2024) 99-114

Synthesis of benzhydrol analogues based on 1'-acetoxychavicol acetate (ACA), as a stable and potent antiproliferative agent on breast cancer cell lines, ADMET analysis and molecular docking study

Mohamad Nurul Azmi ^{1*}, Cheong Siong Tan ¹, Hassan Taiye Abdulameed ^{2,3}, Nik Nur Syazni Nik Mohamad Kamal ², Nur Ezzah Abdul Kahar⁴ and Mohammad Tasyriq Che Omar ⁵

¹Natural Products and Synthesis Organic Research Laboratory (NPSO), School of Chemical Sciences, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

²Advance Medical and Dental Institute, Universiti Sains Malaysia, 13200 Kepala Batas, Penang, Malaysia

³Department of Biochemistry, Kwara State University, PMB1530 Malete, Nigeria.

⁴Science and Engineering Research Centre (SERC), Engineering Campus, Universiti Sains Malaysia, 14300 Nibong Tebal, Penang, Malaysia

⁵Biological Section, School of Distance Education, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

Table of Contents	Page
Figure S1: ¹ H-NMR (500 MHz, MeOH-D ₄) Spectrum of Compound 2	3
Figure S2: ¹³ C-NMR (125 MHz, MeOH-D ₄) Spectrum of Compound 2	3
Figure S3: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3a	4
Figure S4: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 3a	4
Figure S5: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3b	5
Figure S6: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 3b	5
Figure S7: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3c	6
Figure S8: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 3c	6
Figure S9: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3d	7
Figure S10: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 3d	7
Figure S11: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3e	8
Figure S12: ¹³ C-NMR (125 MHz, CDCl ₃) Spectrum of Compound 3e	8
Figure S13: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 3f	9

* Corresponding author: E-Mail: mnazmi@usm.my ; Phone: +6046533562; Fax: +6046574854

Figure S14: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of Compound 3f	9
S1: Molecular Docking	10
Figure S15: Image of docking compared to X-ray diffraction method. Where, Crystal OTH	20

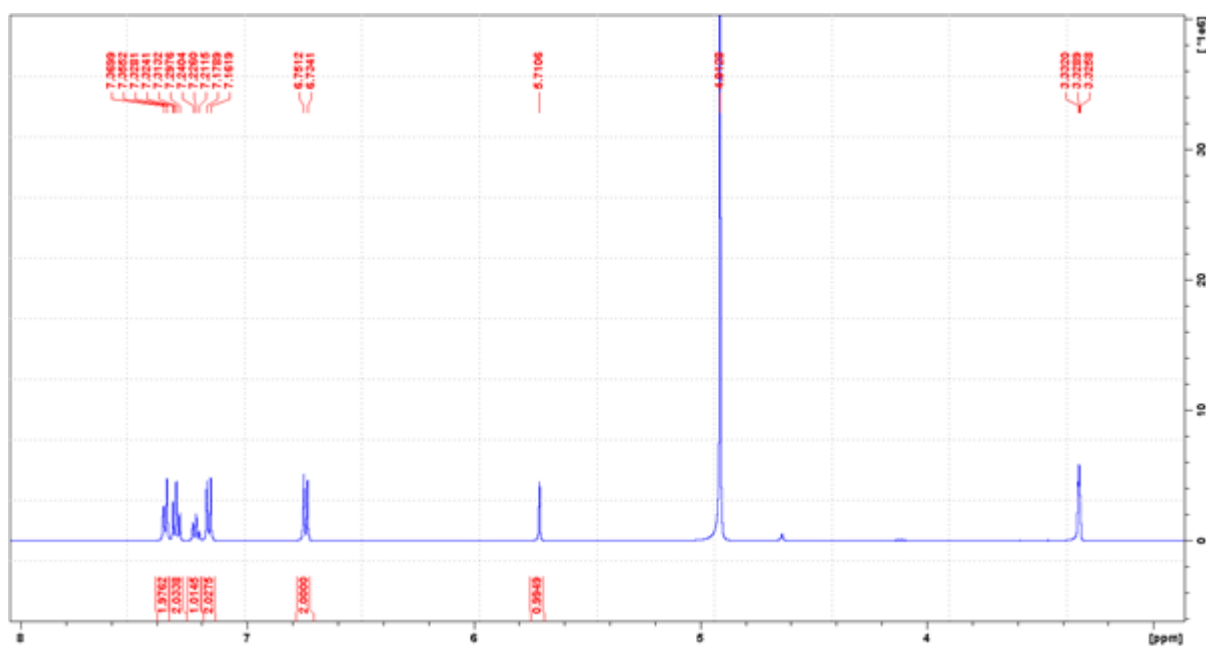


Figure S1: $^1\text{H-NMR}$ (500 MHz, MeOH- D_4) spectrum of compound **2**

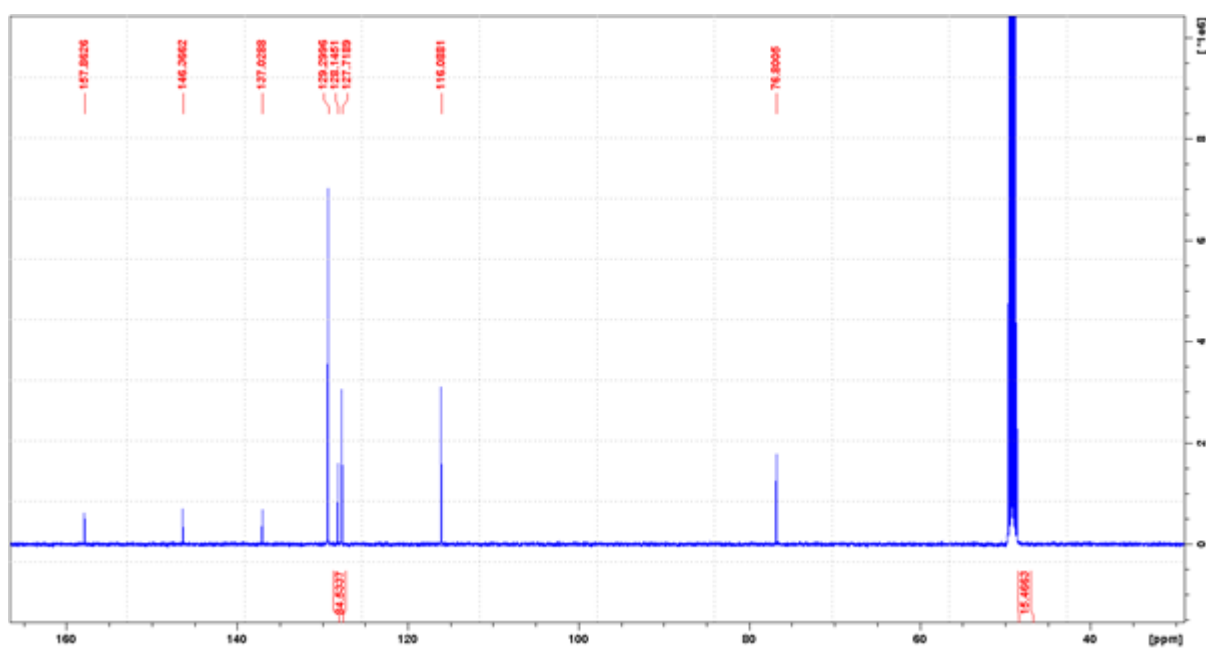


Figure S2: $^{13}\text{C-NMR}$ (125 MHz, MeOH- D_4) spectrum of compound **2**

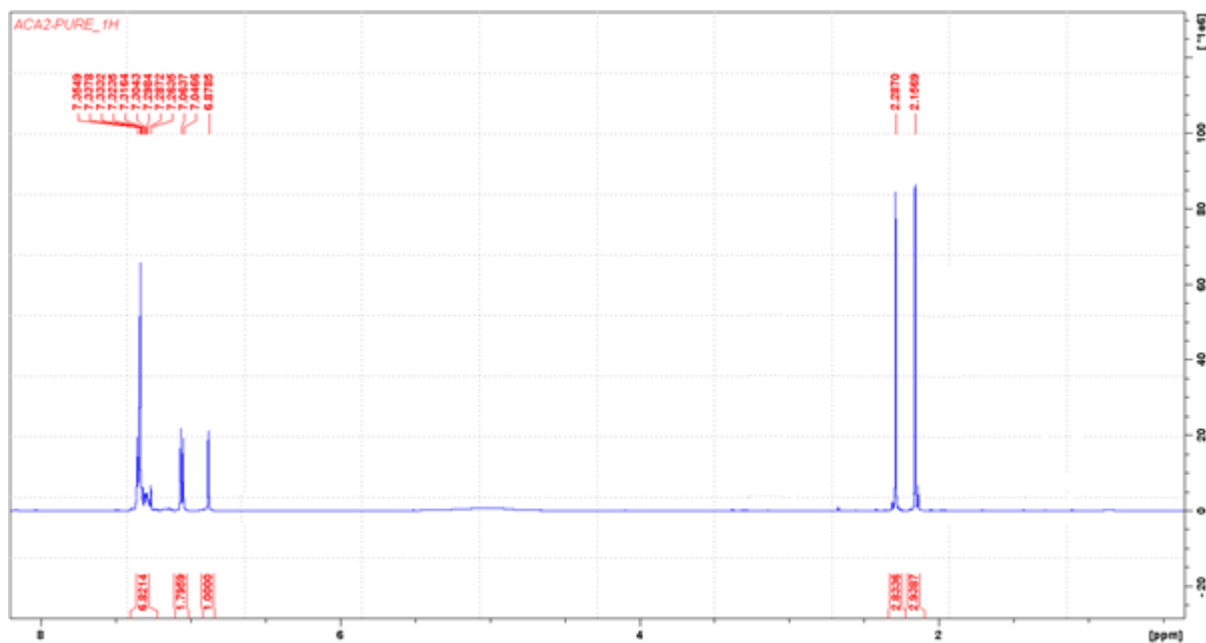


Figure S3: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3a**

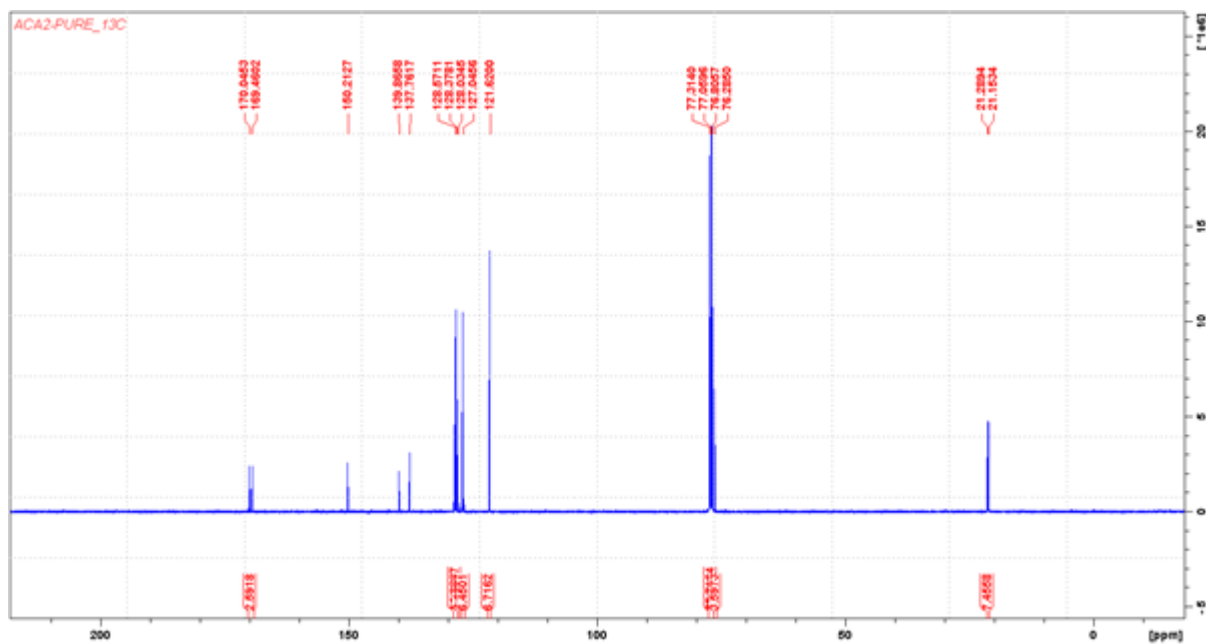


Figure S4: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3a**

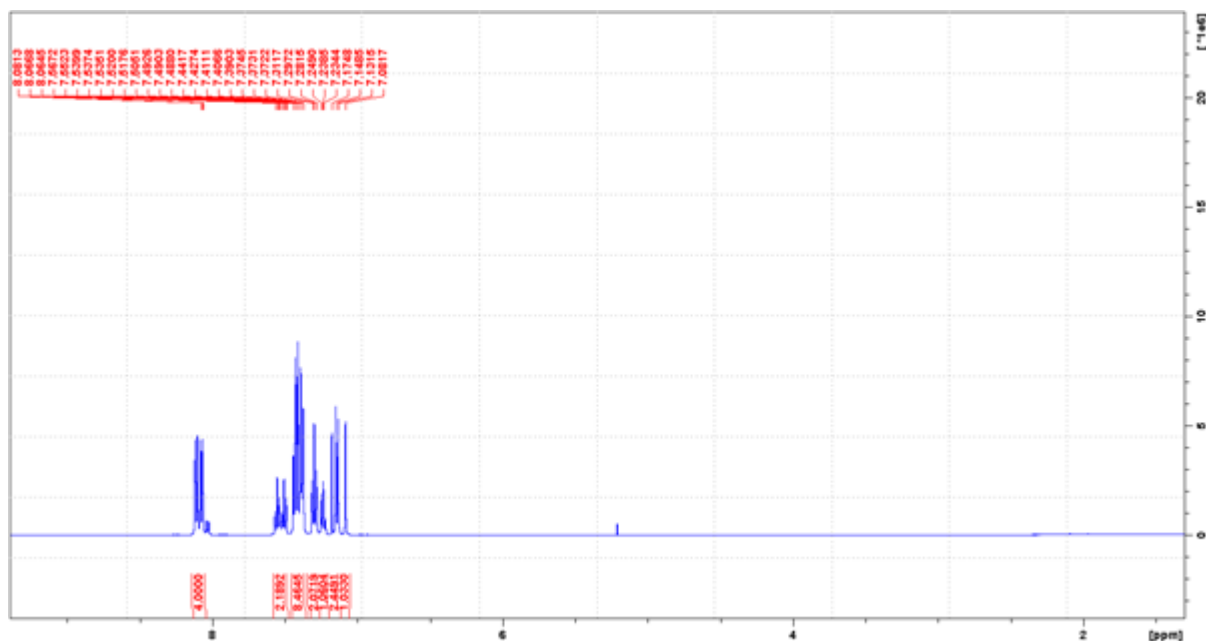


Figure S5: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3b**

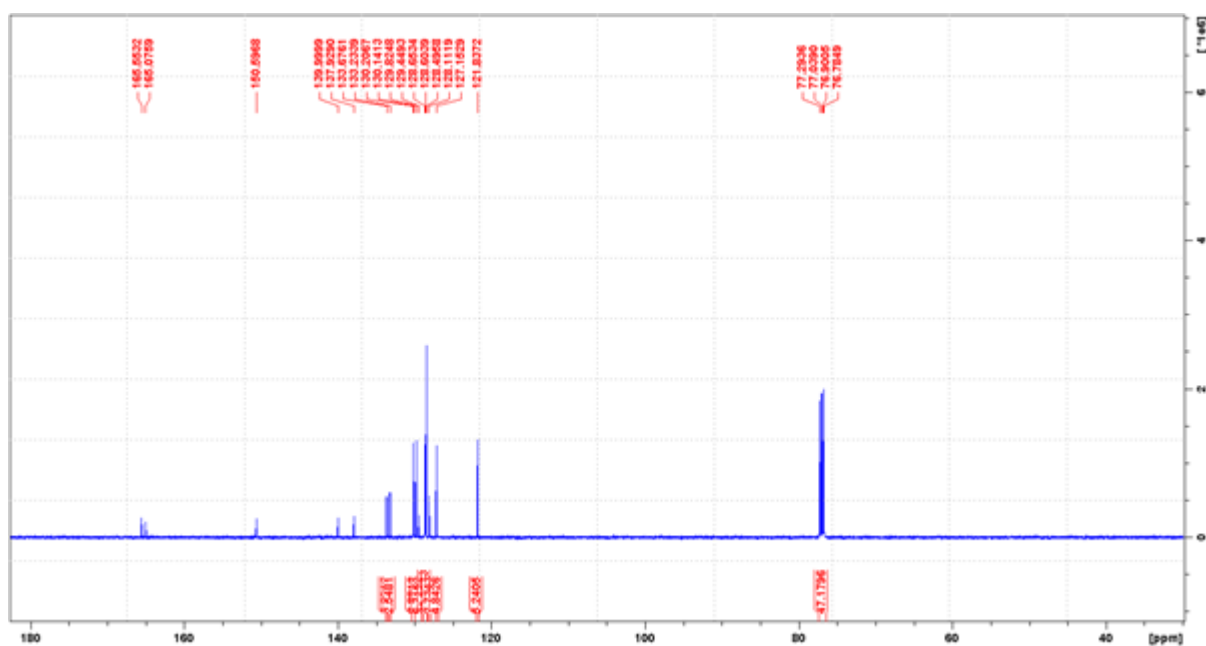


Figure S6: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3b**

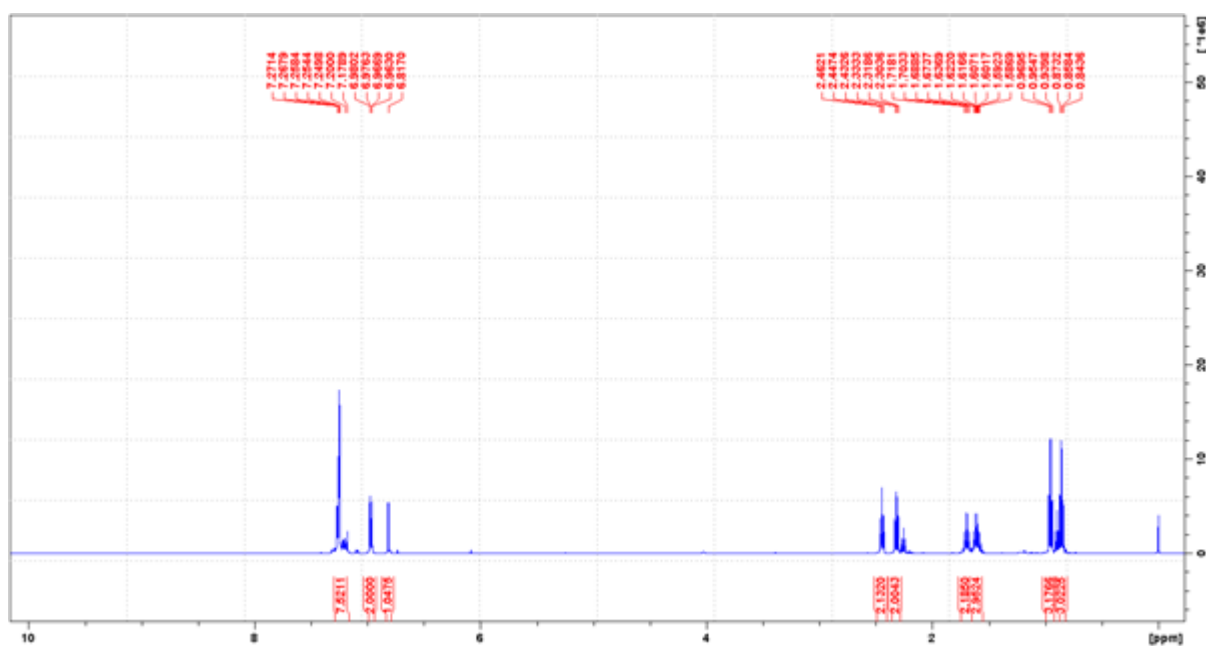


Figure S7: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3c**

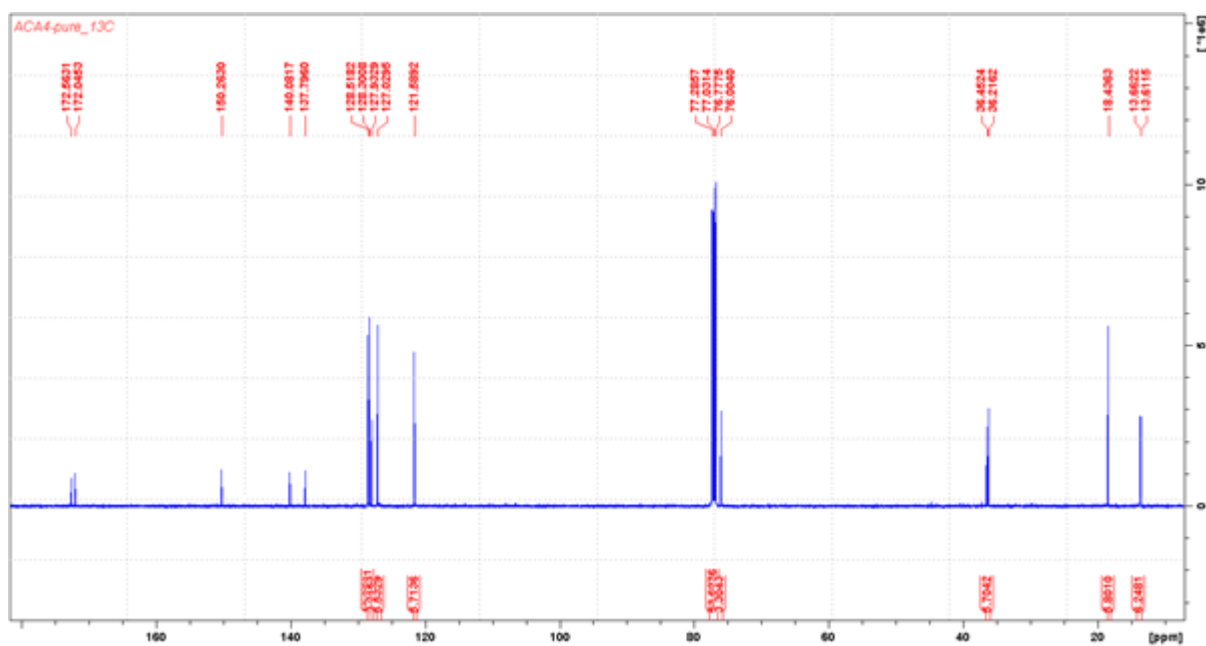


Figure S8: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3c**

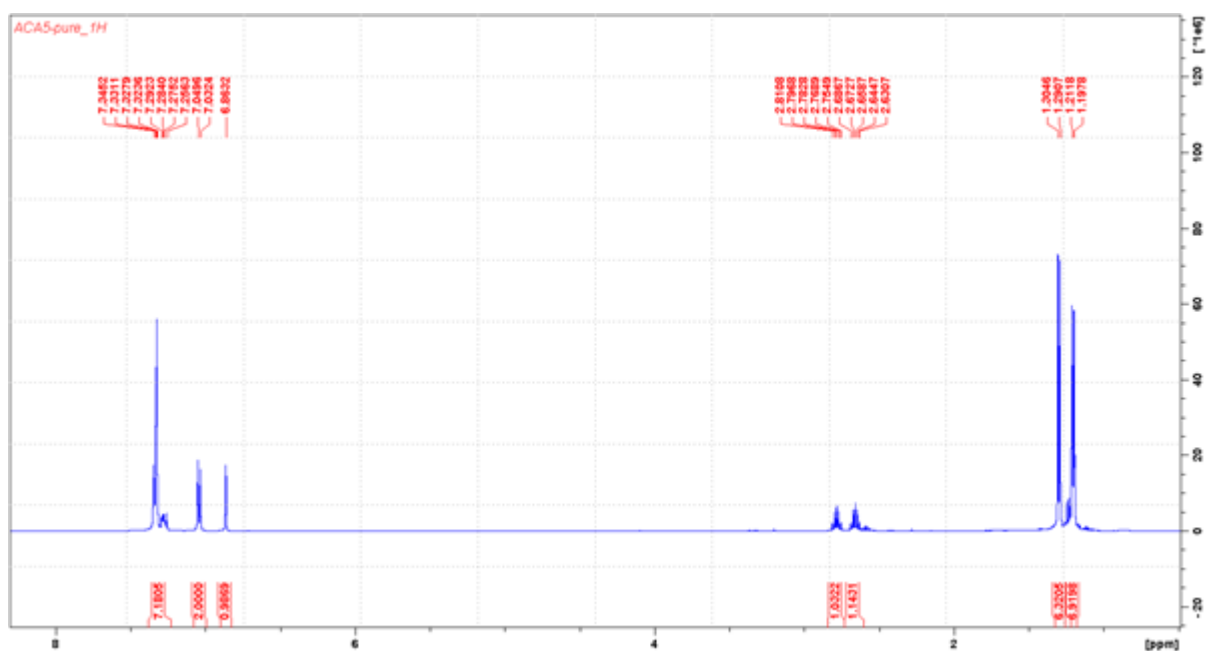


Figure S9: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3d**

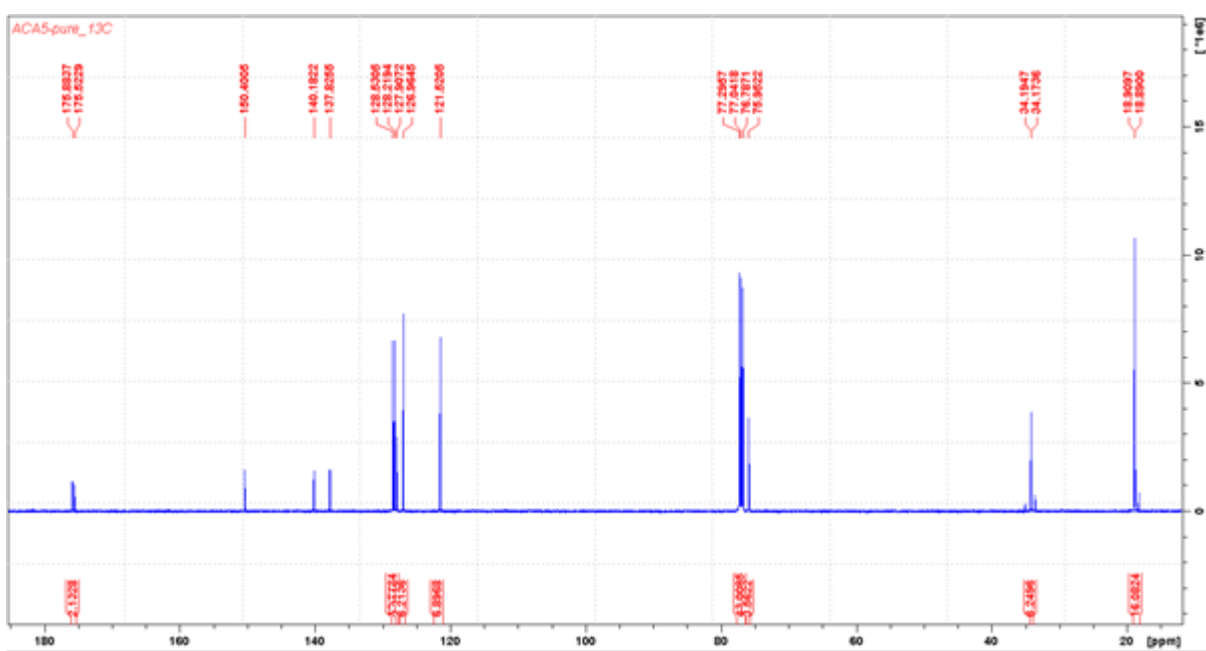


Figure S10: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3d**

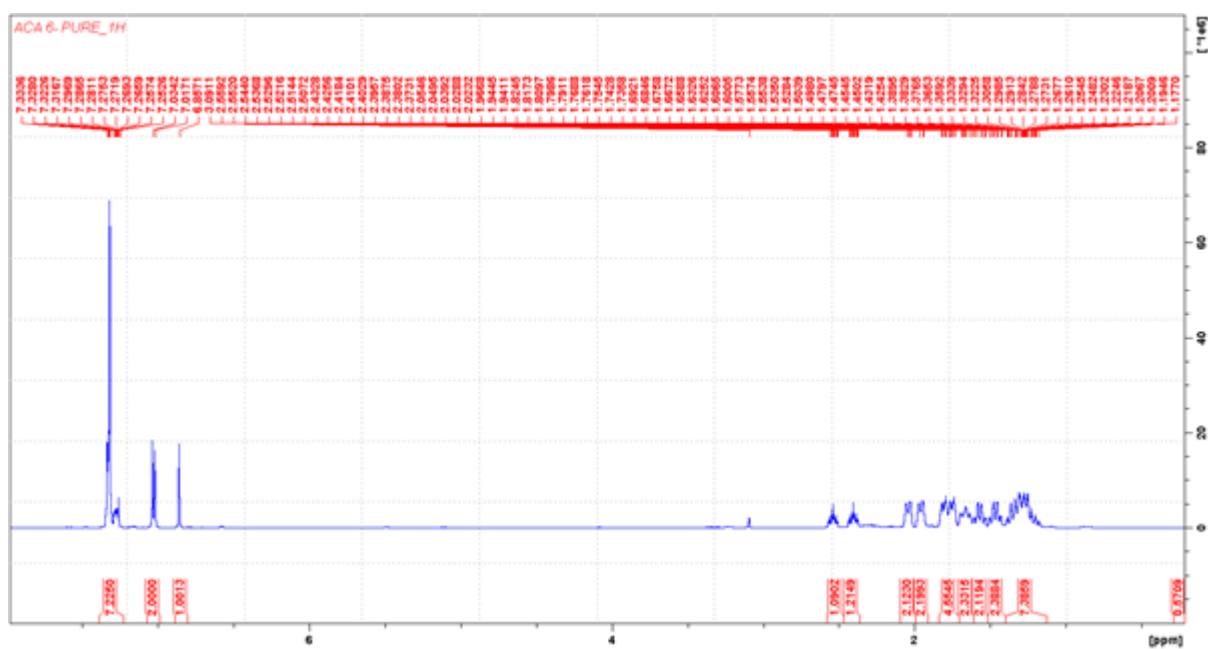


Figure S11: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3e**

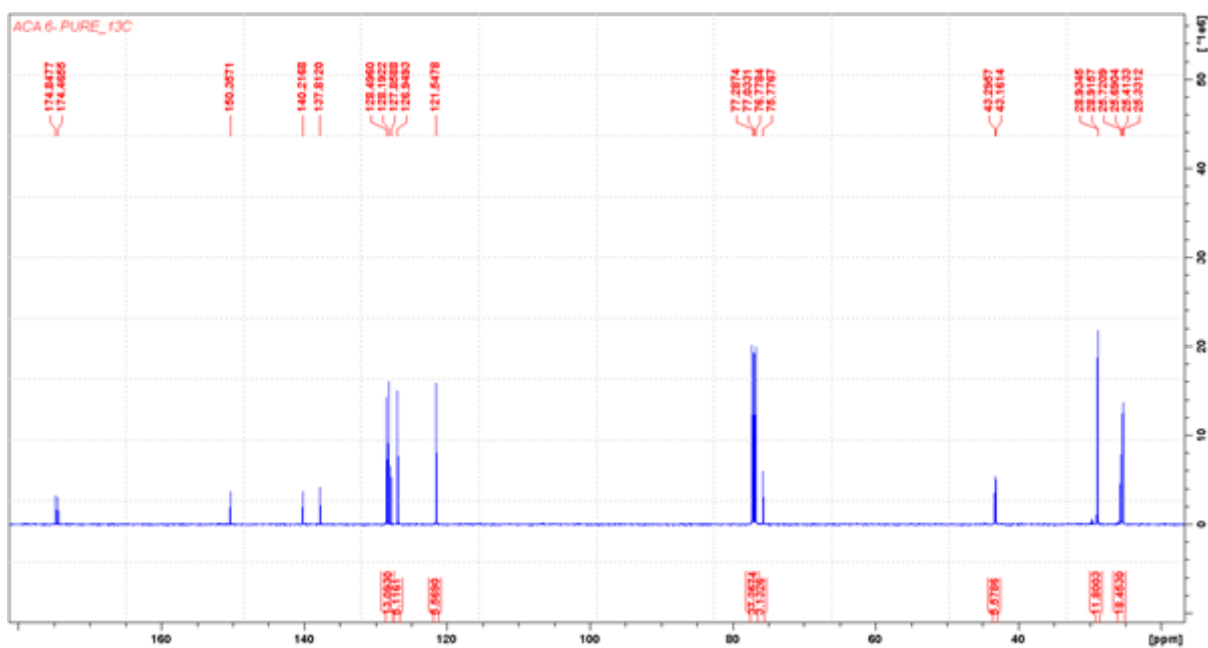


Figure S12: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3e**

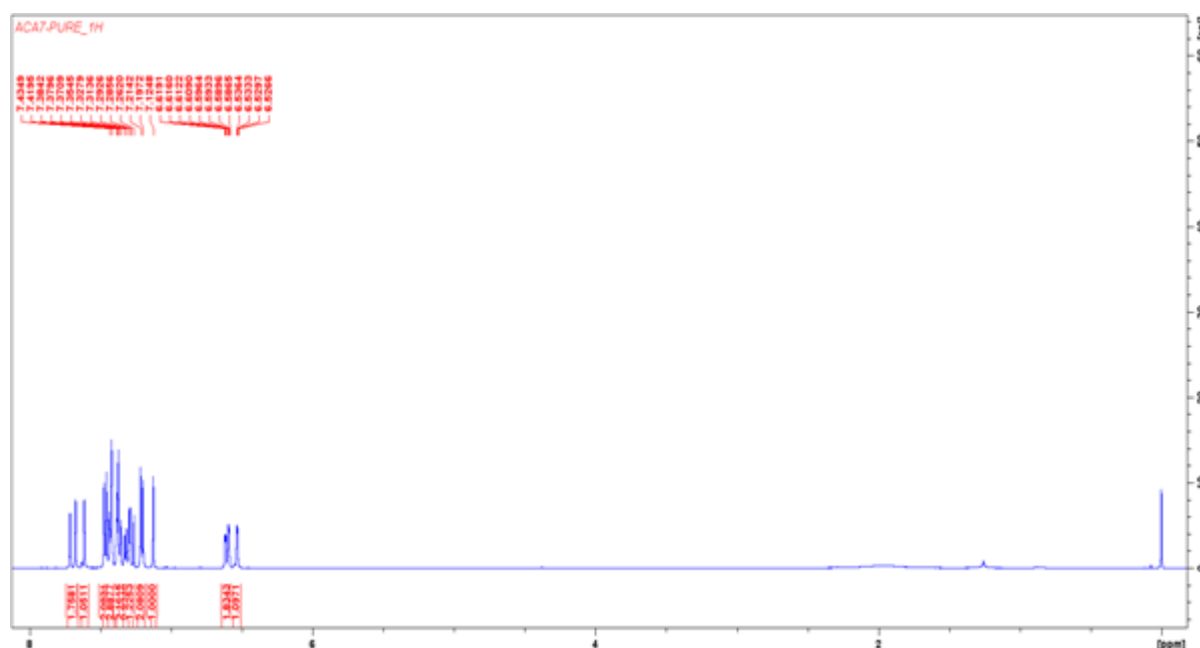


Figure S13: $^1\text{H-NMR}$ (500 MHz, CDCl_3) spectrum of compound **3f**

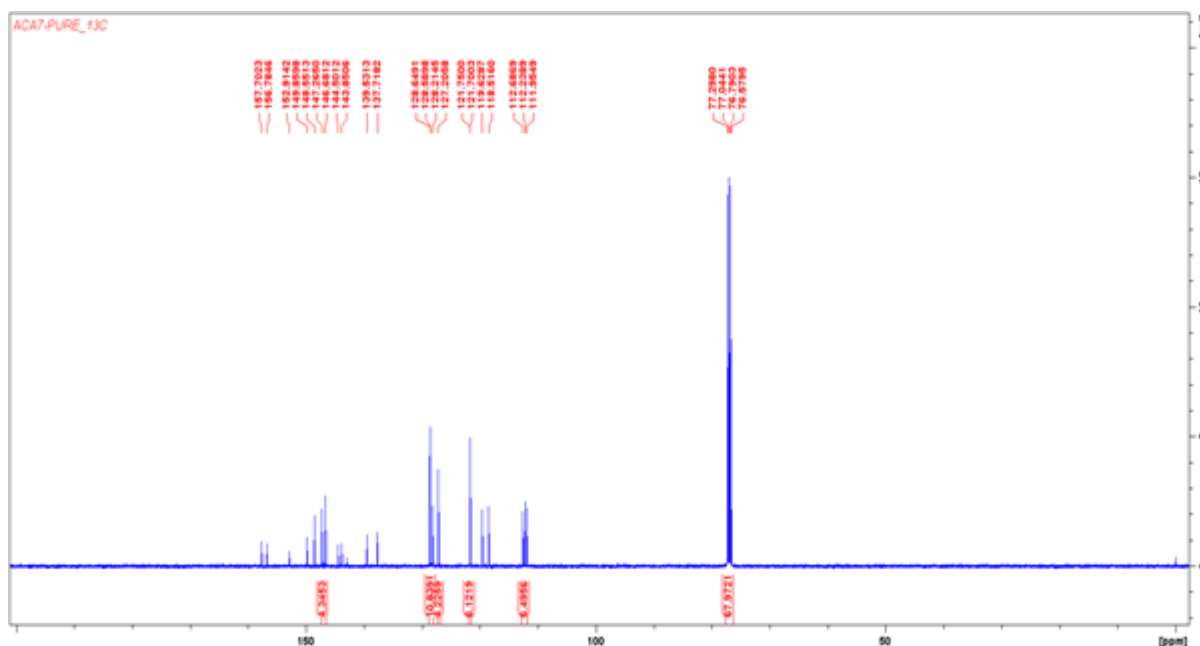


Figure S14: $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) spectrum of compound **3f**

S1 : Molecular Docking

Autodock Vina file from PDB ID: 6SXG

REMARK VINA RESULT: -5.7 0.000 0.000

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK 1 A between atoms: C8_3 and C9_2

REMARK 2 A between atoms: C11_4 and C8_3

REMARK 3 A between atoms: C1_11 and C7_10

REMARK 4 A between atoms: C17_19 and C7_10

REMARK 5 A between atoms: C4_14 and O4_15

REMARK 6 A between atoms: C20_22 and O20_23

REMARK 7 A between atoms: C23_24 and O20_23

REMARK 8 A between atoms: C23_24 and C24_25

REMARK 9 A between atoms: C24_25 and N24_26

REMARK 10 A between atoms: C8_33 and C9_32

REMARK 11 A between atoms: C11_34 and C8_33

REMARK 12 A between atoms: C1_41 and C7_40

REMARK 13 A between atoms: C17_49 and C7_40

REMARK 14 A between atoms: C4_44 and O4_45

REMARK 15 A between atoms: C20_52 and O20_53

REMARK 16 A between atoms: C23_54 and O20_53

REMARK 17 A between atoms: C23_54 and C24_55

REMARK 18 A between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8	OHT	A	305	4.928	3.297	46.592	1.00	88.87	-0.036	C
HETATM	2	C7	OHT	A	305	5.268	4.496	47.115	1.00	90.65	-0.009	C
HETATM	3	C1	OHT	A	305	5.836	4.663	48.482	1.00	86.17	-0.024	A
HETATM	4	C2	OHT	A	305	7.212	4.804	48.676	1.00	84.05	0.015	A
HETATM	5	C3	OHT	A	305	7.732	5.005	49.944	1.00	81.83	0.037	A
HETATM	6	C4	OHT	A	305	6.881	5.061	51.041	1.00	83.97	0.065	A
HETATM	7	C5	OHT	A	305	5.507	4.952	50.858	1.00	83.91	0.037	A
HETATM	8	C6	OHT	A	305	4.992	4.748	49.589	1.00	84.33	0.015	A
HETATM	9	O4	OHT	A	305	7.391	5.137	52.306	1.00	87.85	-0.361	OA
ATOM	10	H4	OHT	A	305	7.734	4.361	52.732	1.00	0.00	0.217	HD
HETATM	11	C17	OHT	A	305	4.989	5.788	46.427	1.00	94.85	-0.024	A
HETATM	12	C18	OHT	A	305	3.699	6.326	46.412	1.00	96.40	0.015	A
HETATM	13	C19	OHT	A	305	3.423	7.481	45.700	1.00	98.59	0.037	A
HETATM	14	C20	OHT	A	305	4.443	8.126	45.006	1.00	99.52	0.068	A
HETATM	15	C21	OHT	A	305	5.732	7.609	45.022	1.00	99.10	0.037	A
HETATM	16	C22	OHT	A	305	5.997	6.446	45.724	1.00	97.40	0.015	A
HETATM	17	O20	OHT	A	305	4.407	9.301	44.298	1.00	98.91	-0.349	OA
HETATM	18	C23	OHT	A	305	5.343	9.494	43.232	1.00	101.18	0.206	C
HETATM	19	C24	OHT	A	305	5.893	10.884	43.422	1.00	104.00	0.297	C
HETATM	20	N24	OHT	A	305	7.301	11.018	43.086	1.00	105.88	0.082	N
HETATM	21	C25	OHT	A	305	8.136	10.654	44.223	1.00	105.91	0.309	C
HETATM	22	C26	OHT	A	305	7.625	10.179	41.942	1.00	106.76	0.309	C
HETATM	23	C11	OHT	A	305	4.439	3.151	45.188	1.00	86.69	-0.029	A
HETATM	24	C16	OHT	A	305	5.288	3.408	44.104	1.00	84.97	0.012	A
HETATM	25	C15	OHT	A	305	4.849	3.207	42.804	1.00	84.10	0.001	A
HETATM	26	C14	OHT	A	305	3.569	2.744	42.563	1.00	85.60	0.000	A
HETATM	27	C13	OHT	A	305	2.716	2.491	43.624	1.00	86.58	0.001	A

HETATM	28	C12 OHT A 305	3.142	2.700	44.929	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	4.991	1.995	47.367	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	5.886	0.949	46.714	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -5.3 4.425 8.473

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	6.674	7.533	54.277	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	6.712	7.864	52.967	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	6.848	9.264	52.478	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	5.721	10.039	52.196	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	5.851	11.356	51.784	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	7.114	11.915	51.641	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	8.243	11.164	51.949	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	8.108	9.848	52.356	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	7.258	13.170	51.122	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	7.583	13.879	51.665	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	6.489	6.873	51.876	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	5.216	6.351	51.632	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	5.026	5.369	50.676	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	6.109	4.906	49.935	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	7.378	5.424	50.158	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	7.563	6.396	51.125	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	6.138	3.996	48.908	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	4.899	3.556	48.340	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	4.696	4.398	47.107	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	5.911	4.645	46.348	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	5.898	3.890	45.101	1.00	105.91	0.309	C
HETATM	22	C26 OHT A 305	6.046	6.066	46.068	1.00	106.76	0.309	C
HETATM	23	C11 OHT A 305	6.620	6.113	54.738	1.00	86.69	-0.029	A
HETATM	24	C16 OHT A 305	7.703	5.251	54.527	1.00	84.97	0.012	A
HETATM	25	C15 OHT A 305	7.675	3.954	55.016	1.00	84.10	0.001	A
HETATM	26	C14 OHT A 305	6.578	3.498	55.725	1.00	85.60	0.000	A

HETATM	27	C13 OHT A 305	5.498	4.337	55.936	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	5.512	5.634	55.441	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	6.667	8.553	55.400	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	8.044	8.785	56.010	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -5.1 3.312 5.505

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	3.953	4.646	51.052	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	5.125	5.041	50.508	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	6.184	5.759	51.273	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	7.339	5.097	51.693	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	8.342	5.778	52.364	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	8.199	7.134	52.631	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	7.068	7.811	52.191	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	6.067	7.125	51.524	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	9.124	7.787	53.396	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	8.937	8.654	53.736	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	5.426	4.915	49.054	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	5.340	6.024	48.207	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	5.536	5.888	46.843	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	5.840	4.640	46.309	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	5.940	3.532	47.140	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	5.730	3.672	48.501	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	6.131	4.294	45.013	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	5.540	3.111	44.464	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	5.003	3.514	43.115	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	3.577	3.287	42.950	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	3.262	1.872	43.107	1.00	105.91	0.309	C
HETATM	22	C26 OHT A 305	2.829	4.073	43.919	1.00	106.76	0.309	C
HETATM	23	C11 OHT A 305	2.945	3.855	50.283	1.00	86.69	-0.029	A
HETATM	24	C16 OHT A 305	2.119	4.476	49.339	1.00	84.97	0.012	A
HETATM	25	C15 OHT A 305	1.231	3.727	48.581	1.00	84.10	0.001	A

HETATM	26	C14 OHT A 305	1.157	2.356	48.744	1.00	85.60	0.000	A
HETATM	27	C13 OHT A 305	1.964	1.729	49.677	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	2.848	2.471	50.449	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	3.535	4.971	52.473	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	2.591	6.164	52.565	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -5.1 1.827 2.626

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	5.070	3.399	46.723	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	5.406	4.603	47.235	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	6.047	4.777	48.569	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	7.421	4.997	48.682	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	8.006	5.203	49.921	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	7.223	5.186	51.068	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	5.849	5.000	50.966	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	5.270	4.790	49.727	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	7.805	5.269	52.301	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	7.275	5.443	53.070	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	5.052	5.892	46.575	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	3.821	6.506	46.819	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	3.458	7.657	46.140	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	4.334	8.220	45.217	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	5.565	7.627	44.973	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	5.916	6.469	45.644	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	4.206	9.376	44.488	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	2.932	9.699	43.922	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	2.601	11.079	44.426	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	1.544	11.112	45.424	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	0.663	9.961	45.274	1.00	105.91	0.309	C
HETATM	22	C26 OHT A 305	2.118	11.128	46.760	1.00	106.76	0.309	C
HETATM	23	C11 OHT A 305	4.505	3.249	45.348	1.00	86.69	-0.029	A
HETATM	24	C16 OHT A 305	3.120	3.224	45.143	1.00	84.97	0.012	A

HETATM	25	C15 OHT A 305	2.600	3.150	43.859	1.00	84.10	0.001	A
HETATM	26	C14 OHT A 305	3.445	3.108	42.765	1.00	85.60	0.000	A
HETATM	27	C13 OHT A 305	4.816	3.126	42.953	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	5.346	3.187	44.234	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	5.213	2.094	47.482	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	3.952	1.697	48.240	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -5.0 3.429 7.072

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	5.153	5.395	52.413	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	4.429	5.097	51.313	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	3.068	4.493	51.364	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	1.936	5.289	51.558	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	0.669	4.730	51.560	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	0.515	3.361	51.375	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	1.631	2.563	51.151	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	2.896	3.126	51.153	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	-0.717	2.784	51.496	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	-0.843	2.041	52.074	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	4.970	5.220	49.929	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	5.919	4.313	49.449	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	6.485	4.479	48.196	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	6.093	5.549	47.397	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	5.143	6.451	47.857	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	4.592	6.287	49.115	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	6.472	5.863	46.116	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	5.572	5.578	45.040	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	5.847	4.150	44.648	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	4.652	3.357	44.408	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	3.485	3.999	44.998	1.00	105.91	0.309	C
HETATM	22	C26 OHT A 305	4.452	3.174	42.979	1.00	106.76	0.309	C
HETATM	23	C11 OHT A 305	6.480	6.076	52.333	1.00	86.69	-0.029	A

HETATM	24	C16 OHT A 305	6.563	7.464	52.169	1.00	84.97	0.012	A
HETATM	25	C15 OHT A 305	7.796	8.099	52.161	1.00	84.10	0.001	A
HETATM	26	C14 OHT A 305	8.959	7.369	52.323	1.00	85.60	0.000	A
HETATM	27	C13 OHT A 305	8.893	5.995	52.480	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	7.665	5.348	52.478	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	4.710	5.062	53.826	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	4.052	6.235	54.542	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -4.9 4.007 8.525

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	5.649	5.224	46.949	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	4.852	4.193	46.594	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	4.420	3.935	45.191	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	3.152	4.316	44.748	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	2.771	4.115	43.432	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	3.654	3.522	42.538	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	4.930	3.166	42.959	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	5.305	3.365	44.277	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	3.247	3.210	41.272	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	2.344	2.967	41.105	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	4.214	3.283	47.587	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	4.704	1.989	47.789	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	4.059	1.115	48.648	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	2.922	1.532	49.333	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	2.432	2.819	49.151	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	3.072	3.682	48.281	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	2.174	0.862	50.268	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	1.242	1.600	51.066	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	1.524	1.203	52.492	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	1.617	2.322	53.415	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	2.355	1.938	54.611	1.00	105.91	0.309	C
HETATM	22	C26 OHT A 305	2.268	3.451	52.769	1.00	106.76	0.309	C

HETATM	23	C11 OHT A 305	6.132	5.410	48.351	1.00	86.69	-0.029	A
HETATM	24	C16 OHT A 305	7.352	4.861	48.765	1.00	84.97	0.012	A
HETATM	25	C15 OHT A 305	7.828	5.092	50.047	1.00	84.10	0.001	A
HETATM	26	C14 OHT A 305	7.106	5.875	50.930	1.00	85.60	0.000	A
HETATM	27	C13 OHT A 305	5.896	6.420	50.536	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	5.405	6.185	49.259	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	6.118	6.295	45.983	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	5.070	7.370	45.720	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -4.9 3.563 6.800

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	4.978	7.060	51.968	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	5.436	5.793	51.869	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	6.404	5.192	52.829	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	6.012	4.855	54.127	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	6.902	4.255	55.002	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	8.203	3.989	54.593	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	8.596	4.291	53.295	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	7.704	4.894	52.424	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	9.121	3.509	55.484	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	9.446	2.620	55.405	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	5.121	4.906	50.713	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	5.956	4.866	49.593	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	5.617	4.108	48.485	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	4.442	3.363	48.490	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	3.608	3.385	49.600	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	3.945	4.155	50.699	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	3.950	2.505	47.538	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	3.529	3.039	46.278	1.00	101.18	0.206	C
HETATM	19	C24 OHT A 305	4.521	2.524	45.267	1.00	104.00	0.297	C
HETATM	20	N24 OHT A 305	5.172	3.565	44.489	1.00	105.88	0.082	N
HETATM	21	C25 OHT A 305	4.922	3.374	43.067	1.00	105.91	0.309	C

HETATM	22	C26 OHT A 305	4.695	4.875	44.907	1.00106.76	0.309 C
HETATM	23	C11 OHT A 305	3.945	7.608	51.039	1.00 86.69	-0.029 A
HETATM	24	C16 OHT A 305	2.598	7.662	51.418	1.00 84.97	0.012 A
HETATM	25	C15 OHT A 305	1.653	8.232	50.578	1.00 84.10	0.001 A
HETATM	26	C14 OHT A 305	2.032	8.763	49.359	1.00 85.60	0.000 A
HETATM	27	C13 OHT A 305	3.359	8.712	48.968	1.00 86.58	0.001 A
HETATM	28	C12 OHT A 305	4.311	8.133	49.796	1.00 86.33	0.012 A
HETATM	29	C9 OHT A 305	5.468	8.050	53.008	1.00 86.72	0.036 C
HETATM	30	C10 OHT A 305	6.664	8.871	52.542	1.00 86.10	0.010 C

ENDMDL

REMARK VINA RESULT: -4.9 1.260 2.010

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK 1 A between atoms: C8_3 and C9_2
 REMARK 2 A between atoms: C11_4 and C8_3
 REMARK 3 A between atoms: C1_11 and C7_10
 REMARK 4 A between atoms: C17_19 and C7_10
 REMARK 5 A between atoms: C4_14 and O4_15
 REMARK 6 A between atoms: C20_22 and O20_23
 REMARK 7 A between atoms: C23_24 and O20_23
 REMARK 8 A between atoms: C23_24 and C24_25
 REMARK 9 A between atoms: C24_25 and N24_26
 REMARK 10 A between atoms: C8_33 and C9_32
 REMARK 11 A between atoms: C11_34 and C8_33
 REMARK 12 A between atoms: C1_41 and C7_40
 REMARK 13 A between atoms: C17_49 and C7_40
 REMARK 14 A between atoms: C4_44 and O4_45
 REMARK 15 A between atoms: C20_52 and O20_53
 REMARK 16 A between atoms: C23_54 and O20_53
 REMARK 17 A between atoms: C23_54 and C24_55
 REMARK 18 A between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	5.158	3.537	46.522	1.00 88.87	-0.036 C
HETATM	2	C7 OHT A 305	5.406	4.749	47.065	1.00 90.65	-0.009 C
HETATM	3	C1 OHT A 305	6.043	4.936	48.399	1.00 86.17	-0.024 A
HETATM	4	C2 OHT A 305	5.301	4.797	49.574	1.00 84.05	0.015 A
HETATM	5	C3 OHT A 305	5.906	4.927	50.813	1.00 81.83	0.037 A
HETATM	6	C4 OHT A 305	7.265	5.206	50.895	1.00 83.97	0.065 A
HETATM	7	C5 OHT A 305	8.020	5.317	49.733	1.00 83.91	0.037 A
HETATM	8	C6 OHT A 305	7.410	5.189	48.497	1.00 84.33	0.015 A
HETATM	9	O4 OHT A 305	7.846	5.456	52.106	1.00 87.85	-0.361 OA
ATOM	10	H4 OHT A 305	8.357	6.245	52.238	1.00 0.00	0.217 HD
HETATM	11	C17 OHT A 305	4.950	6.023	46.442	1.00 94.85	-0.024 A
HETATM	12	C18 OHT A 305	3.691	6.553	46.736	1.00 96.40	0.015 A
HETATM	13	C19 OHT A 305	3.234	7.691	46.092	1.00 98.59	0.037 A
HETATM	14	C20 OHT A 305	4.042	8.325	45.154	1.00 99.52	0.068 A
HETATM	15	C21 OHT A 305	5.301	7.816	44.859	1.00 99.10	0.037 A
HETATM	16	C22 OHT A 305	5.745	6.672	45.497	1.00 97.40	0.015 A
HETATM	17	O20 OHT A 305	3.818	9.484	44.452	1.00 98.91	-0.349 OA
HETATM	18	C23 OHT A 305	4.858	9.993	43.609	1.00101.18	0.206 C
HETATM	19	C24 OHT A 305	4.172	10.909	42.629	1.00104.00	0.297 C
HETATM	20	N24 OHT A 305	4.228	10.453	41.249	1.00105.88	0.082 N

HETATM	21	C25 OHT A 305	2.950	10.675	40.585	1.00105.91	0.309	C
HETATM	22	C26 OHT A 305	5.288	11.148	40.535	1.00106.76	0.309	C
HETATM	23	C11 OHT A 305	4.595	3.380	45.147	1.00 86.69	-0.029	A
HETATM	24	C16 OHT A 305	3.210	3.375	44.938	1.00 84.97	0.012	A
HETATM	25	C15 OHT A 305	2.693	3.295	43.654	1.00 84.10	0.001	A
HETATM	26	C14 OHT A 305	3.540	3.228	42.563	1.00 85.60	0.000	A
HETATM	27	C13 OHT A 305	4.911	3.226	42.755	1.00 86.58	0.001	A
HETATM	28	C12 OHT A 305	5.439	3.293	44.037	1.00 86.33	0.012	A
HETATM	29	C9 OHT A 305	5.406	2.226	47.245	1.00 86.72	0.036	C
HETATM	30	C10 OHT A 305	4.483	1.103	46.789	1.00 86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -4.7 8.259 13.047

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK	1	A	between atoms: C8_3 and C9_2
REMARK	2	A	between atoms: C11_4 and C8_3
REMARK	3	A	between atoms: C1_11 and C7_10
REMARK	4	A	between atoms: C17_19 and C7_10
REMARK	5	A	between atoms: C4_14 and O4_15
REMARK	6	A	between atoms: C20_22 and O20_23
REMARK	7	A	between atoms: C23_24 and O20_23
REMARK	8	A	between atoms: C23_24 and C24_25
REMARK	9	A	between atoms: C24_25 and N24_26
REMARK	10	A	between atoms: C8_33 and C9_32
REMARK	11	A	between atoms: C11_34 and C8_33
REMARK	12	A	between atoms: C1_41 and C7_40
REMARK	13	A	between atoms: C17_49 and C7_40
REMARK	14	A	between atoms: C4_44 and O4_45
REMARK	15	A	between atoms: C20_52 and O20_53
REMARK	16	A	between atoms: C23_54 and O20_53
REMARK	17	A	between atoms: C23_54 and C24_55
REMARK	18	A	between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	8.571	15.427	39.954	1.00 88.87	-0.036	C
HETATM	2	C7 OHT A 305	9.125	14.927	41.080	1.00 90.65	-0.009	C
HETATM	3	C1 OHT A 305	8.820	13.569	41.611	1.00 86.17	-0.024	A
HETATM	4	C2 OHT A 305	8.042	13.405	42.759	1.00 84.05	0.015	A
HETATM	5	C3 OHT A 305	7.724	12.139	43.224	1.00 81.83	0.037	A
HETATM	6	C4 OHT A 305	8.187	11.016	42.550	1.00 83.97	0.065	A
HETATM	7	C5 OHT A 305	8.937	11.166	41.389	1.00 83.91	0.037	A
HETATM	8	C6 OHT A 305	9.256	12.433	40.930	1.00 84.33	0.015	A
HETATM	9	O4 OHT A 305	7.981	9.768	43.066	1.00 87.85	-0.361	OA
ATOM	10	H4 OHT A 305	7.976	9.634	44.006	1.00 0.00	0.217	HD
HETATM	11	C17 OHT A 305	9.998	15.733	41.979	1.00 94.85	-0.024	A
HETATM	12	C18 OHT A 305	11.387	15.579	41.955	1.00 96.40	0.015	A
HETATM	13	C19 OHT A 305	12.190	16.265	42.850	1.00 98.59	0.037	A
HETATM	14	C20 OHT A 305	11.614	17.132	43.772	1.00 99.52	0.068	A
HETATM	15	C21 OHT A 305	10.236	17.305	43.800	1.00 99.10	0.037	A
HETATM	16	C22 OHT A 305	9.438	16.605	42.912	1.00 97.40	0.015	A
HETATM	17	O20 OHT A 305	12.217	17.949	44.696	1.00 98.91	-0.349	OA
HETATM	18	C23 OHT A 305	11.818	17.854	46.067	1.00101.18	0.206	C
HETATM	19	C24 OHT A 305	13.037	17.375	46.812	1.00104.00	0.297	C

HETATM	20	N24 OHT A 305	13.180	17.938	48.145	1.00105.88	0.082	N	
HETATM	21	C25 OHT A 305	11.874	18.261	48.707	1.00105.91	0.309	C	
HETATM	22	C26 OHT A 305	13.876	17.000	49.012	1.00106.76	0.309	C	
HETATM	23	C11 OHT A 305	8.957	16.759	39.400	1.00	86.69	-0.029	A
HETATM	24	C16 OHT A 305	10.114	16.903	38.623	1.00	84.97	0.012	A
HETATM	25	C15 OHT A 305	10.433	18.128	38.057	1.00	84.10	0.001	A
HETATM	26	C14 OHT A 305	9.608	19.221	38.246	1.00	85.60	0.000	A
HETATM	27	C13 OHT A 305	8.464	19.096	39.016	1.00	86.58	0.001	A
HETATM	28	C12 OHT A 305	8.142	17.877	39.597	1.00	86.33	0.012	A
HETATM	29	C9 OHT A 305	7.503	14.706	39.152	1.00	86.72	0.036	C
HETATM	30	C10 OHT A 305	8.029	14.103	37.855	1.00	86.10	0.010	C

ENDMDL

REMARK VINA RESULT: -4.7 1.887 5.100

REMARK 18 active torsions:

REMARK status: ('A' for Active; 'I' for Inactive)

REMARK 1 A between atoms: C8_3 and C9_2
 REMARK 2 A between atoms: C11_4 and C8_3
 REMARK 3 A between atoms: C1_11 and C7_10
 REMARK 4 A between atoms: C17_19 and C7_10
 REMARK 5 A between atoms: C4_14 and O4_15
 REMARK 6 A between atoms: C20_22 and O20_23
 REMARK 7 A between atoms: C23_24 and O20_23
 REMARK 8 A between atoms: C23_24 and C24_25
 REMARK 9 A between atoms: C24_25 and N24_26
 REMARK 10 A between atoms: C8_33 and C9_32
 REMARK 11 A between atoms: C11_34 and C8_33
 REMARK 12 A between atoms: C1_41 and C7_40
 REMARK 13 A between atoms: C17_49 and C7_40
 REMARK 14 A between atoms: C4_44 and O4_45
 REMARK 15 A between atoms: C20_52 and O20_53
 REMARK 16 A between atoms: C23_54 and O20_53
 REMARK 17 A between atoms: C23_54 and C24_55
 REMARK 18 A between atoms: C24_55 and N24_56

REMARK viewdock state: V

HETATM	1	C8 OHT A 305	4.944	3.410	47.333	1.00	88.87	-0.036	C
HETATM	2	C7 OHT A 305	4.316	3.927	46.254	1.00	90.65	-0.009	C
HETATM	3	C1 OHT A 305	3.580	3.099	45.258	1.00	86.17	-0.024	A
HETATM	4	C2 OHT A 305	4.195	2.684	44.075	1.00	84.05	0.015	A
HETATM	5	C3 OHT A 305	3.523	1.877	43.172	1.00	81.83	0.037	A
HETATM	6	C4 OHT A 305	2.219	1.477	43.438	1.00	83.97	0.065	A
HETATM	7	C5 OHT A 305	1.607	1.857	44.626	1.00	83.91	0.037	A
HETATM	8	C6 OHT A 305	2.281	2.667	45.524	1.00	84.33	0.015	A
HETATM	9	O4 OHT A 305	1.506	0.783	42.502	1.00	87.85	-0.361	OA
ATOM	10	H4 OHT A 305	1.089	1.240	41.782	1.00	0.00	0.217	HD
HETATM	11	C17 OHT A 305	4.406	5.366	45.878	1.00	94.85	-0.024	A
HETATM	12	C18 OHT A 305	3.302	6.212	46.016	1.00	96.40	0.015	A
HETATM	13	C19 OHT A 305	3.360	7.527	45.586	1.00	98.59	0.037	A
HETATM	14	C20 OHT A 305	4.535	8.020	45.026	1.00	99.52	0.068	A
HETATM	15	C21 OHT A 305	5.643	7.194	44.893	1.00	99.10	0.037	A
HETATM	16	C22 OHT A 305	5.574	5.877	45.312	1.00	97.40	0.015	A
HETATM	17	O20 OHT A 305	4.830	9.290	44.598	1.00	98.91	-0.349	OA
HETATM	18	C23 OHT A 305	5.665	9.454	43.447	1.00101.18	0.206	C	

HETATM	19	C24 OHT A 305	6.038	10.914	43.420	1.00104.00	0.297	C
HETATM	20	N24 OHT A 305	7.414	11.170	43.028	1.00105.88	0.082	N
HETATM	21	C25 OHT A 305	8.194	11.632	44.169	1.00105.91	0.309	C
HETATM	22	C26 OHT A 305	8.009	9.964	42.473	1.00106.76	0.309	C
HETATM	23	C11 OHT A 305	5.603	4.273	48.360	1.00 86.69	-0.029	A
HETATM	24	C16 OHT A 305	4.852	4.879	49.374	1.00 84.97	0.012	A
HETATM	25	C15 OHT A 305	5.477	5.625	50.362	1.00 84.10	0.001	A
HETATM	26	C14 OHT A 305	6.852	5.771	50.362	1.00 85.60	0.000	A
HETATM	27	C13 OHT A 305	7.607	5.182	49.363	1.00 86.58	0.001	A
HETATM	28	C12 OHT A 305	6.990	4.444	48.362	1.00 86.33	0.012	A
HETATM	29	C9 OHT A 305	5.058	1.922	47.606	1.00 86.72	0.036	C
HETATM	30	C10 OHT A 305	3.970	1.395	48.533	1.00 86.10	0.010	C

ENDMDL



Figure S15: Image of docking compared to X-ray diffraction method. Where, Crystal OTH: Blue in colour and Top Dock Pose: Green in colour