Electronic Supplementary Material for

Prediction of crystal structure of avadomide using machine learning potentials and crystal engineering

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Similar experimental structures in the Cambridge Crystallographic Database Center (CCDC)

The characteristics of the avadomide molecule were determined based on structurally similar experimental molecules in the Cambridge Structural Database (CSD). In these experimental structures, the chiral hydrogen is coplanar with the carbonyl group associated with oxygen atom 3.

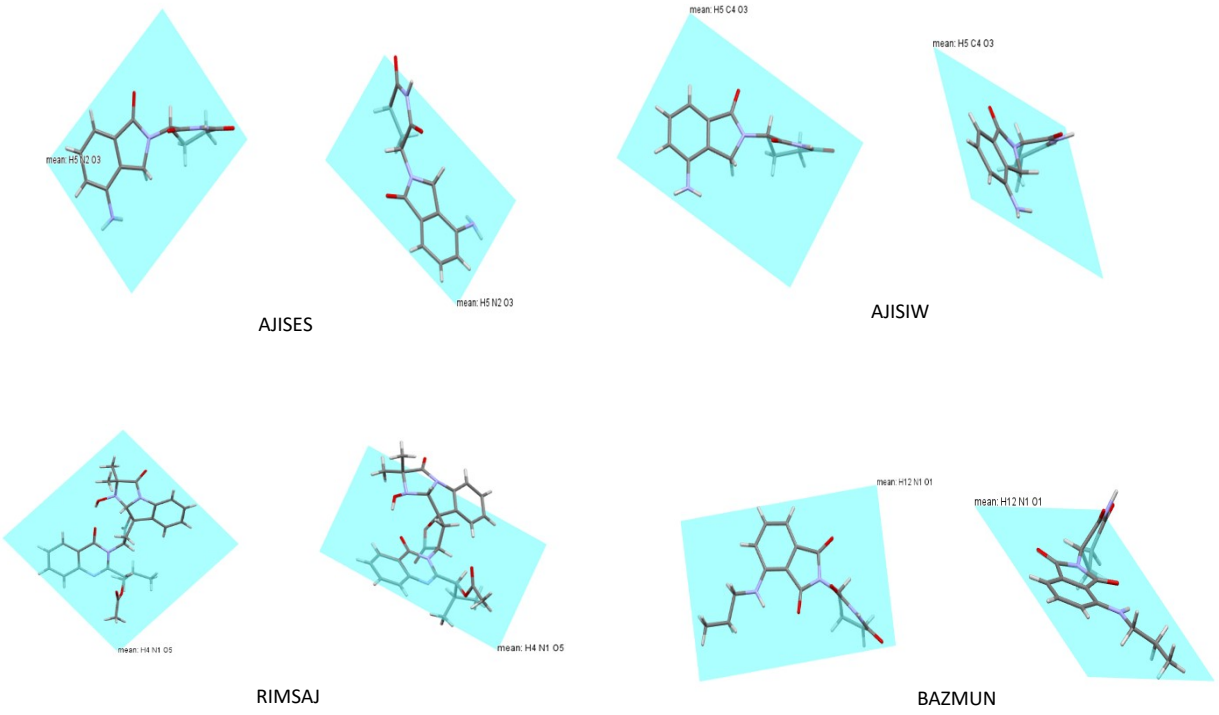

Fig S1. Similar experimental structures to avadomide molecule in the CSD

Energy diagram based on torsion angle of avadomide molecule

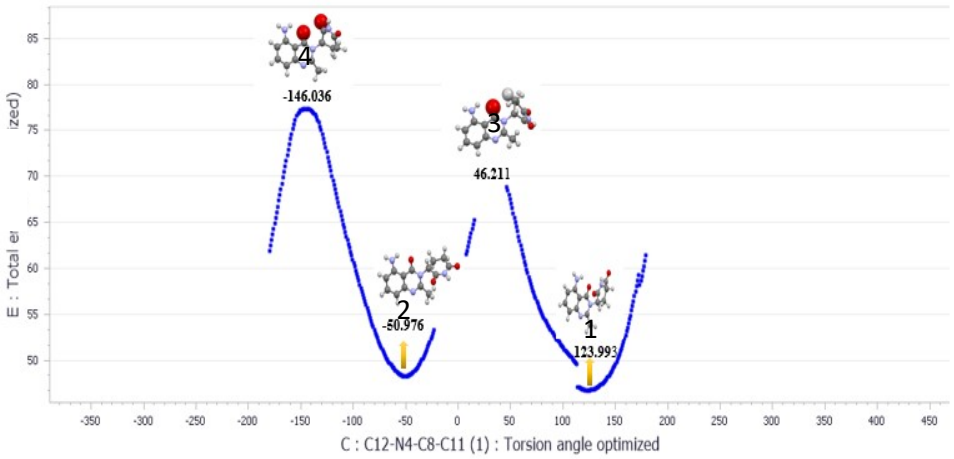

Fig S2. Conformational state of av

Conformation state	Relative energy(kcal/mol)
1	0000
2	6.588
3	109.939
4	118.599

Table S1. Energy comparison of avadomide conformational states

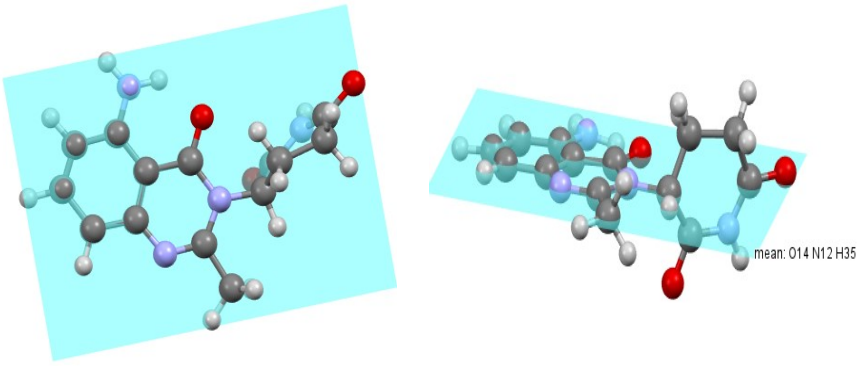

Fig S3. Two-dimensional diagram of avadomide molecule in two conformational forms

Structures of two conformational forms of avadomide molecule

Initial optimization of structures for the conformational form I and II

Table S2. Initial optimization of structures for the conformational form I and II

Rank	Conf	Volume (A^3)	Density (g/cm^3)	SPG	Relative Energy (kJ/mol)
1	1	643.88	1.48	*PI*	0.00
2	1	644.24	1.48	*PI*	0.00
3	1	642.75	1.48	*PI*	0.05
4	1	609.84	1.56	*PI*	0.15
5	1	609.43	1.56	*PI*	0.15
6	1	609.32	1.56	*PI*	0.15
7	1	609.67	1.56	*PI*	0.15
8	1	608.74	1.56	*PI*	0.15
9	1	607.93	1.56	*PI*	0.15

10	1	609.53	1.56	*PI*	0.15
11	1	609.29	1.56	*PI*	0.15
12	1	608.48	1.56	*PI*	0.15
13	1	609.63	1.56	*PI*	0.15
14	1	609.06	1.56	*PI*	0.15
15	1	609.62	1.56	*PI*	0.15
16	1	608.26	1.56	*PI*	0.19
17	1	622.12	1.53	*PI*	0.29
18	2	2634.43	1.44	*C*2/c	1.13
19	2	1320.89	1.44	*C*2/c	1.13
20	1	1251.72	1.52	$P2_1$	1.45
21	2	1348.03	1.41	$P2_1$/c	1.86
22	1	643.22	1.48	*PI*	2.12
23	1	643.24	1.48	*PI*	2.12
24	1	646.33	1.47	*PI*	2.22
25	1	645.79	1.47	*PI*	2.27
26	1	672.15	1.42	*PI*	2.61
27	1	1344.62	1.41	*PI*	3.09
28	1	663.84	1.43	*PI*	3.09
29	1	2557.14	1.49	$P2_1$/c	3.11
30	1	2556.53	1.49	$P2_1$/c	3.11
31	1	658.47	1.44	*PI*	3.52
32	1	658.61	1.44	*PI*	3.52
33	1	656.98	1.45	*PI*	3.57
34	1	658.24	1.44	*PI*	3.57
35	1	2635.85	1.44	*P*bca	3.80
36	1	1266.77	1.5	$P2_1$	3.91
37	1	675.04	1.41	*PI*	3.96
38	1	1357.17	1.4	*PI*	4.00
39	1	666.95	1.43	*PI*	4.29
40	1	666.42	1.43	*PI*	4.34
41	1	667.66	1.42	*PI*	4.34
42	1	667.4	1.43	*PI*	4.39
43	1	666.33	1.43	*PI*	4.39
44	1	666.62	1.43	*PI*	4.39
45	1	2614.17	1.46	*P*mna	4.48
46	1	1224.3	1.55	$P2_1$	4.51
47	1	645.75	1.47	*PI*	4.58
48	1	651.24	1.46	*PI*	4.63
49	1	643.01	1.48	*PI*	4.68
50	2	1377.35	1.38	$Pna2_1$	4.75
51	2	1384.3	1.37	$Pna2_1$	4.75
52	1	1264.5	1.5	$P2_1$	4.80
53	1	685.62	1.39	*PI*	4.82
54	1	1367.45	1.39	$P2_1$	4.87

55	1	688.81	1.38	*PI*	4.92
56	1	2733.67	1.39	*PI*	5.02
57	1	2624.25	1.45	$P2_1/c$	5.02
58	1	2500.57	1.52	*P*bca	5.15
59	1	2504.13	1.52	*P*bca	5.16
60	1	2507.37	1.52	*P*bca	5.21
61	1	2622.44	1.45	$P2_1/c$	5.32
62	1	1295.45	1.47	*PI*	5.45
63	2	1314.73	1.45	$P2_1/c$	5.52
64	2	2771.78	1.37	$P2_1/c$	5.54
65	2	1383.7	1.37	$P2_1/c$	5.55
66	1	1311.07	1.45	*PI*	5.84
67	1	1324.52	1.44	$P2_1$	5.84
68	1	2472.35	1.54	*P*bca	5.85
69	1	1255	1.52	*PI*	5.91
70	1	1254.35	1.52	$P2_1$	5.91
71	1	1258.63	1.51	*PI*	5.93
72	1	1243.4	1.53	$P2_1$	5.96
73	1	663.89	1.43	*PI*	6.08
74	1	664.03	1.43	*PI*	6.08
75	1	662.45	1.44	*PI*	6.08
76	1	1365.86	1.39	*PI*	6.15
77	1	1311.99	1.45	*PI*	6.30
78	1	646.96	1.47	*PI*	6.37
79	1	645.99	1.47	*PI*	6.37
80	1	646.39	1.47	*PI*	6.37
81	1	645.9	1.47	*PI*	6.37
82	1	648.86	1.47	*PI*	6.37
83	1	647.8	1.47	*PI*	6.37
84	1	648.38	1.47	*PI*	6.37
85	1	646.79	1.47	*PI*	6.37
86	1	645.82	1.47	*PI*	6.37
87	1	646.71	1.47	*PI*	6.37
88	1	648.86	1.47	*PI*	6.37
89	1	648	1.47	*PI*	6.37
90	1	646.2	1.47	*PI*	6.37
91	1	648.78	1.47	*PI*	6.37
92	1	646.92	1.47	*PI*	6.42
93	1	646.52	1.47	*PI*	6.42
94	1	646.59	1.47	*PI*	6.42
95	1	646.38	1.47	*PI*	6.42
96	1	647.47	1.47	*PI*	6.42
97	1	646.62	1.47	*PI*	6.42
98	1	648.55	1.47	*PI*	6.42
99	1	644.76	1.48	*PI*	6.42

100	1	646.41	1.47	$P\bar{1}$	6.47

Relative lattice energy plotted against the density for the generated structures of avadomide

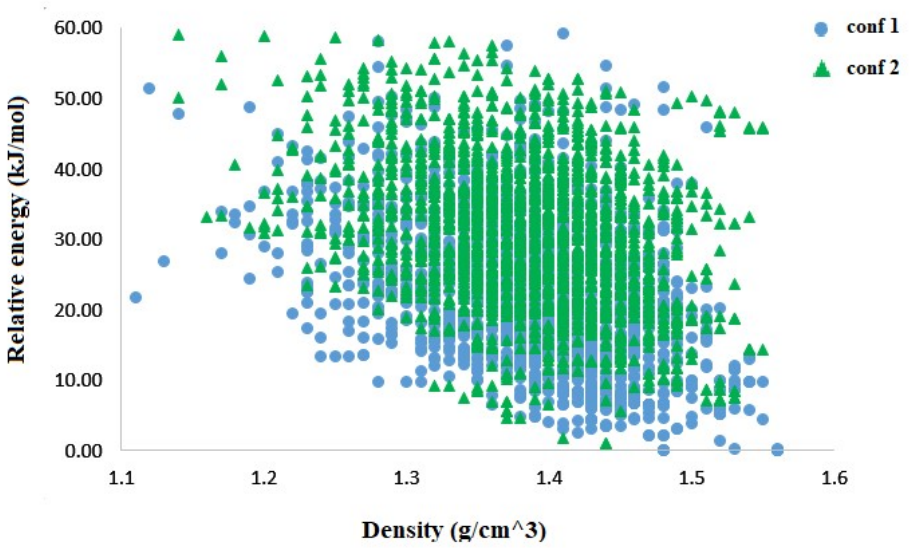

Fig S4. Relative lattice energy (ΔE, kJ/mol) plotted against the density for the generated structures of avadomide

Final Optimization of Structures with PBE-D3 for the Conformational Form I and II.

Table S3. Final Optimization of Structures with PBE-D3 for the Conformational Form I and II.

Rank	conformation	Volume(A^3)	Density(g/cm^3)	SPG	Relative energy (kJ/mol)	Synthons I (I′) II(II′) III
1	**1**	**662.18**	**1.44**	***P*$\bar{1}$**	**0.00**	+ + +
2	1	1317.51	1.44	$P2_1/c$	0.60	+ - -
3	1	1321.99	1.44	$P2_1/c$	0.92	+ - -
4	1	1321.64	1.44	$P2_1/c$	1.01	+ + -
5	1	2877.94	1.32	*P*bca	1.25	- - -
6	1	2863.20	1.33	*P*bcn	1.68	+ - -
7	1	660.52	1.44	$P\bar{1}$	2.17	+ - +

8	1	1358.68	1.40	$Pna2_1$	2.48	- - -
9	1	651.93	1.46	$P\bar{1}$	2.61	+ - +
10	1	2857.41	1.33	*P*bca	2.71	- - -
11	1	653.61	1.46	$P\bar{1}$	2.94	+ - +
12	1	653.79	1.45	$P\bar{1}$	3.04	+ - +
13	1	1369.05	1.39	$Pna2_1$	3.30	- - -
14	1	677.05	1.40	$P\bar{1}$	4.25	+ - +
15	1	2866.88	1.33	*P*bcn	6.26	+ - -
16	1	639.49	1.49	$P\bar{1}$	7.91	- - +
17	1	1378.22	1.38	*P*2/c	7.96	+ - -
18	1	1290.67	1.47	$P2_1/c$	8.13	- - -
19	2	1295.80	1.47	$P2_1/c$	8.13	- - +
20	**2**	**644.32**	**1.48**	$\boldsymbol{P\bar{1}}$	**8.25**	**+ + +**
21	1	655.29	1.45	$P\bar{1}$	8.88	- - +
22	1	1286.17	1.48	$Pna2_1$	9.09	- - -
23	1	677.84	1.40	$P\bar{1}$	9.21	- - +
24	1	640.78	1.48	$P\bar{1}$	9.94	- - +
25	1	674.06	1.41	*P*c	10.81	- - -
26	2	1349.77	1.41	$P2_1/c$	11.00	+ - -
27	2	2731.00	1.39	*P*bcn	11.90	+ + -
28	1	2661.37	1.43	*P*bca	12.31	+ + -
29	1	682.91	1.39	$P\bar{1}$	12.83	- - -
30	1	2989.49	1.27	*P*bca	12.84	+ - -
31	1	1426.06	1.33	$Pna2_1$	13.12	- - -
32	1	682.12	1.39	$P\bar{1}$	13.99	+ - +
33	1	1353.31	1.41	$P2_1/c$	14.21	- - -

34	2	1349.80	1.41	$P2_1/c$	15.20	+ - +
35	1	3138.48	1.21	*P*bca	15.27	- - -
36	2	673.15	1.41	*P*c	15.34	- - -
37	2	1409.18	1.35	*C*c	15.49	- - -
38	2	680.06	1.40	$P\bar{1}$	15.58	+ + -
39	1	1305.21	1.46	$P2_1/c$	15.90	+ - -
40	2	1334.27	1.43	$P2_1/c$	16.26	- + -
41	2	651.87	1.46	$P\bar{1}$	16.31	+ - +
42	2	2665.61	1.43	*C*2/c	16.47	- - +
43	1	1328.28	1.43	$P2_1/c$	16.84	- - -
44	2	638.45	1.49	*P*c	16.84	- - -
45	2	670.22	1.42	$P\bar{1}$	17.32	+ - +
46	1	1356.07	1.40	$Pna2_1$	17.63	+ - -
47	2	666.86	1.43	$P\bar{1}$	17.66	+ - +
48	2	1286.00	1.48	$P2_1/c$	17.70	- - +
49	2	665.89	1.43	$P\bar{1}$	17.85	+ - +
50	2	1429.44	1.33	*C*c	18.31	- - -
51	2	659.22	1.44	$P\bar{1}$	18.91	+ + +
52	2	640.54	1.48	$P\bar{1}$	19.68	+ - +
53	2	663.71	1.43	$P\bar{1}$	19.68	+ + +
54	2	668.01	1.42	$P\bar{1}$	19.73	- - +
55	2	1287.18	1.48	$P2_1/c$	19.80	+ + +
56	2	1304.34	1.46	$P2_1/c$	19.85	+ + -
57	1	640.64	1.48	$P\bar{1}$	19.88	- - +
58	2	640.03	1.49	$P\bar{1}$	19.88	- - +
59	2	666.35	1.43	$P\bar{1}$	19.88	+ - +

Table S4. Refordes of similar experimental structures in the Cambridge Crystallographic Database Center(CCDC)

Quary 1		Quary 2	
REFCODE	SPG	REFCODE	SPG
LOVYIH	$P4_32_12$	CUDCEM	$P1$
QOWJAQ	$P2_1/c$	GOWJOU	$P2_12_12_1$
XOSSOQ	$P\bar{1}$	ZUCRIB	$C2$
ACANLC10	$Pbca$	ABUDIL	$P2_12_12_1$
ACEVIO	$P\bar{1}$	ADIHOK	Pc
ACIBAQ	$P\bar{1}$	ADIJAY	$C2/c$
AKURUU	$P2_1/n$	ADIJOM	$P2_1/c$
APASEQ	$P2_1/n$	ADIJUS	$P2_1/n$
BANNOT	P212121	ADIKAZ	P21/n
BAPRIT	$P\bar{1}$	ADIKED	P21/n
BAPROZ	$P\bar{1}$	AJISES	$P\bar{1}$
BEVPUQ	$P2_1/c$	AJISES01	$Pbca$
BIHDUT	$P2_12_12_1$	AJISIW	$P2_1/c$
BOLGAK	$P\bar{1}$	AJISIX	$P2_1/c$
BUGDEM	$P2_1/n$	AJISOD	$C2/c$
BUGDEM01	$P\bar{1}$	AJOFOW	$P2_1/c$
COFWEA	$P2_1/c$	AJOGAJ	$P2_1/c$
CUJVAE	I2/c	AJOGEN	$P2_1/c$
DAXWAD	$P2_12_12_1$	AGOGIR	$C2/c$
DIVYUC	$P\bar{1}$	AJOGOX	$P\bar{1}$
DIYTOV	$P\bar{1}$	ATEXOM	$P\bar{1}$
DIYVAJ	$Pna2_1$	ATEXUS	$P\bar{1}$
DOHFOV	$P2_1/c$	AWOWUE	$P\bar{1}$
EWUZAY	$C2/c$	AXULOV	$P\bar{1}$
EWUZUS	$P2_1/c$	AXULOV01	$P\bar{1}$
EYAFEQ	$P2_12_12_1$	AZMCHO	$Pccn$
EYOHUV	$P2_1/c$	AZMCHO10	$Pccn$
EZUHUE	$P2_12_12_1$	BAZMUN	$P2_1/c$
FENKER	$P2_1/c$	BAZNAU	$P2_1/c$
FIBBAV	$P2_1/c$	BEYTUV	$P2_1$
FIBBEZ	$P2_1/c$	BOPPIP	$C2$
GIBVAQ	$Pna2_1$	BOQQUT	$P2_1/a$
GIBVUK	Cc	BOQQUT01	$P2_1/c$
GIBWAR	Cc	BOQQUT02	$P2_1/c$
GINKIY	$P\bar{1}$	BOQQUT03	$P2_1/c$

GITLEB	$P2_1/n$	BOQQUT04	$P2_1/c$
GITLEB01	$P2_1/n$	BOQQUT05	$P2_1/c$
GUBODY	$P2_1/c$	BOQQUT06	$P2_1/c$
GUBDUE	$P2_1/c$	BOQQUT07	$P2_1/c$
HALZEB	$P\bar{1}$	BOQQUT08	$P2_1/c$
IGEVEX	$P2_1/c$	BUWMUB	$C2$
IGICIM	$P\bar{1}$	CHEXIM10	$P2_1$
IMIKOE	$P2_1/c$	CIQJOC	$P2_1/c$
IMINAT	$P2_1/n$	CUFYOR	$P2_1/n$
IMINAT01	$P2_1/n$	CUPTEN	$C222_1$
IMINAT02	$P2_1/n$	DAGWEO	$P2_1/a$
IMINAT03	$P2_1/n$	DAWOD	$C2/c$
IXEWAK	$P2_1/c$	DALXOE	$P\bar{1}$
IXIVER	$P\bar{1}$	DOPCUG	$P2_1/n$
IXIVIV	$P2_1/c$	EGUHIZ	$P2_1/n$
JOYZIG	$Pca2_1$	ENELAK	$C2/c$
KICCOQ	$P2_1/c$	GABPHA10	$P\bar{1}$
KIDJAK	$P2_1/n$	GLUTIM	$P2_1/c$
KINQUW	$P2_1/c$	HALKUC	$P\bar{1}$
KINRIL	$P\bar{1}$	HOFFOX	$P\bar{1}$
KINROR	$P2_1/n$	HUGRAD	$P2_1/c$
KUKDIE	$Pna2_1$	HUVFUB	$P\bar{1}$
KUKDOK	$P\text{-}42_1c$	HUVGAI	$P\bar{1}$
KUKDUQ	$P\bar{1}$	ICOSUR	$P2_1/c$
KUKFAY	$P2_1/c$	ICOSUR	$P2_1/c$
LAJNAM	$P2_12_12_1$	ICOTEC	$P\bar{1}$
LAQHES	$C2/c$	ICOTIG	$P\bar{1}$
LEQLIF	$Pbca$	ICOTOM	$P\bar{1}$
LESSIN	$P2_1/c$	JIKHIU	$P2_1/c$
LIFJIV	$P2_1/n$	LASCEN	$P2_12_12_1$
LIFJOB	$P2_1/n$	LERDIV	$P2_1/c$
LIFKAO	$Pnma$	LILTEI	$P2_1/c$
LIFKES	$P\bar{1}$	MEBCEC	$P2_1/c$
LIYBOK	$P\bar{1}$	MICXUU	$P\bar{1}$
LUQTIA	$P2_1/c$	MUWDIS	C2/c
MABRIT	$P2_1/c$	NAHZAZ	$P2_1/c$
MAFNIS	$P1$	NIZJIQ	$P2_1/n$
MAQHOE	$P2_1/c$	NIZJUC	$P\bar{1}$
MAQHUK	$P2_1/c$	NOTRAP	$P2_12_12_1$
MARKOI	$P2_1/n$	PAVYAO	$P2_1/c$
MIRVIU	$Pbca$	REMZOZ	$P2_1/c$
MQAZOX	$P\bar{1}$	PIVFIJ	$P2_1/c$
MXZHQO	$P2_1/n$	POCPED	$P2_1/c$
NAHDEH	$P\bar{1}$	POCPIH	$P\bar{1}$
NALGIT	$Pbcn$	POCPON	$P2_1$

NALQOH	*P*$\bar{1}$
NAXPEJ	*P*2_1/c
NEPVOO	*P*2_1/c
NIJWOU	*P*2_1/c
NUGYOE	*P*2_1
NUMRAP	*P*2_1/c
NUPWAX	*P*2_1/c
OKUQAN	*P*$\bar{1}$
OMOCEY	*P*2_1/c
OMOCEY01	*P*2_1/c
PAPXEM	*P*bca
PUJCON	*P*$\bar{1}$
QANFIW	*P*2_1/n
QANFOC	*P*2_1/c
QANFUI	*P*2_1/c
QANGAP	*P*$2_12_12_1$
QATGIB	*P*$2_12_12_1$
QEQRIN	*C*2/c
QEQROT	*P*c
QESDUO	*P*bca
QEVWAP	*C*222_1
RAPPIK	*C*2/c
RECYIH	*P*$\bar{1}$
RIHSEI	*P*2_1/c
SEPGIE	*P*$\bar{1}$
SODWUG	*P*2_1/c
SODXAN	*P*2_1/n
SODXER	*P*2_1/c
SOFNAC	*P*$2_12_12_1$
SOFNOQ	*P*2_1
SOHCIE	*P*2_1/c
SOKQER	*P*2_1/c
SOKQIV	*P*2_1
SOKQOB	*I*ba2
SOKQUH	*P*2_1
SOKRAO	*P*2_1/c
SONRET	*P*1
TAVFIG	*P*$2_12_12_1$
TERXOD	*P*2_1/c
TOHBIB	*P*$\bar{1}$
TUDZAU	*P*$\bar{1}$
TUFUP	*P*$\bar{1}$
TUXLIJ	P1
TZQXLT	*P*2_1/c
UMOTUM	*P*2_1
REGKIX	*C*2/c
REGKIX01	*C*2/c
SECDEM	*P*nma
SECDIQ	*P*bca
SIKMII	*P*c$a2_1$
THALID03	C2/c
THALID10	*P*2_1/n
THALID11	*C*2/c
THALID12	*P*2_1/n
TOSGUF	*P*$\bar{1}$
UGOHOP	*P*c$a2_1$
UGOHUV	*P*$\bar{1}$
UZAGIN	*P*$\bar{1}$
VINWIZ	*P*bca
VINWOF	*P*2_1/c
VINWUL	*P*2_1/c
VINXAS	*P*2_1/c
WIYTUV	*P*2_1/c
XODPEN	*P*$\bar{1}$
XODPIR	*P*$\bar{1}$
XODPOX	*P*2_1/c
ZORBEP	*P*2_1
ZSPUNT	*P*2_1/a

UMOTUM01	$P2_1$
UMOVAU	$P2_1/c$
UMOVEY	$C2/c$
UMOVIC	$C2/c$
UMOVOI	$P2_1/c$
UMOVUO	$P2_1/c$
UNOBEE	$P2_1/c$
UPAZAN	$P31$
UTITAT	Cc
VATJUW	$P2_1/c$
VATJUW01	$P2_1/c$
VEJVIR	$P2_1/n$
VORLAQ	Cc
VURJUO	$P\bar{1}$
VUZRAJ	$P2_1/c$
WADHUG	$P2_1/c$
WAKGEV	$P\bar{1}$
WELVER	$P2_1/c$
WIQSOH	$P2_1/c$
WULKIZ	$P2_1/n$
WULKOF	$P2_1/n$
WULMIB	$P2_1/n$
WULZAG	$P\bar{1}$
XEBYIP	$C2/c$
XEBYUB	$Pna2_1$
XODZIB	$P2_12_12_1$
XOGJUZ	$P2_1/c$
XOGKAG	$P2_1/c$
XOGKIO	$P2_1/c$
XOTPIH	$C2/c$
YECBUG	$P\bar{1}$
YECBUG01	$P\bar{1}$
YOTTIL	$Pbca$
ZIKHOT	$Cmc2_1$
ZILWOJ	$P2_1/c$
ZILWUP	$C2/c$
ZIXBUG	$P2_1/n$
ZIYYUE	$P2_1/n$
ZODLAH	$P2_1/n$
ZODLAH01	$P2_1/n$
ZODLEL	$C2/c$
ZODLEL01	$C2/c$
ZODLIP	$P2_1/n$
ZODLIP01	$P2_1/n$

Comparison of the PXRD patterns of the predicted and experimental structure

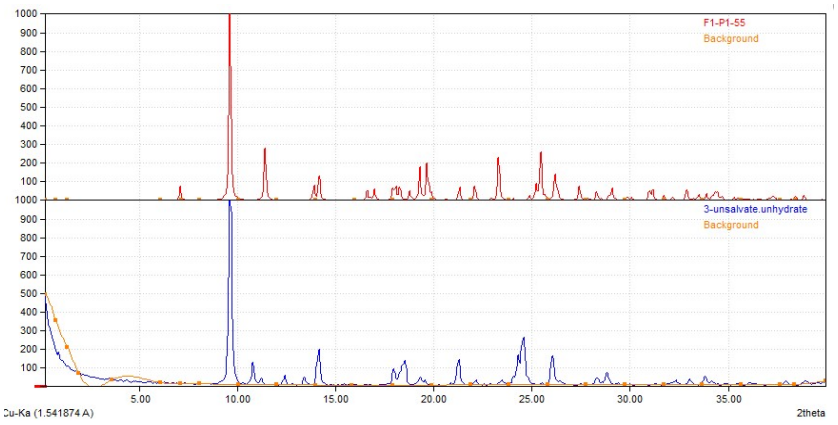

Fig S5. Comparison of the PXRD patterns of the predicted and experimental structure

Table S5.Lattice parameters of the predicted structures of ten lowest structures

Structure rank	Space group	a, Å	b, Å	c, Å	α,	β,	γ,	V, Å3	d, g cm−3
1	*P*$\bar{1}$	15.849	5.469	8.227	106.80	99.26	97.35	662.178	1.44
2	$P2_1/c$	14.351	5.777	15.962	90.00	84.60	90.00	1317.512	1.44
3	$P2_1/c$	5.349	25.020	9.892	90.00	86.94	90.00	1321.99	1.44
4	$P2_1/c$	5.344	25.001	9.906	90.00	86.77	90.00	1321.636	1.44
5	*P*bca	20.012	14.648	9.818	90.00	90.00	90.00	2877.937	1.32
6	*P*bcn	33.524	7.562	11.294	90.00	90.00	90.00	2863.201	1.33
7	*P*$\bar{1}$	5.539	9.528	12.880	85.32	83.78	78.29	660.523	1.44
8	$Pna2_1$	15.117	5.692	15.790	90.00	90.00	90.00	1358.678	1.40
9	*P*$\bar{1}$	5.800	9.489	12.106	85.97	84.82	79.74	651.926	1.46
10	*P*bca	14.046	14.981	13.579	90.00	90.00	90.00	2857.413	1.33

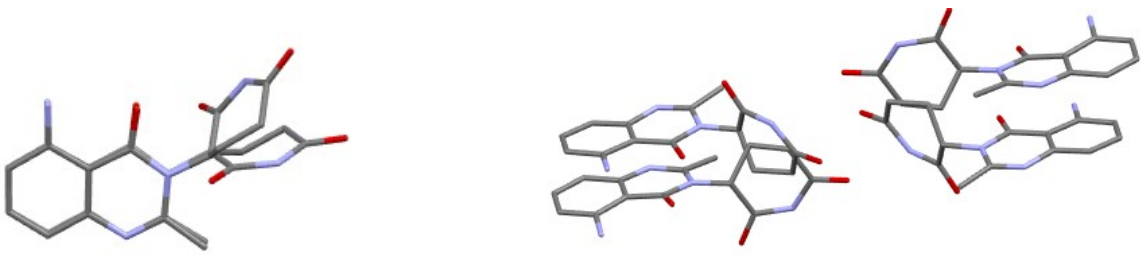

Fig S6. Overlay the first rank and 20th structures(The torsion part of the molecule is not overlaid.)

Overlay the first rank and 20th structures

Top 10 Predicted Crystal Structures (CIF Format)

##

#

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#

```
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data_findsym-STRUC-1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
_space_group_name_Hall          '-P 1'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 15.84900
_cell_length_b                 5.46900
_cell_length_c                 8.22700
_cell_angle_alpha              106.80700
_cell_angle_beta               99.26000
_cell_angle_gamma              97.35500
_cell_volume                   662.148
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H H -0.1465 0.1104 -0.3559
H H -0.0192 -0.0988 -0.3169
H H -0.0047 -0.3603 -0.1106
H H -0.3817 -0.7806 0.0791
H H -0.4204 -0.5193 0.0212
```

H H -0.4281 0.0235 0.4755

H H -0.5327 -0.7234 0.1447

H H -0.4530 -0.7139 0.3245

H H -0.3286 0.0490 -0.1439

H H -0.2857 0.1744 -0.2946

H H -0.1546 -0.4303 0.4471

H H -0.1944 -0.7440 0.2961

H H -0.0837 -0.5959 0.3267

H H -0.2903 -0.4908 0.3443

C C -0.1697 -0.4400 0.1799

C C -0.2664 -0.2162 0.0369

C C -0.2011 -0.1795 -0.0608

C C -0.2094 -0.0320 -0.1792

C C -0.1420 -0.0068 -0.2691

C C -0.0705 -0.1263 -0.2463

C C -0.0615 -0.2715 -0.1327

C C -0.1256 -0.2924 -0.0364

C C -0.3170 -0.4022 0.2477

C C -0.3361 -0.1452 0.3548

C C -0.3987 -0.5894 0.1298

C C -0.4708 -0.6123 0.2300

C C -0.4872 -0.3561 0.3353

C C -0.1502 -0.5599 0.3200

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N N -0.2487 -0.3553 0.1539

N N -0.4188 -0.1493 0.3911

N N -0.2787 0.0871 -0.2014

O O -0.3371 -0.1334 0.0274

O O -0.2816 0.0561 0.4191

O O -0.5580 -0.3260 0.3776

#END

##

#

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# Structural Database, then it will include bibliographic, chemical,
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#
##############################################################################

data_findsym-STRUC-2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
_space_group_name_Hall          '-P 2ybc'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
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2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 14.35100
_cell_length_b                 5.77700
_cell_length_c                 15.96200
_cell_angle_alpha               90.00000
_cell_angle_beta                84.60400
_cell_angle_gamma               90.00000
_cell_volume                   1317.48
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H H 0.2976 0.2492 -0.3014
```

H H 0.4375 0.0085 -0.3488

H H 0.4757 -0.3420 -0.2716

H H 0.1414 -0.8046 -0.0041

H H 0.0751 -0.5477 -0.0133

H H 0.0815 -0.1952 0.2043

H H -0.0054 -0.7990 0.0980

H H 0.1002 -0.8286 0.1463

H H 0.1288 0.0816 -0.1270

H H 0.1528 0.2840 -0.2079

H H 0.3967 -0.6897 0.0465

H H 0.3161 -0.8774 0.0036

H H 0.4287 -0.8300 -0.0512

H H 0.2476 -0.6084 0.0820

C C 0.3377 -0.5481 -0.0620

C C 0.2198 -0.2504 -0.0770

C C 0.2752 -0.1784 -0.1522

C C 0.2509 0.0212 -0.1991

C C 0.3117 0.0880 -0.2692

C C 0.3901 -0.0449 -0.2949

C C 0.4133 -0.2425 -0.2516

C C 0.3577 -0.3064 -0.1785

C C 0.2020 -0.5011 0.0463

C C 0.1775 -0.2960 0.1050

C C 0.1172 -0.6458 0.0282

C C 0.0596 -0.7103 0.1096

C C 0.0350 -0.5065 0.1649

C C 0.3709 -0.7479 -0.0127

N N 0.3856 -0.4925 -0.1323

N N 0.2573 -0.4294 -0.0310

N N 0.0962 -0.3224 0.1592

N N 0.1730 0.1464 -0.1746

O O 0.1425 -0.1653 -0.0488

O O 0.2271 -0.1246 0.1103

O O -0.0361 -0.4967 0.2157

#END

```
##################################################################################
#
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#                             CCDC
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#
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# Structural Database, then it will include bibliographic, chemical,
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data_findsym-STRUC-3
_symmetry_cell_setting          monoclinic
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_symmetry_Int_Tables_number      14
_space_group_name_Hall          '-P 2ybc'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 5.34900
_cell_length_b                 25.02000
_cell_length_c                 9.89200
_cell_angle_alpha              90.00000
_cell_angle_beta               86.94000
_cell_angle_gamma              90.00000
_cell_volume                   1321.98
loop_
_atom_site_label
_atom_site_type_symbol
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_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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H H 0.1686 -0.1312 0.0300

H H 0.5069 -0.1871 0.1261

H H 0.7886 -0.3995 -0.2677

H H 0.4696 -0.3903 -0.3042

H H 0.0738 -0.5115 -0.1262

H H 0.6276 -0.4707 -0.4243

H H 0.7338 -0.4983 -0.2737

H H -0.0853 -0.3082 -0.2428

H H -0.2303 -0.2464 -0.2681

H H 0.7049 -0.3962 0.1985

H H 0.9183 -0.3937 0.0550

H H 0.9166 -0.3419 0.1751

H H 0.6847 -0.4318 -0.0466

C C 0.6084 -0.3380 0.0512

C C 0.2615 -0.3371 -0.0987

C C 0.2276 -0.2816 -0.0654

C C 0.0348 -0.2498 -0.1215

C C 0.0165 -0.1957 -0.0813

C C 0.1871 -0.1734 0.0036

C C 0.3759 -0.2039 0.0575

C C 0.3935 -0.2582 0.0258

C C 0.5266 -0.4163 -0.1009

C C 0.3092 -0.4536 -0.0614

C C 0.5997 -0.4161 -0.2529

C C 0.5903 -0.4720 -0.3142

C C 0.3443 -0.4994 -0.2836

C C 0.7968 -0.3695 0.1227

N N 0.5714 -0.2885 0.0873

N N 0.4719 -0.3624 -0.0473

N N 0.2314 -0.4893 -0.1554

N N -0.1248 -0.2706 -0.2094

O O 0.1220 -0.3649 -0.1690

O O 0.2132 -0.4538 0.0558

O O 0.2440 -0.5311 -0.3587

#END

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_symmetry_space_group_name_H-M 'P21/C'

_symmetry_Int_Tables_number 14

_symmetry_cell_setting monoclinic

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_symmetry_equiv_pos_as_xyz

x,y,z

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-x,-y,-z

x,-y+1/2,z+1/2

_cell_length_a 5.3445

_cell_length_b 25.0012

_cell_length_c 9.9068

_cell_angle_alpha 90.0000

_cell_angle_beta 86.7715

_cell_angle_gamma 90.0000

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

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H5 H 0.17252 0.36941 1.02707 0.01267 Uiso 1.00

H9 H 0.50886 0.31316 1.12383 0.01267 Uiso 1.00

H13 H 0.78931 0.10035 0.73079 0.01267 Uiso 1.00

H17 H 0.47031 0.10972 0.69460 0.01267 Uiso 1.00

H21 H 0.07312 0.98857 0.87356 0.01267 Uiso 1.00

H25 H 0.62676 0.02920 0.57471 0.01267 Uiso 1.00

H29 H 0.73422 0.00153 0.72464 0.01267 Uiso 1.00

H33 H 0.91632 0.19216 0.75567 0.01267 Uiso 1.00

H37 H 0.77201 0.25411 0.72986 0.01267 Uiso 1.00

H41 H 0.70101 0.10388 1.19673 0.01267 Uiso 1.00

H45 H 0.91705 0.10600 1.05406 0.01267 Uiso 1.00

H49 H 0.91483 0.15786 1.17383 0.01267 Uiso 1.00

H53 H 0.68494 0.06830 0.95173 0.01267 Uiso 1.00

C1 C 0.60826 0.16210 1.04930 0.01267 Uiso 1.00

C5 C 0.26181 0.16317 0.89963 0.01267 Uiso 1.00

C9 C 0.22887 0.21869 0.93262 0.01267 Uiso 1.00

C13 C 0.03700 0.25070 0.87628 0.01267 Uiso 1.00

C17 C 0.01976 0.30490 0.91620 0.01267 Uiso 1.00

C21 C 0.19020 0.32711 1.00101 0.01267 Uiso 1.00

C25 C 0.37795 0.29646 1.05523 0.01267 Uiso 1.00

C29 C 0.39470 0.24209 1.02371 0.01267 Uiso 1.00

C33 C 0.52672 0.08373 0.89761 0.01267 Uiso 1.00

C37 C 0.30942 0.04639 0.93775 0.01267 Uiso 1.00

C41 C 0.60004 0.08386 0.74582 0.01267 Uiso 1.00

C45 C 0.59017 0.02786 0.68476 0.01267 Uiso 1.00

C49 C 0.34406 0.00043 0.71602 0.01267 Uiso 1.00

C53 C 0.79506 0.13035 1.12122 0.01267 Uiso 1.00

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N5 N 0.47197 0.13771 0.95099 0.01267 Uiso 1.00

N9 N 0.23064 0.01080 0.84395 0.01267 Uiso 1.00

N13 N 0.87783 0.22995 0.78846 0.01267 Uiso 1.00

O1 O 0.12189 0.13541 0.82977 0.01267 Uiso 1.00

O5 O 0.21429 0.04613 1.05508 0.01267 Uiso 1.00

O9 O 0.24423 0.96843 0.64157 0.01267 Uiso 1.00

##

#

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 # CCDC

#

##

#

```
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_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
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loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
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2 1/2+x,1/2-y,-z
3 -x,1/2+y,1/2-z
4 1/2-x,-y,1/2+z
5 -x,-y,-z
6 1/2-x,1/2+y,z
7 x,1/2-y,1/2+z
8 1/2+x,y,1/2-z
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loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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H H 0.2896 0.5331 -0.4158

H H 0.1752 0.5887 -0.4685

H H -0.0704 0.4794 -0.0156

H H -0.0164 0.3937 0.0519

H H -0.0664 0.1478 -0.0882

H H -0.1298 0.3686 0.1459

H H -0.1651 0.3702 -0.0185

H H 0.1723 0.2899 -0.0736

H H 0.2601 0.2943 -0.1071

H H -0.0886 0.4868 -0.3782

H H -0.0789 0.5556 -0.2296

H H -0.0493 0.5953 -0.3890

H H -0.0844 0.3902 -0.2275

C C 0.0121 0.4933 -0.3002

C C 0.0790 0.3836 -0.1705

C C 0.1368 0.4219 -0.2358

C C 0.2026 0.3883 -0.2072

C C 0.2570 0.4307 -0.2737

C C 0.2468 0.5014 -0.3657

C C 0.1830 0.5338 -0.3956

C C 0.1279 0.4946 -0.3299

C C -0.0427 0.3743 -0.1587

C C -0.0360 0.2706 -0.1713

C C -0.0595 0.4060 -0.0146

C C -0.1194 0.3530 0.0389

C C -0.1104 0.2515 0.0272

C C -0.0551 0.5346 -0.3255

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N N 0.0167 0.4183 -0.2152

N N -0.0694 0.2192 -0.0740

N N 0.2128 0.3184 -0.1195

O O 0.0792 0.3242 -0.0792

O O -0.0079 0.2334 -0.2674

O O -0.1409 0.1973 0.1022

#END

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_symmetry_Int_Tables_number       60
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loop_
_symmetry_equiv_pos_as_xyz
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  -x+1/2,-y+1/2,z+1/2
  -x,y,-z+1/2
  x+1/2,-y+1/2,-z
  -x,-y,-z
  x+1/2,y+1/2,-z+1/2
  x,-y,z+1/2
  -x+1/2,y+1/2,z
_cell_length_a                    33.5242
_cell_length_b                    7.5622
_cell_length_c                    11.2943
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
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H5     H     1.22826   1.09503   1.47970   0.01267  Uiso   1.00
H9     H     1.25202   0.84087   0.60167   0.01267  Uiso   1.00
H13    H     1.11008   1.20511   0.71151   0.01267  Uiso   1.00
H17    H     1.07682   1.37823   0.67596   0.01267  Uiso   1.00
H21    H     1.03113   0.56758   0.98369   0.01267  Uiso   1.00
H25    H     1.03705   1.13381   0.75797   0.01267  Uiso   1.00
```

H29 H 1.06936 1.11524 0.88218 0.01267 Uiso 1.00

H33 H 1.07892 0.90244 0.60743 0.01267 Uiso 1.00

H37 H 1.08973 1.09479 0.52386 0.01267 Uiso 1.00

H41 H 1.19334 1.35825 0.92301 0.01267 Uiso 1.00

H45 H 1.18287 1.22782 0.79642 0.01267 Uiso 1.00

H49 H 1.22934 1.33904 0.80796 0.01267 Uiso 1.00

H53 H 1.13059 1.34861 0.89300 0.01267 Uiso 1.00

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C5 C 1.12348 0.67847 0.69891 0.01267 Uiso 1.00

C9 C 1.15098 0.79084 0.63585 0.01267 Uiso 1.00

C13 C 1.13739 0.93776 0.56673 0.01267 Uiso 1.00

C17 C 1.16625 1.04469 0.51067 0.01267 Uiso 1.00

C21 C 1.20675 1.00934 0.52378 0.01267 Uiso 1.00

C25 C 1.22040 0.86746 0.59103 0.01267 Uiso 1.00

C29 C 1.19268 0.75678 0.64689 0.01267 Uiso 1.00

C33 C 1.11293 1.42681 0.82980 0.01267 Uiso 1.00

C37 C 1.08659 0.54295 0.90760 0.01267 Uiso 1.00

C41 C 1.08954 1.30249 0.74937 0.01267 Uiso 1.00

C45 C 1.05650 1.20887 0.81751 0.01267 Uiso 1.00

C49 C 1.03095 1.33152 0.88902 0.01267 Uiso 1.00

C53 C 1.19744 1.34994 0.82662 0.01267 Uiso 1.00

N1 N 1.20681 0.61346 0.71025 0.01267 Uiso 1.00

N5 N 1.14080 0.53917 0.76385 0.01267 Uiso 1.00

N9 N 1.04805 1.48722 0.92741 0.01267 Uiso 1.00

N13 N 1.09762 0.97230 0.55368 0.01267 Uiso 1.00

O1 O 1.08630 0.69528 0.70101 0.01267 Uiso 1.00

O5 O 1.09980 0.67422 0.95884 0.01267 Uiso 1.00

O9 O 0.99621 1.29529 0.91859 0.01267 Uiso 1.00

##

#

 # Cambridge Crystallographic Data Centre

 # CCDC

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# If this CIF has been generated from an entry in the Cambridge
# Structural Database, then it will include bibliographic, chemical,
# crystal, experimental, refinement or atomic coordinate data resulting
# from the CCDC's data processing and validation procedures.
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#######################################################################

data_findsym-STRUC-7
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
_space_group_name_Hall          '-P 1'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 5.53900
_cell_length_b                 9.52800
_cell_length_c                 12.88000
_cell_angle_alpha               85.32000
_cell_angle_beta               83.78800
_cell_angle_gamma               78.29200
_cell_volume                   660.456
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H H -0.8890 -0.9253 -0.2948
H H -0.5327 -0.9856 -0.4242
H H -0.2514 -0.8108 -0.4802
H H -0.1749 -0.4003 -0.1092
H H -0.4702 -0.4379 -0.0610
H H -0.9574 -0.0545 -0.0914
H H -0.3590 -0.2783 0.0590
```

H H -0.2781 -0.1612 -0.0459

H H -1.0058 -0.6089 -0.1431

H H -1.1033 -0.7687 -0.1648

H H -0.2710 -0.2315 -0.4106

H H -0.0257 -0.3247 -0.3394

H H -0.0483 -0.3739 -0.4677

H H -0.3485 -0.2303 -0.2418

C C -0.3115 -0.4445 -0.3547

C C -0.6476 -0.5025 -0.2306

C C -0.6346 -0.6277 -0.2875

C C -0.8033 -0.7237 -0.2608

C C -0.7621 -0.8512 -0.3133

C C -0.5615 -0.8832 -0.3881

C C -0.4023 -0.7882 -0.4187

C C -0.4411 -0.6582 -0.3698

C C -0.4724 -0.2973 -0.1998

C C -0.7264 -0.1983 -0.1890

C C -0.3721 -0.3538 -0.0950

C C -0.4042 -0.2353 -0.0195

C C -0.6575 -0.1429 -0.0108

C C -0.1556 -0.3378 -0.3949

N N -0.2913 -0.5610 -0.4036

N N -0.4766 -0.4150 -0.2657

N N -0.7901 -0.1273 -0.0964

N N -0.9992 -0.6933 -0.1874

O O -0.7950 -0.4678 -0.1510

O O -0.8656 -0.1719 -0.2589

O O -0.7470 -0.0784 0.0692

#END

data_findsym-STRUC-8

_audit_creation_date 2024-06-30

_symmetry_space_group_name_H-M 'PNA21'

_symmetry_Int_Tables_number 33

_symmetry_cell_setting orthorhombic

loop_

```
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x,-y,z+1/2
  x+1/2,-y+1/2,z
  -x+1/2,y+1/2,z+1/2
_cell_length_a                 15.1173
_cell_length_b                 5.6920
_cell_length_c                 15.7900
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma               90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1    H    0.04421   0.75950  -0.72914   0.01267  Uiso   1.00
H3    H    0.12596   0.01246  -0.63065   0.01267  Uiso   1.00
H5    H    0.20500   0.37395  -0.68228   0.01267  Uiso   1.00
H7    H    0.06766   0.77756  -0.05793   0.01267  Uiso   1.00
H9    H    0.02407   0.49920  -0.08899   0.01267  Uiso   1.00
H11   H    0.19938   0.20512  -0.25242   0.01267  Uiso   1.00
H13   H    0.02886   0.76960  -0.21496   0.01267  Uiso   1.00
H15   H    0.14051   0.83514  -0.19368   0.01267  Uiso   1.00
H17   H    0.00876   0.91407  -0.95083   0.01267  Uiso   1.00
H19   H    0.97837   0.71823  -0.86897   0.01267  Uiso   1.00
H21   H    0.32788   0.67623  -0.99737   0.01267  Uiso   1.00
H23   H    0.24159   0.88376  -0.98583   0.01267  Uiso   1.00
H25   H    0.31352   0.82378  -0.89953   0.01267  Uiso   1.00
H27   H    0.21802   0.63793  -0.07723   0.01267  Uiso   1.00
C1    C    0.22004   0.55251  -0.92117   0.01267  Uiso   1.00
C3    C    0.11281   0.24650  -0.95685   0.01267  Uiso   1.00
C5    C    0.11696   0.17719  -0.86922   0.01267  Uiso   1.00
```

C7 C 0.06929 0.97590 -0.83902 0.01267 Uiso 1.00

C9 C 0.07725 0.91649 -0.75266 0.01267 Uiso 1.00

C11 C 0.12471 0.05952 -0.69765 0.01267 Uiso 1.00

C13 C 0.16972 0.25877 -0.72569 0.01267 Uiso 1.00

C15 C 0.16901 0.31349 -0.81233 0.01267 Uiso 1.00

C17 C 0.16570 0.50614 -0.06878 0.01267 Uiso 1.00

C19 C 0.19442 0.30457 -0.12626 0.01267 Uiso 1.00

C21 C 0.07944 0.62171 -0.09686 0.01267 Uiso 1.00

C23 C 0.08987 0.69639 -0.18870 0.01267 Uiso 1.00

C25 C 0.11954 0.50261 -0.24602 0.01267 Uiso 1.00

C27 C 0.27828 0.74493 -0.95270 0.01267 Uiso 1.00

N1 N 0.22056 0.49964 -0.84061 0.01267 Uiso 1.00

N3 N 0.16762 0.43554 -0.97975 0.01267 Uiso 1.00

N5 N 0.17029 0.32407 -0.21083 0.01267 Uiso 1.00

N7 N 0.01953 0.84432 -0.89239 0.01267 Uiso 1.00

O1 O 0.06606 0.15315 -0.01312 0.01267 Uiso 1.00

O3 O 0.24128 0.14182 -0.10181 0.01267 Uiso 1.00

O5 O 0.10087 0.49973 -0.32215 0.01267 Uiso 1.00

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 # Cambridge Crystallographic Data Centre

 # CCDC

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data_findsym-STRUC-9

_symmetry_cell_setting triclinic

_symmetry_space_group_name_H-M 'P -1'

_symmetry_Int_Tables_number 2

_space_group_name_Hall '-P 1'

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 -x,-y,-z

_cell_length_a 5.80000

_cell_length_b 9.48900

_cell_length_c 12.10600

_cell_angle_alpha 85.97100

_cell_angle_beta 84.82600

_cell_angle_gamma 79.74100

_cell_volume 651.946

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

H H -0.4304 -0.8663 0.2243

H H -0.1017 -0.9501 0.0894

H H 0.2078 -0.7986 0.0306

H H 0.2368 -0.1266 0.3661

H H 0.3394 -0.3119 0.3632

H H -0.4438 -0.0251 0.4006

H H -0.0054 -0.3578 0.4948

H H 0.1403 -0.2351 0.5521

H H -0.4783 -0.5459 0.3782

H H -0.5990 -0.7004 0.3584

H H 0.2946 -0.2324 0.0577

H H 0.4760 -0.3010 0.1653

H H 0.5056 -0.3895 0.0378

H H 0.1097 -0.1681 0.2027

C C 0.2054 -0.4236 0.1430

C C -0.1281 -0.4547 0.2749

C C -0.1295 -0.5873 0.2245

C C -0.3067 -0.6731 0.2563

C C -0.2926 -0.8023 0.2040

C C -0.1068 -0.8478 0.1263

C C 0.0657 -0.7652 0.0934

C C 0.0514 -0.6325 0.1402

C C 0.0345 -0.2316 0.2714

C C -0.2177 -0.1523 0.2900

C C 0.1792 -0.2312 0.3709

C C 0.0404 -0.2497 0.4823

C C -0.1855 -0.1447 0.4906

C C 0.3803 -0.3321 0.0995

N N 0.2146 -0.5477 0.1021

N N 0.0383 -0.3733 0.2280

N N -0.2839 -0.0951 0.3935

N N -0.4873 -0.6312 0.3337

O O -0.2638 -0.4072 0.3563

O O -0.3507 -0.1260 0.2152

O O -0.2851 -0.1037 0.5813

#END

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Cambridge Crystallographic Data Centre

CCDC

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data_findsym-STRUC-10

_symmetry_cell_setting orthorhombic

_symmetry_space_group_name_H-M 'P b c a'

_symmetry_Int_Tables_number 61

_space_group_name_Hall '-P 2ac 2ab'

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2+x,1/2-y,-z

3 -x,1/2+y,1/2-z

4 1/2-x,-y,1/2+z

5 -x,-y,-z

6 1/2-x,1/2+y,z

7 x,1/2-y,1/2+z

8 1/2+x,y,1/2-z

_cell_length_a 14.04600

_cell_length_b 14.98100

_cell_length_c 13.57900

_cell_angle_alpha 90.00000

_cell_angle_beta 90.00000

_cell_angle_gamma 90.00000

_cell_volume 2857.34

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

H H -0.2702 0.3963 -0.5833

H H -0.3341 0.5362 -0.5128

H H -0.2440 0.6196 -0.3837

H H 0.2271 0.4827 -0.2956

H H 0.1827 0.3999 -0.3767

H H 0.1178 0.1793 -0.2133

H H 0.3381 0.3481 -0.3060

H H 0.2939 0.3653 -0.1860

H H -0.0415 0.3003 -0.5171

H H -0.1340 0.3022 -0.6042

H H 0.0283 0.5438 -0.1079

H H 0.1112 0.5932 -0.1910

H H 0.0004 0.6463 -0.1677

H H 0.1183 0.4436 -0.1690

C C -0.0103 0.5325 -0.2606

C C -0.0102 0.4038 -0.3714

C C -0.0933 0.4419 -0.4173

C C -0.1423 0.3965 -0.4955

C C -0.2313 0.4313 -0.5256

C C -0.2664 0.5100 -0.4857

C C -0.2166 0.5577 -0.4141

C C -0.1307 0.5228 -0.3786

C C 0.1076 0.4087 -0.2392

C C 0.0775 0.3138 -0.2097

C C 0.1991 0.4144 -0.2995

C C 0.2728 0.3482 -0.2619

C C 0.2343 0.2551 -0.2576

C C 0.0353 0.5815 -0.1771

N N -0.0847 0.5676 -0.3032

N N 0.0271 0.4516 -0.2899

N N 0.1423 0.2458 -0.2238

N N -0.1071 0.3218 -0.5379

O O 0.0285 0.3319 -0.3948

O O -0.0004 0.2999 -0.1713

O O 0.2817 0.1879 -0.2785

#END