Supporting Information for

Solution Conformations Shed Light on PROTAC Cell Permeability

Yoseph Atilaw,[a] Vasanthanathan Poongavanam,[a] Caroline Svensson Nilsson,[a] Duy Nguyen,[b] Anja Giese,[c] Daniel Meibom,[d] Mate Erdelyi[a] and Jan Kihlberg[a,*]

[a]Department of Chemistry - BMC, Uppsala University, SE-75123 Uppsala, Sweden

[b]Nuvisan Innovation Campus Berlin GmbH, Muellerstrasse 178, 13353 Berlin, Germany

[c]Bayer AG, Drug Discovery Sciences, 13342 Berlin, Germany

[d]Bayer AG, Drug Discovery Sciences, 42113 Wuppertal, Germany

Corresponding author

Jan Kihlberg, jan.kihlberg@kemi.uu.se, ORCID: 0000-0002-4205-6040

Table of Contents

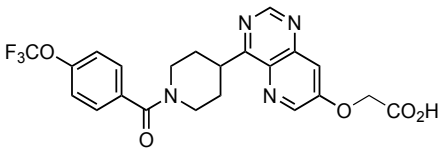
1. Synthesis and characterization of PROTAC 1

1.1. Analytical LCMS methods

Method 1: Instrument: Waters Acquity UPLCMS Single Quad; column: Acquity UPLC BEH C18 1.7 µm, 50x2.1 mm; Eluent A: water + 0. 1% formic acid (99%), Eluent B: acetonitrile; gradient: 0-1.6 min 1-99% B, 1.6-2.0 min 99% B; flow 0.8 ml/min; temperature: 60 °C; DAD scan: 210-400 nm.

Method 2: Instrument: Agilent 1290 UPLCMS 6230 TOF; column: BEH C 18 1.7 µm, 50x2.1 mm; Eluent A: water + 0.05% formic acid (99%); Eluent B: acetonitrile + 0.05% formic acid (99%); gradient: 0-1.7 2-90% B, 1.7-2.0 90% B; flow 1.2 ml/min; temperature: 60°C; DAD scan: 190-400 nm.

1.2. [(4-{1-[4-(Trifluoromethoxy)benzoyl]piperidin-4-yl}pyrido[3,2-d]pyrimidin-7-yl)oxy]acetic acid (3)



Potassium carbonate (396 mg, 2.87 mmol) and ethyl bromoacetate (0.19 mL, 1.70 mmol) were added to a solution of [4-(7-hydroxypyrido[3,2-d]pyrimidin-4-yl)piperidin-1-yl][4-(trifluoro-methoxy)phenyl]methanone[1] (**2**, 600 mg, 1.64 mmol) in THF (18 mL). The reaction mixture was stirred at 100 °C for 8 h in a sealed tube. After cooling to room temperature, water was added, and the resulting mixture was extracted with ethyl acetate. The combined organic layers were washed with water, brine, dried over anhydrous sodium sulfate, and concentrated in vacuo. The crude product was used in the next step without prior purification (809 mg).

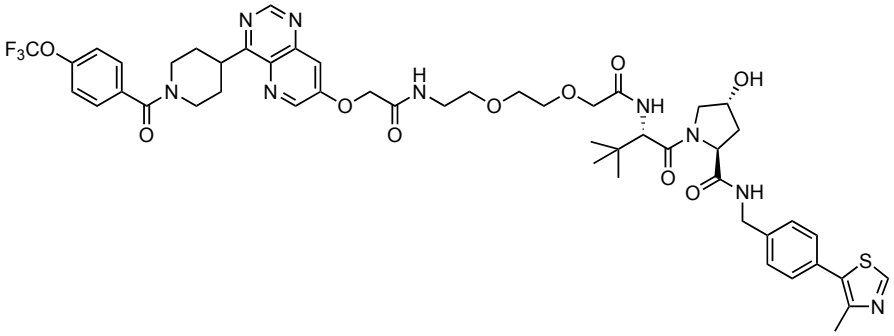
Aqueous sodium hydroxide (14 mL, 2.0 M, 28 mmol) was added to a solution of ethyl [(4-{1-[4-(trifluoromethoxy)benzoyl]piperidin-4-yl}pyrido[3,2-d]pyrimidin-7-yl)oxy]acetate (809 mg) in ethanol (42 mL). The reaction mixture was stirred at room temperature overnight. After removal of ethanol, water was added, followed by extraction with dichloromethane. The aqueous phase was acidified with saturated aqueous citric acid

solution. The precipitates were then filtered and dried in vacuum to afford **3** (304 mg, 38% yields over 2 steps).

LC-MS (method 1): RT = 1.01 min; MS (ESI pos) m/z calcd for $C_{22}H_{20}N_4O_5F_3$ $[M+H]^+$ 477, found 477.

^{1}H-NMR (400 MHz, DMSO-d_6): δ [ppm] 13.50-13.10 (br, 1H, -COOH), 9.21 (s, 1H, pyrimidine -H), 8.90 (d, J = 2.79 Hz, 1H, pyridine-H), 7.73 (d, J = 3.00 Hz, 1H, pyridine-H), 7.61-7.56 (AA´BB´ system, 2H, Phenyl-H), 7.49-7.41 (AA´BB´ system, 2H, Phenyl-H), 5.07 (s, 2H, -CH_2), 4.70-4.60 (br, 1H, piperidine-H), 4.45-4.35 (br, 1H, piperidine-H), 3.75-3.65 (br, 1H, piperidine-H), 3.14-2.99 (br, 1H, piperidine-H), 2.09-1.80 (br m, 4H, piperidine-H). One piperidine proton is not visible.

1.3. 3-Methyl-N-{[2-(2-{2-[(4-{1-[4-(trifluoromethoxy)benzoyl]piperidin-4-yl}pyrido[3,2-d]pyrimidin-7-yl)oxy]acetamido}ethoxy)ethoxy]acetyl}-L-valyl-(4R)-4-hydroxy-N-{[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl}-L-prolinamide (1)



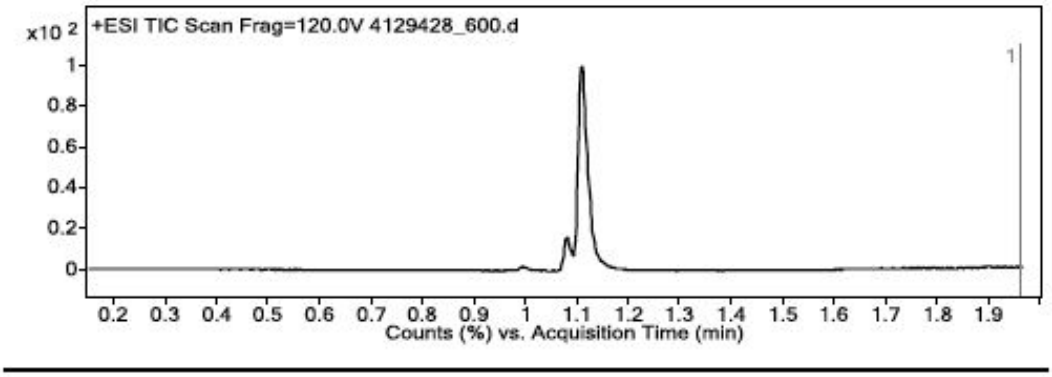
N-{[2-(2-Aminoethoxy)ethoxy]acetyl}-3-methyl-L-valyl-(4R)-4-hydroxy-N-{[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl}-L-prolinamide[2] (**4**, 133 mg, 0,23 mmol), followed by HATU (88 mg, 0.23 mmol) and N,N-diisopropylethylamine (0.11 mL, 0.63 mmol) were added to a solution of [(4-{1-[4-(trifluoromethoxy)benzoyl]piperidin-4-yl}pyrido[3,2-d]pyrimidin-7-yl)oxy]acetic acid (**3**, 100 mg, 0.21 mmol) in DMF (3 mL). The reaction mixture was stirred at room temperature overnight and purified by HPLC (Instrument: Waters auto purification MS Single Quad; column: Waters X Brigde C18 5 µm 100 x 30 mm; Eluent A: water + 0.1% formic acid (99%), Eluent B: acetonitrile; gradient: 0-5.5 min 5-100% B; flow 70 ml/min; temp: 25 °C; DAD scan: 210-400 nm) to afford PROTAC **1** (112 mg, 48% yield).

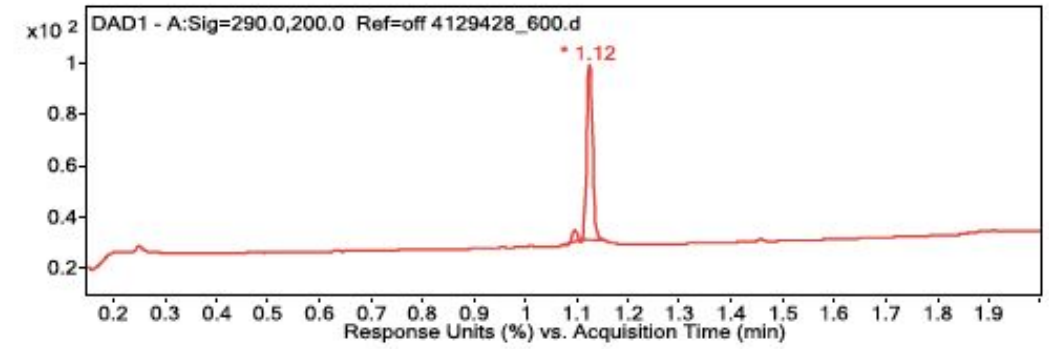
HRMS (ESI) m/z calcd for $C_{50}H_{59}N_9O_{10}F_3S$ $[M+H]^+$ 1034.4058, found 1034.4078.

^{1}H-NMR (400 MHz, DMSO-d_6): δ [ppm] 9.20 (s, 1H, pyrimidine H), 8.97 (s, 1H, thiazole-H), 8.89 (d, J = 2.79 Hz, 1H, pyridine-H), 8.59 (t, J = 5.96 Hz, 1H, amide-NH), 8.36 (t, J = 5.45 Hz, 1H, amide-NH), 7.66 (d, J = 2.79 Hz, 1H, pyridine-H), 7.60-7.55 (AA´BB´ system, 2H, Phenyl-H), 7.47-7.49 (m, 3H, 2 Phenyl-H, amide-NH), 7.39-7.35 (m, 4H, Phenyl-H), 5.16 (d, J = 3.65 Hz, 1H, OH), 4.83 (s, 2H, -CH_2), 4.65-4.20 (m, 8H), 3.95 (s, 2H, -CH_2), 3.75-3.45 (m, 11H), 2.45-2.40 (m, 4H), 2.10-1.77 (m, 6H), 0.93 (s, 9H, *t*-Bu).

^{13}C-NMR (101 MHz, $CDCl_3$): δ [ppm] 173.8, 171.1, 170.8, 169.7, 169.1, 166.7, 156.4, 155.9, 150.3, 150.0, 148.5, 147.4, 145.4, 138.1, 134.7, 133.9, 131.5, 131.0, 129.4, 128.8, 128.2, 120.9, 113.6, 71.3, 70.3, 70.1, 70.0, 69.5, 67.5, 58.9, 57.2, 56.8, 43.1, 38.8, 37.7, 36.6, 35.9, 30.7, 30.6, 29.7, 26.4, 16.1.

LC-MS determination of purity (method 2): RT = 1.12 min; MS (ESI pos) m/z calcd for $C_{50}H_{59}N_9O_{10}F_3S$ $[M+H]^+$ 1034, found 1034, purity 93.6%.





Integration Peak List

Peak	RT	Height	Area	AreaSumPercent
1	1.09	3.88	2.79	6.38
2	1.12	51.4	40.97	93.62

2. Determination of physicochemical properties and *in vitro* potencies of PROTAC 1

Determination of aqueous solubility and LogD. The aqueous solubility and LogD of **1** were determined as reported previously.[1]

Determination of permeability using the PAMPA assay. The permeability of **1** in the parallel artificial membrane permeability assay (PAMPA) was determined at Pharmaron: https://www.pharmaron.com/services/biosciences/dmpk-for-discovery-preclinical-development/in-vitro-admet

Biochemical ERK5 inhibition assay. The potency (IC_{50}) of **1** in inhibition of ERK5 in a biochemical assay was determined as reported previously.[1]

Biochemical VHL inhibtion assay. Von Hippel Lindau (VHL) protein, Elongin B and Elongin C protein (VBC) were labeled with an amine reactive (isothiocyanate group) terbium chelate. A HIF-1alpha derived peptide with hydroxyproline was labeled with fluorescein on the C terminus. The hydroxyproline is essential for the binding of the peptide to the VBC complex, leading to an energy transfer from terbium to fluorescein and the generation of FRET signals (ex 340 nm, em 520 nm). The decrease in the FRET signal is proportional to the binding of a compound to VHL. IC_{50} values are determined by interpolation from plots of relative FRET signal vs inhibitor concentration.

Cellular VHL inhibtion assay. Cellular VHL inhibition was determined using the Promega NanoBRET™ VHL ternary complex starter kit: https://promega.media/-/media/files/resources/application-notes/nanobret/assessing-protac-permeability-and-quantifying-vhl-engagement.pdf?la=en.

Table S1. Potencies for binding of **1** to ERK5 and VHL determined in biochemical and cell-based assays, followed by the ratio between the two potencies.

Potency	Biochemical IC_{50} (μM)	Cellular IC_{50} (μM)	Cell/Biochem. ratio
ERK5	1.23±0.044 (N=2)		
VHL	0.307±0.009 (N=3)	4.31±6.11 (N=5)[a]	14

[a]Geometric mean

3. NMR spectroscopic analysis of PROTAC 1

3.1. ^{1}H-NMR chemical shift assignment

Assignment of protons for PROTAC **1** was derived from ^{1}H, TOCSY, NOESY, HSQC and HMBC NMR specta (Figure S4-S20), recoreded at 25 °C on a 800 MHz BRUKER Avance III HD NMR spectrometer equipped with a TCI cryogenic probe using $CDCl_3$, DMSO-d_6 or DMSO-d_6:D_2O (10:1) as solvent. ^{1}H NMR chemical shifts are listed in Table S2.

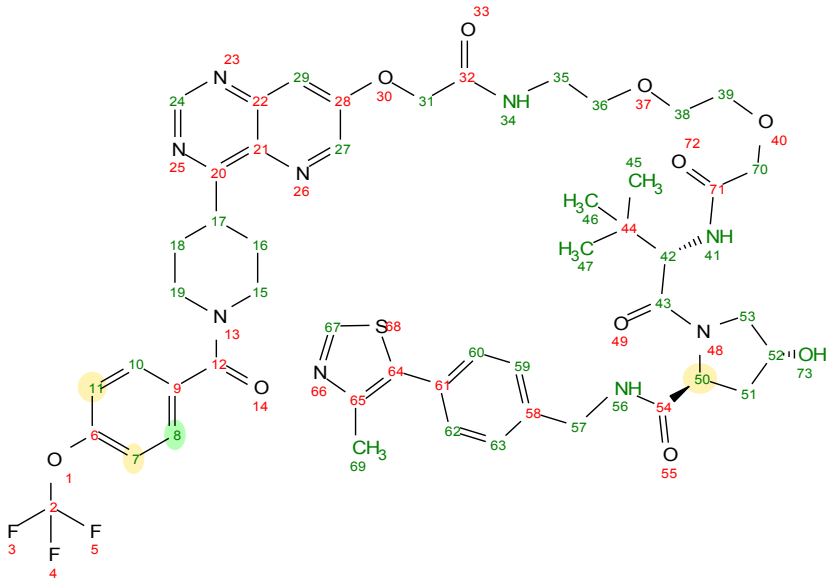


Figure S1. Structure and numbering of PROTAC **1**

Table S2. ^{1}H-NMR chemical shift assignment (δ, ppm) for PROTAC **1** in $CDCl_3$, DMSO-*d*$_6$ and DMSO-*d*$_6$:D_2O (10:1)

Proton no.	δ, $CDCl_3$	Proton no.	δ, DMSO-*d*$_6$	Proton no.	δ, DMSO-*d*$_6$:D_2O (10:1)
7/11	7.27	7/11	7.45	7/11	7.42
8/10	7.52	8/10	7.58	8/10	7.55
17	4.38	16`/18`	4.64	16`/18`	1.83
24	9.18	16``/18``	3.68	16``/18``	1.83
27	8.80	17	4.38	17	4.34
29	7.62	24	9.20	24	9.16
31`	4.79	27	8.89	27	8.85
31``	4.68	29	7.65	29	7.60
34	7.31	31`/31``	4.82	31`/31``	4.78
35`/35``	3.51	34	8.34	34	8.38
36`/36``	3.60	35`	3.49	35`	3.34
38`/38``	3.60	35``	3.35	35``	3.29
39``/39``	3.60	36`/36``	3.60	36`/36``	3.47
41	7.35	38`/38``	3.60	38`/38``	3.36
42	4.59	39`/39``	3.60	39`/39``	3.52
50	4.71	41	7.42	41	7.39
51`	2.45	42	4.57	42	4.54
51``	2.22	50	4.44	50	4.43
52	4.59	51`	2.05	51`	1.89
53`	4.06	51``	1.89	51``	2.05
53``	3.69	52	4.36	52	4.34
56	7.55	53`	3.66	53`	3.60
57`	4.61	53``	3.60	53``	3.63
57``	4.35	56	8.56	56	8.56
59/62	7.34	57`	4.36	57`	4.23
60/63	7.34	57``	4.25	57``	4.33
67	8.70	59/63	7.37	59/63	7.34
70`	3.90	60/ 62	7.37	60/62	7.34
70``	3.77	67	9.00	67	8.91
73	4.59	70`/70``	3.95	70`/70``	3.92

3.2. Interproton distances

NOE build-ups were recorded without solvent suppression using mixing times of 100, 200, 300, 400, 500, 600 and 700 ms. The relaxation delay was set to 2.5 s, and 16 scans were recorded with 8192 and 512 data points in the direct (F2) and indirect (F1) dimension, respectively. Distances were calculated using germinal methylene protons (ref=1.78 Å) as reference (Table S3-S5). Interproton distances (r_{ij}) were claculated according to the equation $r_{ij}=r_{ref}(\sigma_{ref}/\sigma_{ij})^{(1/6)}$. The NOE peak intensities were calculated according to the equation ([cross peak1 × cross peak2]/[diagonal peak1 × diagonal peak2])$^{0.5}$. A minimum of 4 mixing times giving a linear ($R^2 \geq 0.93$) build-up rate (σ_{ij}) were used for quantification.

Table S3. Interproton distances (Å) for PROTAC **1** derived from NOE build-up measurements in $CDCl_3$ (δ in ppm)

No.	Proton A	Proton B	δA (ppm)	δA (ppm)	σ	R^2	Dis. r_{ij}(Å)
1	27	31``	8.80	4.68	6.09 E-07	0.98	3.4
2	27	31`	8.80	4.79	4.48 E-07	0.99	3.6
3	27	70``	8.80	3.77	3.82 E-07	0.97	3.7
4	29	31``	7.26	4.68	3.23 E-06	0.99	2.6
5	56	57`	7.55	4.61	2.86 E-06	0.97	2.6
6	56	70``	7.55	3.77	5.83 E-06	0.96	3.4
7	8/10	51`	7.52	2.45	5.30 E-06	0.99	4.5
8	34	31``	7.31	4.68	2.26 E-06	0.97	2.7
9	34	31`	7.31	4.79	6.90 E-06	0.95	2.7
10	50	51``	4.71	2.22	2.07 E-06	0.97	2.3
11	17	16`/18`	4.38	4.64	2.06 E-06	0.99	1.9
12	17	16``/18``	4.38	3.68	1.23 E-06	0.99	2.1
13	53`	51`	4.06	2.45	1.28 E-06	0.95	3.0

Table S4. Interproton distances (Å) for PROTAC **1** derived from NOE build-up measurements in DMSO-d_6 (δ in ppm)

No.	Proton A	Proton B	δA (ppm)	δA (ppm)	σ	R^2	Dis. r_{ij}(Å)
1	27	17	8.89	4.38	3.05 E-06	0.99	3.47
2	27	31	8.89	4.82	5.71 E-07	0.99	3.13
3	56	31	8.56	4.82	6.99 E-07	0.98	4.44
4	56	51``	8.56	1.89	5.02 E-06	0.99	3.2
5	56	51`	8.56	2.05	9.24 E-06	0.99	3.1
6	56	53`	8.56	3.66	5.63 E-07	0.98	4.6
7	56	57`	8.56	4.36	2.61 E-05	0.98	2.43
8	56	50	8.56	4.44	1.20 E-07	0.99	1.94
9	34	29	8.34	7.65	9.11 E-06	0.99	2.89
10	34	31	8.34	4.82	1.91 E-05	0.99	2.56
11	34	41	8.34	7.42	1.19 E-06	0.97	4.06
12	29	35``	7.65	3.35	4.94 E-06	0.97	4.63
13	29	31	7.65	4.82	1.48 E-06	0.99	2.1
14	41	53``	7.42	3.60	8.23 E-06	0.99	2.78
15	41	70	7.42	3.95	1.02 E-05	0.99	2.84
16	41	53`	7.42	3.66	7.35 E-05	0.96	4.02
17	42	53``	4.57	3.60	6.69 E-05	0.99	2.08
18	42	53`	4.57	3.66	6.48 E-06	0.99	2.09
19	42	70	4.57	3.95	1.58 E-06	0.99	3.87
20	50	53`	4.44	3.66	2.11 E-06	0.96	3.69
21	50	51`	4.44	2.05	6.48 E-05	0.98	2.09
22	50	51``	4.44	1.89	1.60 E-07	0.98	2.14
23	52	53`	4.36	4.36	5.50 E-06	0.99	2.16
24	52	53``	4.36	3.60	6.11 E-06	0.99	2.29
25	53`	51`	3.60	2.05	5.52 E-06	0.95	3.15
26	53``	51``	3.60	1.89	1.01 E-05	0.99	3.14
27	53``	51`	3.60	2.05	4.52 E-06	0.96	2.14

Table S5. Interproton distances (Å) for PROTAC **1** derived from NOE build-up measurements in DMSO-d_6:D_2O (10:1) (δ in ppm)

No.	Proton A	Proton B	δA (ppm)	δA (ppm)	σ	R^2	Dis. r_{ij}(Å)
1	42	50	4.54	4.43	5.48E-06	0.99	3.87
2	42	70	4.54	3.92	5.39E-06	0.99	3.94
3	41	70	7.42	3.92	5.87E-05	0.98	2.61
4	50	51''	4.43	2.06	0.000141	0.99	2.11
5	50	51'	4.43	1.89	5.85E-05	0.93	2.44
6	57'	51''	4.22	2.06	2.14E-06	0.93	4.24
7	53'	51'	3.61	1.89	4.97E-05	0.99	2.68
8	56	53'	3.60	3.61	3.02E-06	0.92	4.00
9	42	53'	4.54	3.61	0.00038235	0.99	1.90
10	50	53'	4.43	3.61	1.61E-05	0.99	3.23
11	27	31	8.85	4.78	1.94E-05	0.99	2.94
12	27	18	8.85	1.83	2.48E-06	0.96	4.14
13	31	35'	4.78	3.34	2.5E-06	0.92	4.13
14	31	35''	4.78	3.29	1.53E-06	0.95	4.48
15	36	35'	3.47	3.32	5.37E-05	0.99	2.64
16	29	50	7.59	4.43	1.51E-06	0.96	4.49
17	31	57'	4.78	3.61	1E-06	0.94	4.81
18	31	50	4.78	4.43	3.08E-06	0.99	3.99

Table S6. $^3J_{HH}$ coupling constants for PROTAC **1** in $CDCl_3$, DMSO-d_6 and DMSO-d_6:D_2O (10:1) (δ ppm)

$CDCl_3$					DMSO-d_6					DMSO-d_6:D_2O (10:1)				
^{1}H A	^{1}H B	δA	δB	$^3J_{HH}$ (Hz)	^{1}H A	^{1}H B	δA	δB	$^3J_{HH}$ (Hz)	^{1}H A	^{1}H B	δA	δB	$^3J_{HH}$ (Hz)
57`	56	4.61	7.55	5.42	57`	56	4.36	8.56	4.3	57`	56	4.22	3.60	5.6
53`	52	4.06	4.59	3.42	53`	52	3.66	4.36	3.96	42	41	4.54	7.42	9.6
51`	50	2.22	4.71	7.62	42	41	4.57	7.42	9.54	34	35`	8.38	3.32	5.9

4. Monte Carlo molecular mechanics (MCMM) conformational search

The theoretical conformation ensemble of PROTAC **1** was identified by performing careful Monte Carlo conformational analysis using five different (OPLS, OPLS-2005, OPLS3e, AMBER* and MMFF) force fields, each with the GB/SA solvation models chloroform and

water. These conformational searches were done using the Monte Carlo algorithm with intermediate torsion sampling, 50 000 Monte Carlo steps and a RMSD cut-off set to 2.0 Å. A Molecular Mechanics energy minimization was performed as implemented in the Macromodel BatchMin V12.1 of the Schrödinger Package.[10] Each conformation was energy minimized using Polak-Ribière type conjugate gradient (PRCG) with a maximum of 5000 iterative steps. All conformations within 42 kJ/mol from the global minimum were saved. Results of all the different conformational searches are given in Table S7. All ensembles generated by the conformational searches were combined and elimination of redundant conformations was performed by comparison of heavy atom coordinates applying an RMSD cutoff set to 3.0 Å giving the final ensemble used for NAMFIS-analysis.

Table S7. Result of the MCMM conformational analysis

Force fields	Solvent		Following redundant conformer elimination
	$CHCl_3$	H_2O	
OPLS	134	967	
OPLS3e	508	1733	
OPLS 2005	1259	3037	152
MMFF	1935	1394	
AMBER*	2323	2263	
Final ensemble used			152

5. Identifications of solution ensemble using the NAMFIS algorithm

Solution ensembles were determined by fitting the experimentally measured distances and coupling constants to those back-calculated from computationally predicted conformations using NAMFIS algorithm.[3,4] Methylene protons were treated according to the equation $d = (((d_1^{-6}) + (d_2^{-6}))/2)^{-1/6}$, and methyl protons according to $d = (((d_1^{-6}) + (d_2^{-6}) + (d_3^{-6}))/3)^{-1/6}$. The back-calculated *J*-coupling constants were generated according to the following Karplus equation ${}^3J_{HH} = 9.4*((COS(\theta))^2) - (1.1*(COS(\theta))) + 0.4$.

The NAMFIS output solution ensembles were validated using standard methods, i.e. through evaluation of the reliability of the conformational restraints by the addition of 10% random noise to the experimental data, by the random removal of individual restraints, and by comparison of the experimentally observed and back-calculated distances.

Additional validation step was performed by comparing the solution ensembles for specific parts of the PROTAC **1**, when feeding the NAMFIS algorithm with specific sets of NOE proton-proton distances, which describe certain parts of the molecule. Thus, the NAMFIS output obtained using all distances was compared to the NAMFIS outputs obtained using distances from the POI-ligand part only (H27-H34), and the VHL E3 ligase ligand part only (H70-H56). Using this, we evaluated whether long-range restraints (distances from POI ligand to VHL E3 ligase ligand) over-restrained the compound, possibly falsifying the conformation of parts of the molecule that are well-described by local NOE- and *J*-restraints. Comparison of RMSD values and dihedral angles of these specific regions of the molecule ij ensembles derived from NAMFIS analysis including either restraints for a specific region only, or for the entire molecule indicated that the long-range restraints did not distort the conformation of the well-described (NOE, *J*) POI a and VHL E3 parts of the molecule. The interatomic distances, *J*-couplings and populations of the validated conformational ensembles are given in Tables S8-S10.

Table S8. Experimentally determined and back-calculated distances (NAMFIS output) interproton distances (Å)

Interproton distances $CDCl_3$		Interproton distances DMSO-d_6		Interproton distances DMSO-d_6:D_2O (10:1)	
$Exp._{dist(Å)}$	$Calc._{dist(Å)}$	$Exp._{dist(Å)}$	$Calc._{dist(Å)}$	$Exp._{dist(Å)}$	$Calc._{dist(Å)}$
3.40	3.38	3.47	3.87	3.87	3.88
3.58	3.57	3.13	3.13	3.94	4.50
3.67	3.72	4.44	4.00	2.61	2.64
2.57	2.51	3.20	3.35	2.11	2.39
2.63	2.65	3.10	3.35	2.44	2.90
3.42	3.74	4.60	4.71	4.24	4.44
4.51	4.39	2.43	2.61	2.68	3.08
2.70	2.74	1.94	2.24	4.00	3.85
2.73	2.77	2.89	3.04	1.90	2.15
2.27	2.72	2.56	2.92	3.23	3.67
1.89	2.37	4.06	3.91	2.94	2.40
2.06	2.55	4.63	4.76	4.14	4.47
3.00	3.60	2.10	2.50	4.13	4.53
		2.78	3.25	4.48	4.62
		2.84	3.00	2.64	2.68
		4.02	3.50	4.49	4.50
		2.08	2.36	4.81	4.80
		2.09	2.36	3.99	4.04
		3.87	4.27		
		3.69	3.87		
		2.09	2.54		
		3.15	3.12		
		3.14	2.86		
		3.62	3.55		
		2.14	2.54		
		2.16	2.51		
		2.29	2.51		
		1.78	1.76		
RMSD	0.49	RMSD	0.37	RMSD	0.30

Table S9. Experimentally determined and back-calculated coupling constants (NAMFIS output)

$CDCl_3$		DMSO-d_6		DMSO-d_6:D_2O (10:1)	
Exp.dist(Å)	Calc.dist(Å)	Exp.dist(Å)	Calc.dist(Å)	Exp.dist(Å)	Calc.dist(Å)
5.4	5.5	4.3	5.3	5.6	5.6
3.4	2.4	4.0	3.8	9.6	8.9
7.6	6.6	9.5	8.7	5.8	5.5
RMSD	0.82	RMSD	0.74	RMSD	0.42

Table S10. Conformational populations derived by NAMFIS-analysis of PROTAC **1** in $CDCl_3$, DMSO-d_6 and DMSO-d_6:D_2O (10:1) solution. Coordinates for the conformations below are available at pages S23-S86 of the Supporting Information.

$CDCl_3$		DMSO-d_6		DMSO-d_6:D_2O (10:1)	
Conf. No.	Population (%)	Conf. No.	Population (%)	Conf. No.	Population (%)
1	30	9	40	15	17
2	20	10	20	16	16
3	15	11	16	17	15
4	10	12	13	18	13
5	7	13	4	19	11
6	4	14	3	20	7
7	3			21	5
8	3			22	5
				23	5
				24	4

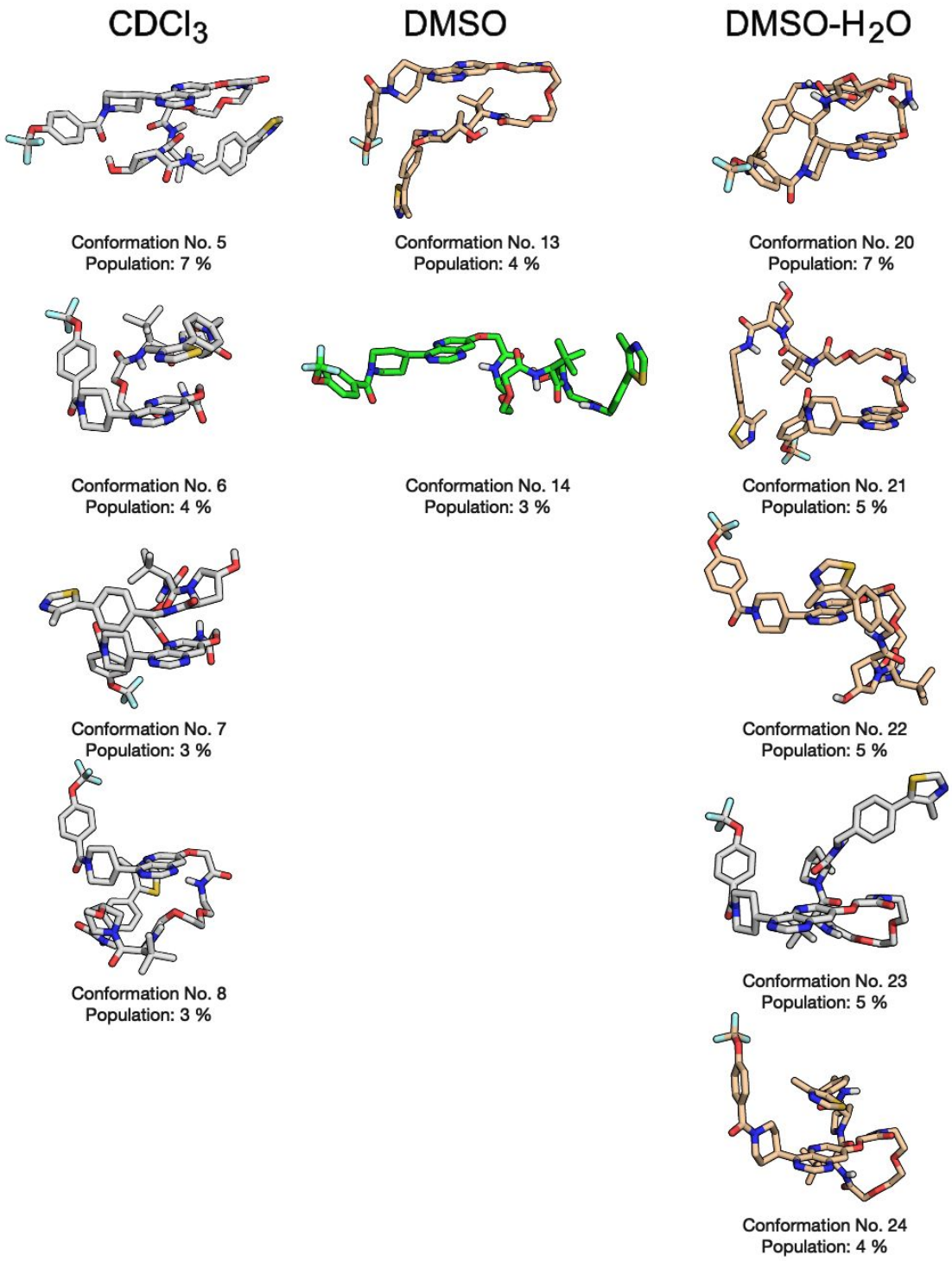


Figure S2. Structures of the minor conformations (population <10%) in the ensembles adopted by **1** in chloroform, DMSO and DMSO-water (10:1). Conformations that are predominantly linear are in green, those that are folded with one turn are in wheat, while folded conformations with two turns are in grey. The number and population in % is given below each conformation. To facilitate comparisons, all conformations are shown having the pyrimidine moiety of the ERK5 binding ligand of **1** in the same orientation. Intramolecular hydrogen bonds are indicated with dashed black lines.

6. Computational characterization of reported VHL PROTACs and of PROTAC 1

6.1. Molecular property analysis

We compared the molecular properties of VHL PROTAC **1** to the set of VHL PROTACs compiled by Maple et al.[5] In brief, Maple et al. compiled a set of 218 VHL PROTACs from the literature and analyzed them in detail from a chemical space perspective. Herein, we first removed duplicates from the set of Maple et al. by analysis of their SMILES representations. The SMILES code for each compound was then converted into structures using the MOE modeling software (version 2014.09).[6] Subsequently, physicochemical descriptors that are commonly used to characterize compounds in drug discovery were calculated, i.e. the molecular weight (MW) and descriptor of molecular polarity (HBA, HBD and TPSA), lipophilicity (cLogP) and flexibility (NRotB). Molecular properties were analyzed and plotted using RStudio (version 3.4.4).[7]

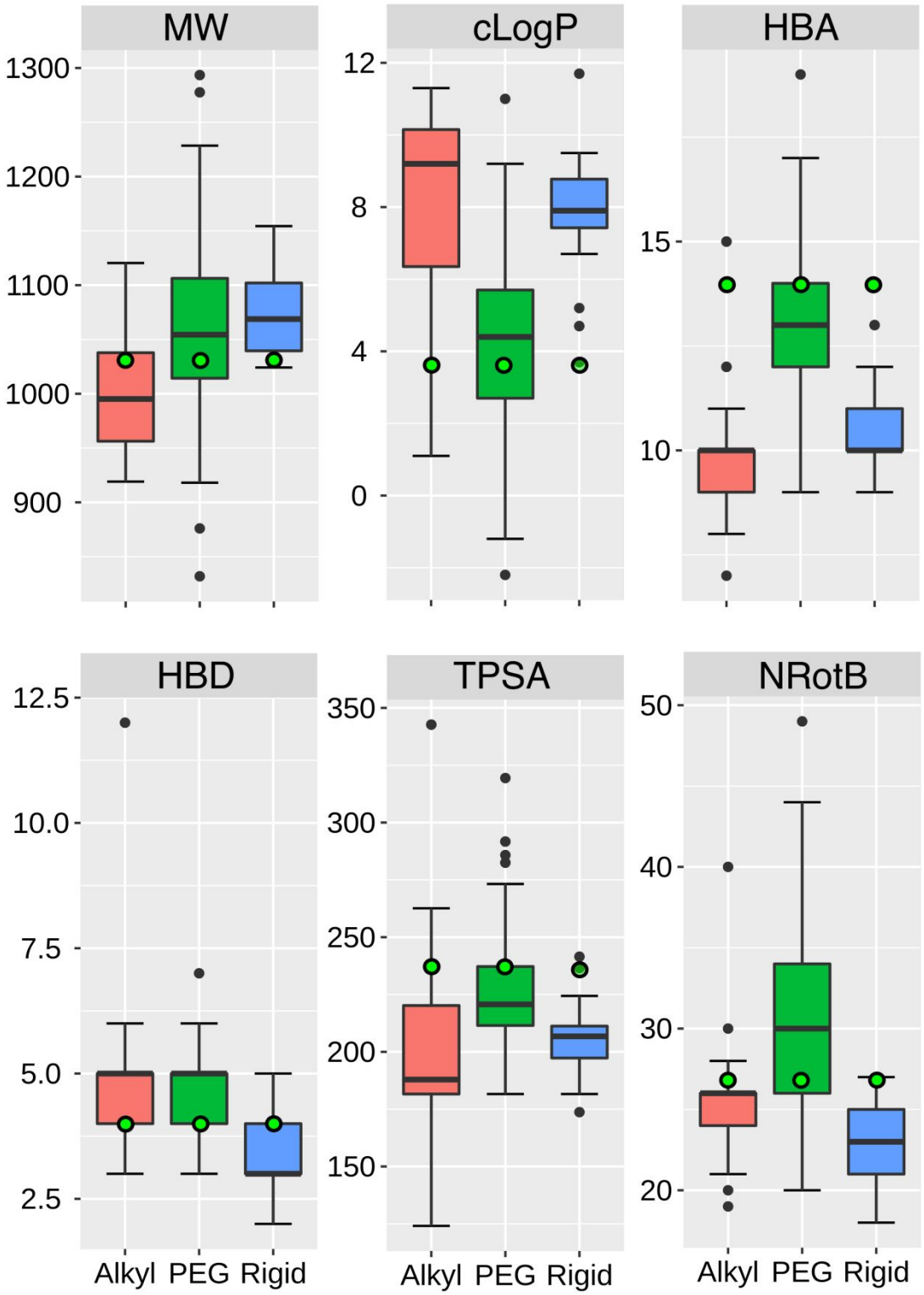


Figure S3. Molecular weight (MW, Da), lipophilicity (cLogP), hydrogen bond acceptors and donors (HBA and HBD), topological polar surface area (TPSA, Å^2), and the number of rotatable bonds (NRotB) calculated for PROTAC **1** and the three subsets of VHL PROTACs that have aliphatic (alkyl, n=63), ethylene glycol based (PEG, n=135) or rigid (n=19) linkers

reported by Maple, et al.[5] The values of the six descriptors calculated for **1** are shown as green circles (MW = 1034 Da, cLogP = 3.55, HBA = 14, HBD = 4, TPSA = 237 Å^2, NRotB = 27). Boxplots show the 50th percentiles as horizontal bars, the 25th and 75th percentiles as boxes, the 25th percentile minus 1.5 x the interquartile range and the 75th percentile plus 1.5 x the interquartile range as whiskers for the three subset of PROTACs.

6.2. Calculation of descriptors for conformers in the solution ensembles

Prior to the calculation of 3D molecular descriptors for the 24 solution conformers of **1**, each conformer was thoroughly checked so that its structure was represented correctly. Subsequently, 3D descriptors that represent the molecular size (radius of gyration, R_{gyr}) and surface polarity (solvent-accessible 3D polar surface area, SA 3D PSA) were calculated as described previously.[8] The two descriptors were then analyzed using the Data Warrior program.[9]

Intramolecular hydrogen bonds (IMHBs) were identified in the solution conformers using the Maestro program (available in the Schrödinger Suite)[10] with the default distance and angle parameters, i.e. a maximum distance between acceptor and donor of 2.8 Å and a minimum angle for donor and acceptor of 120° and 80°, respectively.

Table S11. Overview of solution conformations, calculated descriptors and intramolecular hydrogen bonds in each conformation of PROTAC **1** in the three solvents used for NMR spectroscopy.

Solvent	Conf. No.	Popul. (%)	Descriptors[a]			Conf. category
			SA 3D PSA (Å²)[a]	R_{gyr} (Å)[b]	IMHB[c]	
$CDCl_3$	1	30	202.0	5.5	1	Major
	2	20	182.6	5.8	2	Major
	3	15	194.5	5.6	2	Major
	4	10	241.5	8.1	1	Major
	5	7	172.4	6.2	2	Minor
	6	4	207.3	5.4	1	Minor
	7	3	207.1	5.8	1	Minor
	8	3	242.1	5.6	1	Minor
DMSO-d_6	9	40	198.8	7.4	1	Major
	10	20	205.9	5.2	1	Major
	11	16	202.3	9.2	3	Major
	12	13	258.9	9.7	0	Major
	13	4	200.5	6.3	1	Minor
	14	3	191.9	8.2	2	Minor
DMSO-d_6 - D_2O	15	17	238.9	6.0	1[d]	Major
	16	16	246.0	7.0	1	Major
	17	15	211.8	8.9	1	Major
	18	13	186.0	6.9	2	Major
	19	11	240.0	6.3	1	Major
	20	7	209.0	6.9	2	Minor
	21	5	248.8	7.1	1	Minor
	22	5	219.8	6.3	1	Minor
	23	5	242.6	6.1	2	Minor
	24	4	237.0	6.6	1	Minor

[a]SA 3D PSA = solvent accessible 3D polar surface area. [b]R_{gyr} (Å) = radius of gyration. [c]IMHB = intramolecular hydrogen bond. [d]A three centered (bifurcated) intramolecular hydrogen bond.

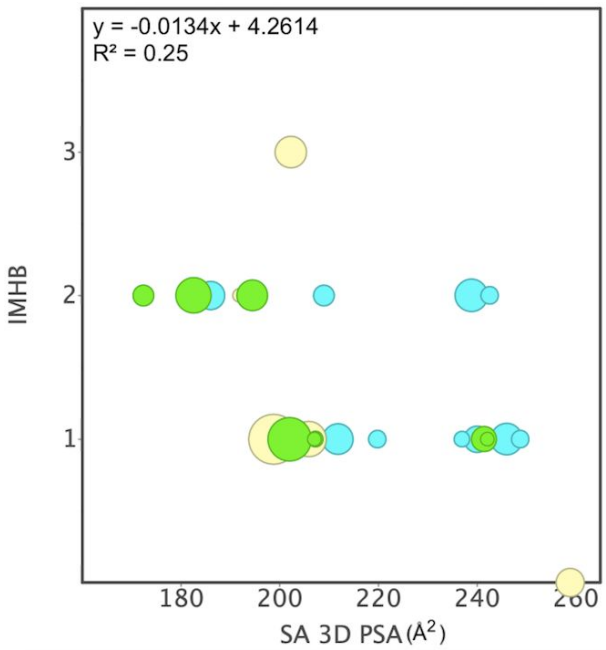


Figure S4. The number of intramolecular hydrogen bonds (IMHB) versus the solvent accessible 3D polar surface area (SA 3D PSA) for all solution conformations populated by **1**. Conformations in $CDCl_3$ are in green, those in DMSO-d_6 are in wheat while those in DMSO-d_6–D_2O are in blue. The area of each circle is proportional to the population of the corresponding conformation (in %).

6.3. **Structural comparison of conformers in solution ensembles**

Table S12. RMSD matrix for all conformations

Conf. No	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1	0																						
2	3.78																						
3	4.87	5.19																					
4	6.46	6.41	4.83																				
5	5.26	6.23	4.60	4.63																			
6	4.51	5.29	5.44	6.62	5.53																		
7	6.11	5.85	5.88	6.21	4.98	4.82																	
8	3.37	4.52	5.39	5.74	5.25	5.25	5.50																
9	6.14	6.51	5.74	4.24	5.70	5.82	6.78	5.20															
10	4.41	4.78	5.59	7.47	6.01	4.73	4.12	4.75	7.13														
11	8.28	7.60	7.61	5.47	5.98	7.31	6.86	7.11	5.48	8.32													
12	8.46	7.73	8.56	6.06	6.69	7.21	7.34	7.93	6.01	8.92	3.12												
13	4.32	3.20	5.53	6.42	5.75	6.01	6.42	4.95	6.20	6.08	8.03	8.22											
14	7.44	6.40	6.67	4.71	5.73	6.50	5.66	6.85	4.92	7.85	3.95	3.45	6.84										
15	4.38	4.73	5.00	7.64	6.51	3.92	6.40	5.49	6.62	5.25	9.26	9.42	4.86	8.22									
16	6.37	5.23	4.69	5.13	4.22	6.92	6.29	5.73	5.70	6.91	5.31	6.13	5.23	5.14	6.46								
17	8.23	7.10	6.86	4.42	5.37	7.01	6.54	7.71	5.64	8.56	3.39	3.77	7.24	4.17	8.38	5.11							
18	5.83	5.97	4.61	4.18	5.49	5.52	6.14	4.93	3.80	6.78	6.33	6.51	5.95	4.90	6.17	5.39	5.92						
19	4.69	4.30	3.70	6.14	6.00	6.11	6.53	5.38	6.33	4.95	8.72	9.18	4.65	7.30	3.86	4.80	8.00	5.32					
20	5.64	5.06	5.00	4.74	5.20	5.90	5.49	5.49	4.37	6.92	5.94	5.99	4.91	3.86	6.32	4.29	5.45	3.91	4.97				
21	4.86	5.01	5.81	6.89	6.53	4.79	5.54	5.37	6.21	5.49	8.17	7.63	4.97	6.29	4.38	6.37	7.32	5.76	4.90	4.51			
22	6.07	6.01	4.04	3.54	5.23	5.74	6.25	5.73	3.89	7.03	6.42	6.85	5.97	5.51	5.75	4.84	5.24	3.75	4.86	4.50	5.62		
23	4.23	4.32	5.58	5.85	5.43	4.10	4.75	4.89	6.48	5.05	6.72	7.06	4.84	6.57	5.08	6.68	5.60	6.15	6.38	6.16	5.87	5.50	
24	4.05	4.53	4.93	5.82	6.21	4.65	6.65	3.92	4.68	5.97	7.17	7.50	4.79	6.63	4.69	6.79	7.06	4.46	5.01	5.34	5.37	5.43	4.48

7. Coordinates for the conformations (1-24)

conformer_1

F	-3.692904	8.516063	-0.727684
C	-3.039904	7.299463	-0.704484
F	-3.770704	6.471463	0.131416
F	-3.036904	6.824863	-2.005584
O	-1.707304	7.564163	-0.203684
C	-0.763004	6.575363	-0.040684
C	-0.968304	5.211563	-0.337284
C	0.056596	4.275063	-0.138084
C	1.307596	4.677963	0.350916
C	2.384196	3.673663	0.569416
N	2.759696	2.855963	-0.432484
C	2.615696	3.135763	-1.864684
C	1.832596	2.015663	-2.550884
C	2.491596	0.646563	-2.300984
C	1.755996	-0.482137	-3.027084
C	2.246996	-1.803337	-3.073484
N	3.390296	-2.131237	-2.458884
C	3.759496	-3.417137	-2.488784
C	3.045196	-4.429237	-3.121084
O	3.513396	-5.721237	-3.011784
C	2.789396	-6.835837	-3.593684
C	1.539296	-7.215037	-2.793984
N	1.474496	-6.754637	-1.545184
C	0.357596	-6.953637	-0.637884
C	-0.789804	-6.001237	-0.986284
O	-0.296204	-4.653137	-1.034484
C	-1.237004	-3.702537	-1.567484
C	-2.389804	-3.438637	-0.592284
O	-1.841504	-3.205037	0.705216
C	-2.838004	-3.156637	1.736216
C	-2.066104	-2.915137	3.025816
N	-0.749704	-2.839237	2.852316
C	0.258696	-2.513337	3.839416
C	1.159996	-3.742937	4.149516
C	1.755596	-4.441837	2.911116
C	0.330296	-4.795637	4.905116
C	2.311996	-3.327937	5.080216
C	0.993096	-1.301137	3.235116
N	1.004196	-0.106437	3.850216
C	0.393596	0.279163	5.124616
C	-1.086604	0.612963	4.892216
N	-1.440604	0.758163	3.616116
C	-2.776404	1.001063	3.120716
C	-2.676404	1.214063	1.624216
C	-1.866804	0.379363	0.831716
C	-1.782604	0.581863	-0.554684

C	-2.518104	1.610763	-1.164084
C	-2.452704	1.813563	-2.625584
C	-2.962604	0.918863	-3.568284
C	-3.692004	-0.382637	-3.295784
N	-2.734904	1.370163	-4.891784
C	-2.124804	2.502563	-4.866984
S	-1.734404	3.192563	-3.333184
C	-3.319004	2.449363	-0.374484
C	-3.394704	2.254363	1.013816
O	-1.880304	0.711463	5.826516
C	1.173096	1.516663	5.575316
C	1.528396	2.190363	4.253016
O	2.689996	3.012263	4.372516
C	1.778796	1.002263	3.321116
O	1.496996	-1.411937	2.119716
O	-2.632004	-2.792837	4.111316
O	0.651596	-7.897737	-3.303884
C	1.889696	-4.058437	-3.807884
C	1.484496	-2.730437	-3.779084
N	0.368796	-2.375237	-4.415984
C	-0.025404	-1.101037	-4.357684
N	0.628596	-0.161537	-3.669484
C	2.575696	0.457563	-0.774584
C	3.420996	1.582563	-0.171484
O	2.889296	3.605063	1.690216
C	1.516796	6.028863	0.660016
C	0.489996	6.967563	0.460816
H	-1.904804	4.840263	-0.719684
H	-0.121904	3.232563	-0.355484
H	3.611296	3.177963	-2.307184
H	2.128696	4.084563	-2.082484
H	1.807396	2.232563	-3.619384
H	0.816696	2.019763	-2.155684
H	3.504696	0.684663	-2.702984
H	4.666696	-3.697137	-1.971684
H	3.457696	-7.696837	-3.579284
H	2.530696	-6.636237	-4.633784
H	2.256596	-6.203237	-1.219584
H	0.693496	-6.738037	0.376716
H	0.007596	-7.985437	-0.680484
H	-1.555504	-6.104837	-0.217884
H	-1.210404	-6.282437	-1.951884
H	-1.625204	-4.029337	-2.541284
H	-0.702604	-2.753137	-1.701484
H	-3.069704	-4.300437	-0.571984
H	-2.947404	-2.552337	-0.921984
H	-3.376304	-4.102537	1.801716
H	-3.532704	-2.335037	1.558616
H	-0.449804	-2.923137	1.885916
H	-0.241104	-2.247937	4.765316

H	2.440996	-3.783037	2.380716
H	2.316396	-5.322437	3.224416
H	0.969996	-4.764337	2.227716
H	-0.103504	-4.359537	5.805216
H	-0.472504	-5.175037	4.273216
H	0.960396	-5.636037	5.197016
H	1.914496	-2.813337	5.955416
H	2.861696	-4.209337	5.410916
H	3.010596	-2.667537	4.566516
H	0.500096	-0.484537	5.894416
H	-0.705904	0.635363	2.934716
H	-3.207804	1.878363	3.603316
H	-3.398104	0.127463	3.318216
H	-1.309004	-0.433237	1.271316
H	-1.156704	-0.063937	-1.154684
H	-3.860204	-0.545737	-2.232484
H	-4.657404	-0.357537	-3.800684
H	-3.104904	-1.211237	-3.691384
H	-1.867904	3.004263	-5.789484
H	-3.885504	3.245963	-0.835784
H	-4.017504	2.905563	1.610416
H	2.088196	1.195163	6.073616
H	0.592596	2.167063	6.230116
H	0.683896	2.775363	3.887116
H	2.899296	3.316563	3.466616
H	1.458496	1.254063	2.309816
H	2.837496	0.740063	3.329816
H	1.278296	-4.765937	-4.343184
H	-0.922004	-0.813437	-4.889284
H	3.049196	-0.484137	-0.507184
H	1.574396	0.478563	-0.341684
H	3.531696	1.375863	0.891516
H	4.414096	1.581963	-0.621584
H	2.473396	6.346063	1.049816
H	0.666696	8.006663	0.698616

conformer_2

F	-3.558004	3.753676	-1.863362
C	-2.340265	3.930701	-1.241011
F	-2.174082	5.290561	-1.044912
F	-2.367903	3.256562	-0.035468
O	-1.348340	3.373772	-2.123014
C	0.003103	3.562688	-1.940571
C	0.596593	4.042984	-0.749967
C	1.990100	4.222498	-0.664660
C	2.826256	3.931489	-1.759458
C	4.294524	4.141684	-1.700391
N	5.035597	3.646561	-0.691011
C	6.479282	3.861043	-0.632436
C	7.246094	2.555765	-0.909600

C	6.438163	1.293307	-0.537813
C	5.584238	0.726410	-1.677742
C	4.912544	-0.507156	-1.545416
N	4.988490	-1.230837	-0.417692
C	4.342930	-2.404142	-0.388865
C	3.563003	-2.900124	-1.448894
O	2.918318	-4.099266	-1.284592
C	2.031525	-4.571112	-2.310106
C	1.419074	-5.901455	-1.879921
N	0.873610	-5.950302	-0.665021
C	0.247843	-7.137385	-0.113918
C	-1.248685	-7.112774	-0.420972
O	-1.823566	-5.937466	0.160601
C	-3.233794	-5.833379	-0.065917
C	-3.839979	-4.926916	1.007230
O	-3.521432	-5.471400	2.294692
C	-3.726539	-4.554476	3.376655
C	-2.558454	-3.582512	3.543502
N	-1.501446	-3.750074	2.746107
C	-0.320437	-2.903740	2.776561
C	0.831575	-3.602621	3.547684
C	0.424800	-3.787442	5.020560
C	2.092118	-2.722450	3.526855
C	1.196613	-4.992412	2.996304
C	0.020290	-2.562228	1.314768
N	-0.011300	-1.289843	0.884066
C	-0.110299	-0.110671	1.746089
C	-1.542549	0.161791	2.207652
N	-2.498634	-0.589276	1.656703
C	-3.892349	-0.542691	2.061268
C	-4.553170	0.712339	1.526635
C	-4.713169	1.844195	2.345321
C	-5.332311	3.006279	1.853302
C	-5.791631	3.069199	0.522831
C	-6.440820	4.287900	-0.023019
C	-6.032128	5.603048	0.223976
C	-4.847660	6.018260	1.072551
N	-6.831281	6.536886	-0.418507
C	-7.747149	5.941816	-1.094892
S	-7.795428	4.217279	-1.065459
C	-5.635251	1.930769	-0.292927
C	-5.019631	0.767341	0.201444
O	-1.767959	1.026851	3.048260
C	0.413657	1.058838	0.910199
C	1.411433	0.366618	-0.007129
O	2.548012	0.055290	0.775555
C	0.635554	-0.901177	-0.356904
O	0.273834	-3.473382	0.529173
O	-2.623385	-2.688426	4.382230
O	1.439658	-6.872125	-2.634873

C	3.482924	-2.119667	-2.618578
C	4.174570	-0.899667	-2.680248
N	4.103808	-0.174432	-3.797114
C	4.800241	0.968458	-3.815927
N	5.535279	1.442496	-2.805668
C	5.592786	1.676706	0.687279
C	4.515783	2.694981	0.290117
O	4.810030	4.773952	-2.619796
C	2.235257	3.453900	-2.941059
C	0.846029	3.261032	-3.025912
H	0.009561	4.295466	0.121238
H	2.424812	4.615802	0.243083
H	6.722191	4.206337	0.373509
H	6.824190	4.629322	-1.325626
H	8.145955	2.578919	-0.293445
H	7.578982	2.524999	-1.947439
H	7.148898	0.518441	-0.247131
H	4.409935	-3.000227	0.512478
H	2.581345	-4.730155	-3.238946
H	1.222875	-3.857796	-2.474461
H	0.810576	-5.087670	-0.130531
H	0.395227	-7.149649	0.965831
H	0.689586	-8.042867	-0.532852
H	-1.705790	-8.005990	0.007368
H	-1.402820	-7.112291	-1.501266
H	-3.708752	-6.821832	0.004605
H	-3.420240	-5.412523	-1.063241
H	-4.930508	-4.884766	0.882868
H	-3.428219	-3.914997	0.892020
H	-3.815928	-5.129678	4.298318
H	-4.649919	-3.992407	3.230492
H	-1.523750	-4.497495	2.061702
H	-0.549146	-1.999713	3.332744
H	1.263653	-4.178896	5.596833
H	0.122274	-2.832569	5.451973
H	-0.403796	-4.490373	5.104535
H	2.444699	-2.578310	2.505238
H	1.877219	-1.749011	3.968086
H	2.888612	-3.196254	4.101322
H	0.315499	-5.632116	2.952195
H	1.634514	-4.913974	2.002722
H	1.931832	-5.464893	3.648061
H	0.545481	-0.218203	2.610883
H	-2.206469	-1.270185	0.971255
H	-3.959368	-0.565075	3.150378
H	-4.406456	-1.421260	1.671350
H	-4.349113	1.820101	3.363099
H	-5.454793	3.849186	2.516643
H	-5.168046	6.157879	2.104845
H	-4.056197	5.272337	1.029839

H	-4.452770	6.962666	0.697641
H	-8.462936	6.516866	-1.664053
H	-5.980328	1.948705	-1.317094
H	-4.902278	-0.091440	-0.442799
H	0.866611	1.836306	1.526380
H	-0.394384	1.475608	0.309770
H	1.667254	0.961867	-0.885562
H	3.170620	-0.469034	0.260224
H	-0.126935	-0.676219	-1.104227
H	1.306130	-1.662735	-0.748578
H	2.913743	-2.432424	-3.479873
H	4.773615	1.567255	-4.716868
H	6.245879	2.112998	1.444164
H	5.118268	0.804794	1.134892
H	3.685779	2.135028	-0.133575
H	4.172499	3.218699	1.182898
H	2.864940	3.248489	-3.794406
H	0.419526	2.898135	-3.951343

conformer_3

F	-3.467394	6.284528	3.422430
C	-3.295379	5.338483	2.427634
F	-2.368164	4.419044	2.897904
F	-4.526025	4.732854	2.224904
O	-2.829963	6.037797	1.256683
C	-2.573806	5.404280	0.061098
C	-2.690578	4.011441	-0.152320
C	-2.406451	3.454013	-1.411336
C	-1.990265	4.258980	-2.487931
C	-1.696415	3.641580	-3.806686
N	-0.607350	3.962523	-4.530316
C	-0.315527	3.288418	-5.786599
C	0.611751	2.103036	-5.500722
C	1.614708	2.404855	-4.362959
C	1.191420	1.793293	-3.023848
C	1.071969	0.397109	-2.860742
N	1.336223	-0.454916	-3.864331
C	1.199984	-1.764136	-3.613216
C	0.788591	-2.294773	-2.375457
O	0.652005	-3.657049	-2.245442
C	-0.075082	-4.201225	-1.127057
C	-1.539320	-3.745014	-1.147790
N	-2.002886	-3.110812	-0.069088
C	-3.320235	-2.499231	0.003008
C	-4.376820	-3.555879	0.329393
O	-4.011948	-4.223351	1.542564
C	-4.934255	-5.256300	1.908008
C	-4.483275	-5.887323	3.227898
O	-3.174636	-6.453614	3.065268
C	-2.523066	-6.721747	4.313744

C	-1.981476	-5.430068	4.925777
N	-1.247394	-4.659170	4.123812
C	-0.550807	-3.448593	4.528635
C	0.888226	-3.789886	5.017174
C	1.624977	-2.519286	5.472937
C	1.738503	-4.474850	3.931508
C	0.855105	-4.732129	6.233393
C	-0.547052	-2.511213	3.307695
N	-0.816711	-1.206774	3.453932
C	-0.601288	-0.235148	2.392155
C	0.902001	0.071562	2.302216
N	1.696462	-0.947406	1.968271
C	3.144796	-0.876098	1.879909
C	3.562678	-0.496637	0.473328
C	3.624055	0.851788	0.081861
C	4.030855	1.206880	-1.216227
C	4.405518	0.221149	-2.151815
C	4.864947	0.570571	-3.522095
C	5.655709	1.676234	-3.857077
C	6.229296	2.685123	-2.883842
N	5.909149	1.758373	-5.218212
C	5.367699	0.766147	-5.828040
S	4.489134	-0.384948	-4.891801
C	4.318370	-1.130554	-1.762481
C	3.899371	-1.485193	-0.467782
O	1.339989	1.189279	2.576877
C	-1.427296	0.982517	2.811527
C	-1.290365	0.960313	4.333943
O	-2.365535	1.633729	4.958413
C	-1.276185	-0.537836	4.662499
O	-0.287041	-2.969115	2.191990
O	-2.235556	-5.135178	6.093349
O	-2.235355	-3.932651	-2.147480
C	0.529295	-1.381502	-1.336724
C	0.661122	-0.006449	-1.575344
N	0.392291	0.847024	-0.585744
C	0.576047	2.146230	-0.845242
N	0.970635	2.649902	-2.019713
C	1.842052	3.930526	-4.301787
C	0.543924	4.716218	-4.028965
O	-2.488576	2.794439	-4.220296
C	-1.889172	5.647325	-2.281581
C	-2.171123	6.207582	-1.023340
H	-3.000900	3.328820	0.625448
H	-2.503742	2.386475	-1.558008
H	0.185967	3.988624	-6.456465
H	-1.214559	2.940629	-6.297815
H	1.159853	1.873199	-6.415482
H	-0.008664	1.241906	-5.254337
H	2.565377	1.944180	-4.629250

H	1.408637	-2.458167	-4.417519
H	0.415975	-3.948954	-0.187171
H	-0.065418	-5.287323	-1.219712
H	-1.406237	-3.038757	0.749319
H	-3.569345	-2.013539	-0.941820
H	-3.314726	-1.743754	0.789486
H	-4.440857	-4.273666	-0.489872
H	-5.343910	-3.064542	0.447046
H	-4.961669	-6.026927	1.125109
H	-5.939094	-4.830931	2.036247
H	-5.188187	-6.678660	3.516890
H	-4.480226	-5.108411	4.002646
H	-1.684139	-7.394620	4.134337
H	-3.212450	-7.206744	5.006877
H	-1.149220	-4.928565	3.154179
H	-1.097745	-2.989903	5.351403
H	1.096676	-2.060277	6.308387
H	2.633968	-2.770073	5.801807
H	1.704308	-1.799574	4.659602
H	1.237230	-5.366055	3.553873
H	1.930214	-3.796065	3.101612
H	2.700322	-4.772992	4.349581
H	0.495297	-5.720484	5.949516
H	1.857806	-4.848553	6.645671
H	0.208097	-4.321523	7.009056
H	-0.963476	-0.598421	1.429937
H	1.250299	-1.840337	1.792310
H	3.560495	-1.850317	2.138884
H	3.537688	-0.145529	2.588679
H	3.350046	1.623752	0.787173
H	4.040330	2.253227	-1.481854
H	6.489834	2.204911	-1.940632
H	7.134769	3.117139	-3.310720
H	5.510178	3.486057	-2.713163
H	5.468424	0.664519	-6.899340
H	4.584668	-1.916105	-2.456260
H	3.846718	-2.529064	-0.191994
H	-2.468146	0.812263	2.533948
H	-1.073226	1.911715	2.364191
H	-0.338398	1.405096	4.631230
H	-2.299268	2.571027	4.740120
H	-0.622504	-0.715997	5.515857
H	-2.288164	-0.874870	4.893950
H	0.239727	-1.703716	-0.352635
H	0.388741	2.855801	-0.049074
H	2.246378	4.247556	-5.264200
H	2.585290	4.173056	-3.540346
H	0.487015	4.911234	-2.960466
H	0.597557	5.680155	-4.536644
H	-1.598316	6.292062	-3.099668

H -2.080210 7.278487 -0.893647

conformer_4

F	-0.140288	13.347796	-3.244025
C	-0.615437	14.114317	-2.238389
F	0.353082	14.300501	-1.315579
F	-0.943202	15.321827	-2.751354
O	-1.772778	13.537751	-1.657840
C	-1.653844	12.303909	-1.084778
C	-2.842140	11.808916	-0.532091
C	-2.874941	10.558671	0.090008
C	-1.713987	9.785896	0.146599
C	-1.750964	8.479697	0.844876
N	-1.215779	7.353948	0.203992
C	-1.311266	7.190095	-1.249434
C	-0.286767	6.194471	-1.790953
C	-0.234953	4.865607	-1.013911
C	-1.356283	3.888886	-1.359522
C	-1.153077	2.520009	-1.174559
N	0.008858	1.990256	-0.710476
C	0.075200	0.646896	-0.575376
C	-0.963976	-0.215576	-0.880667
O	-0.720763	-1.541795	-0.683845
C	-1.753135	-2.452754	-1.048395
C	-1.271799	-3.889903	-0.837467
N	-2.283116	-4.828497	-0.883628
C	-2.034480	-6.226639	-0.566678
C	-2.039497	-6.480906	0.942300
O	-3.372687	-6.300179	1.442193
C	-3.470517	-6.610221	2.834525
C	-3.177806	-5.395679	3.714431
O	-3.201712	-5.796968	5.088391
C	-2.908024	-4.716769	5.973766
C	-1.413844	-4.387437	6.053430
N	-0.602864	-5.502783	5.964717
C	0.828456	-5.355390	5.676829
C	1.674613	-6.528308	6.263281
C	3.170270	-6.314272	5.959149
C	1.262314	-7.907730	5.712978
C	1.508679	-6.554149	7.799334
C	0.899827	-5.249293	4.130584
N	1.642757	-4.236503	3.573058
C	1.645983	-4.025963	2.126810
C	2.629500	-4.971572	1.408355
N	2.461491	-5.015381	0.039904
C	3.219741	-5.946779	-0.757700
C	3.060163	-5.664681	-2.227775
C	2.016547	-6.250812	-2.956144
C	1.863349	-5.982101	-4.319642
C	2.745640	-5.116188	-4.979640

C	2.588306	-4.826321	-6.405186
C	2.381936	-3.619760	-7.062184
C	2.235376	-2.275321	-6.441614
N	2.300851	-3.710344	-8.446194
C	2.442468	-4.963056	-8.815844
S	2.677972	-6.099606	-7.559233
C	3.778387	-4.516637	-4.247047
C	3.932518	-4.785694	-2.883305
O	3.531495	-5.574168	1.988497
C	2.082105	-2.572726	1.953678
C	3.006235	-2.350459	3.148967
O	3.110200	-0.973133	3.465677
C	2.315889	-3.144023	4.259596
O	0.263913	-6.037789	3.419580
O	-0.991957	-3.243848	6.194914
O	-0.094190	-4.192397	-0.649705
C	-2.142720	0.354740	-1.350843
C	-2.264936	1.730389	-1.508276
N	-3.427803	2.223403	-1.962879
C	-3.502591	3.551644	-2.092236
N	-2.523652	4.417015	-1.809406
C	-0.162344	5.140550	0.495197
C	-1.241904	6.108532	0.964706
O	-2.226564	8.458141	1.978686
C	-0.516786	10.280523	-0.381887
C	-0.489690	11.534745	-1.003337
H	-3.752121	12.404248	-0.578382
H	-3.799777	10.192536	0.529754
H	-1.175817	8.143918	-1.764239
H	-2.337692	6.879557	-1.470618
H	0.703613	6.664169	-1.716695
H	-0.467407	6.017444	-2.858051
H	0.704653	4.382910	-1.317183
H	1.022546	0.265682	-0.202959
H	-2.003823	-2.347271	-2.110477
H	-2.635053	-2.288880	-0.418171
H	-3.245713	-4.520851	-0.807164
H	-1.068571	-6.518883	-0.991428
H	-2.827376	-6.802192	-1.054896
H	-1.361566	-5.789236	1.448619
H	-1.719295	-7.511390	1.131663
H	-2.827862	-7.458566	3.100942
H	-4.498296	-6.940541	3.023925
H	-3.937279	-4.624793	3.537543
H	-2.205818	-4.962002	3.460702
H	-3.231574	-5.010455	6.977687
H	-3.467002	-3.820610	5.682853
H	-1.060728	-6.304984	5.537089
H	1.159498	-4.417568	6.132296
H	3.527054	-5.366601	6.376302

H	3.780329	-7.113180	6.396710
H	3.367218	-6.308764	4.882241
H	0.205782	-8.123051	5.902104
H	1.438483	-7.983963	4.635393
H	1.843921	-8.706918	6.187984
H	0.474998	-6.770703	8.090221
H	2.143337	-7.323899	8.253542
H	1.787935	-5.591515	8.242450
H	0.638608	-4.193950	1.736170
H	1.560144	-4.702703	-0.333701
H	2.873629	-6.960044	-0.520377
H	4.276400	-5.899602	-0.468120
H	1.313285	-6.919839	-2.464579
H	1.042430	-6.449290	-4.859578
H	3.210658	-1.894452	-6.124108
H	1.806833	-1.562992	-7.153798
H	1.573248	-2.316687	-5.570919
H	2.412869	-5.266059	-9.854337
H	4.478584	-3.840822	-4.733507
H	4.740303	-4.305943	-2.333833
H	1.216030	-1.901417	2.018641
H	2.584551	-2.361230	1.004460
H	4.006412	-2.754588	2.953694
H	3.549436	-0.534343	2.715523
H	3.030645	-3.527080	4.991635
H	1.568289	-2.541240	4.787154
H	-3.004641	-0.252636	-1.607950
H	-4.438198	3.962548	-2.456750
H	0.818095	5.583122	0.717100
H	-0.224881	4.212920	1.075757
H	-2.242696	5.671279	0.867149
H	-1.085483	6.322447	2.028306
H	0.397864	9.696521	-0.305032
H	0.461249	11.876127	-1.403301

conformer_5

F	1.785164	10.627747	1.181429
C	0.505795	11.144477	1.284198
F	0.025817	11.036649	2.577185
F	0.592666	12.491297	0.998447
O	-0.398651	10.573089	0.310547
C	-0.725717	9.236604	0.279711
C	-0.240356	8.260285	1.177389
C	-0.637156	6.918075	1.055520
C	-1.515769	6.522050	0.036299
C	-1.936299	5.095073	-0.070191
N	-1.872520	4.439718	-1.246577
C	-2.418476	3.094606	-1.382022
C	-1.273218	2.090904	-1.280539
C	-0.193849	2.357793	-2.343503

C	0.978829	1.394664	-2.159765
C	0.882316	0.024244	-2.470657
N	-0.258118	-0.485816	-2.951650
C	-0.279449	-1.796421	-3.212925
C	0.794064	-2.657160	-3.025473
O	0.610888	-3.984322	-3.316790
C	1.747304	-4.871554	-3.449839
C	1.159939	-6.269999	-3.575469
N	-0.153959	-6.316284	-3.392242
C	-0.977563	-7.495100	-3.272971
C	-1.953076	-7.214742	-2.136531
O	-2.349785	-5.837312	-2.209891
C	-3.029567	-5.401894	-1.028236
C	-3.795729	-4.104122	-1.301411
O	-2.892174	-3.037709	-1.628488
C	-3.556225	-1.764697	-1.705028
C	-3.444444	-1.066234	-0.354483
N	-2.364111	-1.379608	0.355832
C	-2.016884	-0.890255	1.676292
C	-2.047211	-2.054287	2.710650
C	-3.480105	-2.601522	2.830451
C	-1.643292	-1.582500	4.117017
C	-1.129000	-3.231212	2.340116
C	-0.633328	-0.254410	1.475074
N	-0.299636	0.903830	2.068396
C	1.002817	1.540218	1.911133
C	2.027863	0.853776	2.821733
N	2.320472	-0.398567	2.487058
C	3.224013	-1.280495	3.189418
C	2.996361	-2.637302	2.563603
C	2.640185	-3.744998	3.349421
C	2.381483	-4.988199	2.746256
C	2.460537	-5.130753	1.349054
C	2.177734	-6.419277	0.672594
C	1.042631	-7.217608	0.864604
C	-0.135758	-6.963169	1.784232
N	1.069370	-8.369332	0.040375
C	2.137380	-8.373674	-0.674450
S	3.248998	-7.067439	-0.491616
C	2.845932	-4.026936	0.573208
C	3.114105	-2.788567	1.173569
O	2.526028	1.419082	3.791334
C	0.779452	3.017784	2.242390
C	-0.319268	2.955747	3.297083
O	-1.071580	4.168278	3.331725
C	-1.176744	1.777062	2.833968
O	0.160251	-0.827037	0.724385
O	-4.307285	-0.281579	0.027852
O	1.863162	-7.251950	-3.797206
C	1.980284	-2.107160	-2.546284

C	2.021222	-0.748655	-2.257999
N	3.148666	-0.214048	-1.789749
C	3.180784	1.097848	-1.542285
N	2.131386	1.905554	-1.716371
C	0.242007	3.834093	-2.258207
C	-0.968639	4.764097	-2.350843
O	-2.297970	4.530354	0.961092
C	-2.011767	7.490806	-0.850580
C	-1.615120	8.832657	-0.729872
H	0.439113	8.504672	1.979135
H	-0.263121	6.182661	1.753240
H	-2.896054	2.988842	-2.356450
H	-3.167317	2.865271	-0.623840
H	-1.687520	1.091204	-1.384255
H	-0.825606	2.185595	-0.296521
H	-0.630059	2.199467	-3.330203
H	-1.193388	-2.225212	-3.598419
H	2.378323	-4.857468	-2.563995
H	2.329634	-4.622149	-4.337065
H	-0.604876	-5.431344	-3.186572
H	-1.528957	-7.636837	-4.202331
H	-0.391909	-8.386823	-3.047314
H	-1.438674	-7.390648	-1.192779
H	-2.815396	-7.877587	-2.211537
H	-2.300119	-5.235121	-0.225086
H	-3.750203	-6.166850	-0.709417
H	-4.369050	-3.847711	-0.400905
H	-4.489943	-4.270523	-2.136001
H	-4.604490	-1.873606	-1.985208
H	-3.058767	-1.146420	-2.450822
H	-1.672209	-1.959069	-0.099438
H	-2.745965	-0.144755	1.984951
H	-4.172280	-1.790112	3.056114
H	-3.536629	-3.341289	3.629119
H	-3.787788	-3.082015	1.902730
H	-0.623968	-1.196018	4.122028
H	-2.326845	-0.805104	4.456082
H	-1.692493	-2.413708	4.820578
H	-0.084191	-2.926514	2.361384
H	-1.260359	-4.034830	3.064111
H	-1.364093	-3.620056	1.350479
H	1.353110	1.471164	0.883736
H	1.780159	-0.784806	1.715429
H	2.996344	-1.299519	4.255615
H	4.252345	-0.959428	3.023049
H	2.555218	-3.642161	4.421447
H	2.114592	-5.832579	3.365164
H	-0.074643	-5.995525	2.272892
H	-1.055549	-6.996646	1.201851
H	-0.168839	-7.744303	2.543272

H	2.320926	-9.173793	-1.377339
H	2.938650	-4.129582	-0.494844
H	3.406111	-1.949606	0.557924
H	0.391940	3.519775	1.356065
H	1.673806	3.534300	2.590749
H	0.111536	2.740246	4.274929
H	-1.580120	4.243969	2.501086
H	-1.602111	1.280766	3.702941
H	-1.972503	2.137997	2.182722
H	2.868536	-2.693205	-2.381715
H	4.100916	1.532891	-1.176021
H	0.928087	4.062763	-3.074249
H	0.729797	4.040317	-1.304141
H	-0.598847	5.786354	-2.343877
H	-1.475555	4.603240	-3.302729
H	-2.704759	7.199712	-1.626383
H	-2.001228	9.568101	-1.420371

conformer_6

F	0.407378	7.992557	2.196007
C	0.226381	6.706891	2.673950
F	1.295897	6.298934	3.453259
F	-0.879741	6.736627	3.499951
O	-0.084401	5.767219	1.620363
C	0.869652	5.299436	0.747153
C	2.100717	5.934744	0.478548
C	3.012857	5.368015	-0.428435
C	2.720814	4.160026	-1.079713
C	3.730485	3.551464	-2.001853
N	3.393056	3.102737	-3.230215
C	2.151197	3.389197	-3.955207
C	1.392158	2.083798	-4.199320
C	2.282890	1.084508	-4.948885
C	1.555319	-0.217279	-5.271152
C	1.085433	-1.144416	-4.312502
N	1.270852	-0.948116	-2.999109
C	0.780597	-1.862849	-2.152490
C	0.088327	-3.010584	-2.554035
O	-0.444901	-3.956592	-1.707976
C	-0.389266	-3.789805	-0.272967
C	0.969234	-4.177036	0.308167
N	1.358519	-3.512487	1.391578
C	2.625074	-3.704920	2.071925
C	3.701050	-2.879193	1.370890
O	3.155441	-1.591765	1.072678
C	4.143855	-0.658769	0.631814
C	3.444589	0.638161	0.222045
O	2.390600	0.944458	1.142947
C	2.819824	1.705584	2.284790
C	1.657254	1.669110	3.269530

N	0.661182	0.872415	2.895447
C	-0.580298	0.565212	3.578347
C	-1.762166	1.382211	2.969938
C	-1.911385	1.182059	1.451790
C	-1.562890	2.885528	3.229766
C	-3.108228	1.022550	3.618683
C	-0.684675	-0.958522	3.379145
N	-1.166553	-1.768389	4.337101
C	-1.149544	-3.224148	4.199144
C	-2.365272	-3.726497	3.410278
N	-3.372868	-2.864964	3.252611
C	-4.588173	-3.109671	2.495164
C	-4.361392	-2.654834	1.069505
C	-4.586723	-1.318789	0.705289
C	-4.323415	-0.887053	-0.605407
C	-3.818345	-1.785041	-1.562755
C	-3.481006	-1.344152	-2.937270
C	-2.694778	-0.232437	-3.260716
C	-1.988872	0.709204	-2.307225
N	-2.555860	-0.077359	-4.662150
C	-3.182916	-1.020624	-5.270321
S	-4.013532	-2.197351	-4.319402
C	-3.639810	-3.130836	-1.206856
C	-3.907511	-3.562904	0.101986
O	-2.377625	-4.862968	2.938460
C	-1.141402	-3.773966	5.626012
C	-1.890990	-2.703708	6.411612
O	-1.520183	-2.725707	7.792647
C	-1.447823	-1.410541	5.721640
O	-0.262654	-1.427146	2.319990
O	1.658716	2.332900	4.305672
O	1.659193	-5.041409	-0.233272
C	-0.081057	-3.200190	-3.917617
C	0.419239	-2.261615	-4.810047
N	0.245741	-2.447981	-6.118970
C	0.724543	-1.535660	-6.969362
N	1.369803	-0.434302	-6.575116
C	3.633622	0.894875	-4.241065
C	4.296499	2.256020	-4.012066
O	4.888250	3.482144	-1.591457
C	1.500029	3.522308	-0.803163
C	0.578845	4.098900	0.082928
H	2.379320	6.864191	0.950598
H	3.954501	5.861897	-0.621733
H	2.401304	3.829668	-4.920716
H	1.496773	4.095099	-3.448192
H	0.495413	2.286814	-4.784926
H	1.103507	1.673656	-3.237870
H	2.511531	1.547486	-5.909751
H	0.948192	-1.666760	-1.103919

H	-1.125304	-4.463050	0.165088
H	-0.664918	-2.774124	0.010640
H	0.767925	-2.747894	1.723617
H	2.909766	-4.757089	2.099419
H	2.516614	-3.340540	3.093740
H	3.990945	-3.370399	0.441596
H	4.569687	-2.795791	2.024402
H	4.698395	-1.058909	-0.227472
H	4.842799	-0.454418	1.453752
H	2.988000	0.490082	-0.765368
H	4.172964	1.456356	0.163418
H	3.030093	2.735519	1.994363
H	3.698050	1.262216	2.753436
H	0.840718	0.336377	2.050547
H	-0.474180	0.817253	4.631933
H	-2.162007	0.147012	1.226576
H	-2.712115	1.815235	1.069536
H	-0.992594	1.440921	0.927349
H	-1.433584	3.066559	4.296943
H	-0.685432	3.253446	2.702485
H	-2.426780	3.451101	2.880384
H	-3.068421	1.223933	4.688599
H	-3.907676	1.623009	3.184395
H	-3.351432	-0.026338	3.457686
H	-0.241234	-3.572134	3.707897
H	-3.245547	-1.946913	3.650284
H	-5.394775	-2.524694	2.937122
H	-4.855761	-4.166329	2.519026
H	-4.949847	-0.613068	1.438533
H	-4.495393	0.147865	-0.865064
H	-1.969707	0.317497	-1.294007
H	-0.961589	0.831464	-2.638659
H	-2.484582	1.679469	-2.317522
H	-3.182356	-1.068502	-6.350401
H	-3.267883	-3.838340	-1.934485
H	-3.738857	-4.595756	0.372036
H	-0.110276	-3.821309	5.978045
H	-1.613112	-4.753764	5.705658
H	-2.966496	-2.838589	6.292032
H	-2.000300	-2.009732	8.235424
H	-2.234963	-0.664536	5.806691
H	-0.532424	-1.047570	6.190555
H	-0.607268	-4.068558	-4.281691
H	0.583205	-1.691689	-8.030941
H	4.283069	0.275560	-4.859798
H	3.505697	0.417346	-3.271232
H	5.252131	2.073726	-3.522471
H	4.499328	2.726989	-4.974417
H	1.267981	2.572177	-1.254922
H	-0.360016	3.601684	0.272275

conformer_7

F	2.419333	-0.277596	7.136049
C	2.855743	-0.330111	5.827557
F	3.708767	-1.415492	5.730709
F	1.731585	-0.509719	5.041161
O	3.523912	0.927056	5.569150
C	4.076014	1.245523	4.348674
C	4.678872	2.510170	4.240240
C	5.266306	2.932094	3.036168
C	5.251686	2.094252	1.910992
C	5.875767	2.513125	0.624315
N	5.301103	3.465317	-0.139930
C	4.025941	4.133796	0.129762
C	2.934042	3.430506	-0.673561
C	3.302375	3.390716	-2.169295
C	2.259471	2.653814	-3.003504
C	1.929869	1.288248	-2.852251
N	2.568950	0.514305	-1.964346
C	2.159786	-0.751615	-1.837975
C	1.126277	-1.320987	-2.571236
O	0.796401	-2.628754	-2.315059
C	-0.337520	-3.230222	-2.981927
C	-0.588366	-4.557064	-2.275269
N	0.130363	-4.724392	-1.172526
C	0.131386	-5.865374	-0.286083
C	1.411495	-5.766053	0.543169
O	1.687425	-4.378833	0.799908
C	1.139374	-3.905093	2.038078
C	0.925418	-2.386804	1.948619
O	0.177264	-2.049488	0.767239
C	-1.247098	-2.166176	0.924525
C	-1.817370	-0.857762	1.458909
N	-1.105505	0.226196	1.166478
C	-1.452227	1.606664	1.428910
C	-0.651399	2.174074	2.640477
C	-1.085134	1.465443	3.934733
C	-0.939552	3.670430	2.845780
C	0.874335	2.009853	2.515750
C	-1.112070	2.254427	0.080024
N	-1.925664	3.133594	-0.522046
C	-3.206122	3.656808	-0.050502
C	-4.358304	2.781748	-0.560137
N	-4.031264	1.841005	-1.449548
C	-4.957774	0.972091	-2.153786
C	-4.762455	-0.461758	-1.712290
C	-4.129439	-1.385572	-2.558014
C	-3.986161	-2.725010	-2.162012
C	-4.467481	-3.155600	-0.913953
C	-4.310428	-4.563018	-0.477612

C	-4.685324	-5.689546	-1.219017
C	-5.375964	-5.725724	-2.568589
N	-4.375700	-6.891990	-0.535370
C	-3.847362	-6.624368	0.605450
S	-3.632517	-4.968549	1.038291
C	-5.079587	-2.223898	-0.060275
C	-5.226751	-0.884325	-0.457673
O	-5.507042	2.959356	-0.157035
C	-3.283812	5.066511	-0.637420
C	-2.572980	4.917617	-1.981117
O	-2.020567	6.164041	-2.411775
C	-1.477398	3.889997	-1.681428
O	-0.095926	1.867829	-0.491064
O	-2.852933	-0.834630	2.121768
O	-1.394956	-5.381270	-2.702528
C	0.492877	-0.516012	-3.516629
C	0.899501	0.806394	-3.657010
N	0.290728	1.587196	-4.551324
C	0.678610	2.861200	-4.666520
N	1.631811	3.409438	-3.907516
C	4.739968	2.902528	-2.426226
C	5.717519	3.663118	-1.526250
O	6.891597	1.917807	0.266583
C	4.655164	0.829251	2.009862
C	4.074009	0.403390	3.215150
H	4.692598	3.168248	5.097088
H	5.730842	3.905548	2.971917
H	4.083798	5.172974	-0.194748
H	3.739165	4.147639	1.178605
H	1.990784	3.962251	-0.546440
H	2.829375	2.429152	-0.262194
H	3.282312	4.429297	-2.501882
H	2.656798	-1.377064	-1.109690
H	-0.120833	-3.400275	-4.036892
H	-1.221272	-2.603629	-2.870038
H	0.765628	-3.967801	-0.934274
H	0.114712	-6.802812	-0.842490
H	-0.739044	-5.807662	0.366951
H	2.232939	-6.158408	-0.056218
H	1.331295	-6.351381	1.460027
H	1.838988	-4.127089	2.854619
H	0.180983	-4.395567	2.252095
H	1.908083	-1.903608	1.869130
H	0.427436	-2.021910	2.856578
H	-1.525532	-2.985144	1.584864
H	-1.676730	-2.346327	-0.060183
H	-0.298934	0.106334	0.562379
H	-2.518405	1.668839	1.636744
H	-0.805112	0.413070	3.906729
H	-0.601563	1.922259	4.798407

H	-2.165701	1.541409	4.057307
H	-0.630347	4.252251	1.977494
H	-2.004315	3.822525	3.019081
H	-0.393308	4.041014	3.713429
H	1.260520	2.605814	1.691229
H	1.355480	2.355087	3.430504
H	1.146630	0.965940	2.361253
H	-3.265613	3.739780	1.032163
H	-3.049260	1.765228	-1.676636
H	-4.761542	1.054577	-3.222799
H	-5.991483	1.261063	-1.965037
H	-3.761355	-1.072612	-3.524721
H	-3.504971	-3.426760	-2.828162
H	-5.692676	-4.737897	-2.898216
H	-4.693900	-6.148958	-3.305894
H	-6.257872	-6.361606	-2.493416
H	-3.549483	-7.423165	1.270322
H	-5.443097	-2.534950	0.909111
H	-5.705236	-0.175448	0.203364
H	-2.710882	5.741624	-0.000824
H	-4.306977	5.427136	-0.746327
H	-3.259956	4.518315	-2.728021
H	-2.758955	6.755297	-2.619218
H	-1.329058	3.238611	-2.542683
H	-0.547174	4.405945	-1.438771
H	-0.307773	-0.876945	-4.141657
H	0.185645	3.488955	-5.397619
H	4.998926	3.074697	-3.470958
H	4.838245	1.840263	-2.209033
H	6.731032	3.316119	-1.724402
H	5.684113	4.723574	-1.777867
H	4.646237	0.179350	1.146408
H	3.633117	-0.580734	3.228299

conformer_8

F	0.218153	7.245498	-5.838008
C	0.887952	8.136186	-5.104771
F	2.142905	7.733926	-4.897193
F	0.937299	9.273251	-5.795809
O	0.216549	8.418566	-3.878121
C	0.017486	7.420347	-2.945696
C	0.428965	6.088557	-3.094506
C	0.177939	5.157900	-2.089495
C	-0.476109	5.543089	-0.910946
C	-0.790170	4.540968	0.179886
N	0.172226	3.675082	0.606007
C	1.616649	3.822260	0.330638
C	2.093050	2.511923	-0.336053
C	1.730083	1.253720	0.494087
C	2.151220	-0.068177	-0.176338

C	1.598559	-0.503083	-1.420768
N	0.655885	0.204807	-2.108263
C	0.218849	-0.294522	-3.290312
C	0.652033	-1.496022	-3.846349
O	0.095221	-1.860045	-5.058056
C	0.390801	-3.136572	-5.661064
C	-0.438077	-4.289961	-5.050883
N	-1.323016	-3.991008	-4.090155
C	-2.197727	-4.928553	-3.373292
C	-1.469033	-5.952490	-2.474467
O	-0.569654	-5.289744	-1.586149
C	-0.158634	-6.080347	-0.471082
C	1.047685	-5.433453	0.246543
O	0.961792	-4.013910	0.438227
C	-0.192474	-3.484190	1.109921
C	-0.146113	-3.679518	2.637360
N	1.038941	-3.937278	3.211832
C	1.260062	-3.963241	4.672599
C	2.551019	-4.757430	5.114512
C	3.844778	-4.025002	4.690262
C	2.577847	-6.153626	4.439957
C	2.608137	-4.988382	6.644740
C	0.984111	-2.593015	5.388575
N	1.062133	-1.423940	4.692509
C	0.583706	-0.129588	5.240517
C	-0.835144	0.276331	4.742772
N	-1.704301	-0.691241	4.412210
C	-3.070066	-0.490287	3.919396
C	-3.136707	-0.329471	2.403151
C	-3.116647	-1.458322	1.581490
C	-3.193935	-1.320643	0.198502
C	-3.327217	-0.054474	-0.380183
C	-3.423878	0.097623	-1.866639
C	-2.999769	1.120061	-2.732370
C	-2.239757	2.386688	-2.402539
N	-3.279783	0.946724	-4.012158
C	-3.897014	-0.181714	-4.231686
S	-4.197049	-1.141361	-2.830977
C	-3.383283	1.070970	0.447992
C	-3.292864	0.935356	1.832100
O	-1.172143	1.461006	4.748976
C	1.694247	0.890275	4.859662
C	2.853589	0.061943	4.323131
O	3.670727	-0.363712	5.401587
C	2.122658	-1.141118	3.715819
O	0.521960	-2.632889	6.534478
O	-1.177539	-3.551720	3.300709
O	-0.283572	-5.440524	-5.461455
C	1.613441	-2.234744	-3.144521
C	2.114234	-1.741428	-1.918064

N	3.077079	-2.449152	-1.261876
C	3.512001	-1.930601	-0.087407
N	3.098050	-0.778783	0.490173
C	0.254249	1.276002	0.965723
C	-0.142278	2.629525	1.599142
O	-1.931297	4.539835	0.653223
C	-0.907228	6.868662	-0.776883
C	-0.652236	7.795784	-1.783830
H	0.938400	5.748329	-3.983375
H	0.482561	4.132831	-2.246294
H	2.118292	3.941562	1.293156
H	1.881768	4.716276	-0.235102
H	3.177384	2.581902	-0.434827
H	1.687612	2.457122	-1.344483
H	2.333197	1.318125	1.403294
H	-0.519736	0.297282	-3.811095
H	1.455107	-3.369882	-5.634147
H	0.127097	-3.064723	-6.715984
H	-1.361539	-3.019304	-3.811338
H	-2.837872	-5.456883	-4.083363
H	-2.873199	-4.341978	-2.748349
H	-0.907799	-6.664297	-3.081955
H	-2.219114	-6.525087	-1.924147
H	0.132470	-7.081208	-0.797489
H	-0.990910	-6.206131	0.223627
H	1.950976	-5.625310	-0.333510
H	1.205220	-5.926691	1.206522
H	-1.123455	-3.881504	0.705344
H	-0.215016	-2.409555	0.926069
H	1.850362	-4.025019	2.618024
H	0.435084	-4.584917	5.029335
H	3.920126	-3.037617	5.144804
H	4.733583	-4.574573	5.004508
H	3.919248	-3.911420	3.608345
H	1.676102	-6.725451	4.663820
H	2.667174	-6.089343	3.355140
H	3.425091	-6.750542	4.781452
H	1.721597	-5.511191	7.006360
H	3.471906	-5.591178	6.929597
H	2.693725	-4.053256	7.199150
H	0.440181	-0.195355	6.320476
H	-1.354339	-1.640866	4.371602
H	-3.550878	0.364994	4.401988
H	-3.670850	-1.356962	4.202666
H	-3.037957	-2.446257	2.011117
H	-3.154570	-2.207100	-0.418287
H	-2.906945	3.239196	-2.274791
H	-1.668871	2.283196	-1.481590
H	-1.517302	2.657201	-3.173660
H	-4.208925	-0.511568	-5.213381

H	-3.503415	2.058257	0.025099
H	-3.337453	1.817241	2.456710
H	1.967802	1.558226	5.677513
H	1.375742	1.523823	4.031435
H	3.478508	0.560832	3.578058
H	4.008731	0.422723	5.854030
H	1.661782	-0.813219	2.784285
H	2.783065	-1.963130	3.449690
H	2.001780	-3.173986	-3.502596
H	4.270536	-2.492425	0.443736
H	0.091909	0.510366	1.724634
H	-0.431764	1.055602	0.148255
H	-1.180462	2.637812	1.934383
H	0.457382	2.826069	2.488305
H	-1.437517	7.190925	0.110414
H	-0.981795	8.818196	-1.663873

conformer_9

F	1.897399	10.939694	-7.267178
C	0.916040	11.060151	-8.196736
F	-0.005901	11.958866	-7.767858
F	1.487971	11.581821	-9.309134
O	0.352048	9.858647	-8.498179
C	-0.298320	9.111016	-7.537664
C	-0.851661	7.884248	-7.958315
C	-1.534563	7.049294	-7.052212
C	-1.660598	7.421914	-5.695317
C	-2.417985	6.562578	-4.719714
N	-2.060727	5.259646	-4.577576
C	-2.864366	4.320985	-3.781550
C	-2.107217	3.952940	-2.492774
C	-0.711189	3.376941	-2.811095
C	0.096789	3.074987	-1.548067
C	0.520464	1.764129	-1.206595
N	0.250660	0.675749	-1.968167
C	0.696228	-0.530030	-1.563946
C	1.410616	-0.739952	-0.367648
O	1.784351	-2.027917	-0.040461
C	2.199731	-2.274813	1.305183
C	2.539850	-3.756720	1.490002
N	2.820189	-4.437092	0.376426
C	3.128292	-5.855212	0.261771
C	2.080634	-6.518174	-0.637001
O	1.985245	-5.762795	-1.842819
C	0.702427	-5.805389	-2.455949
C	-0.173486	-4.652559	-1.935174
O	-0.572633	-4.928314	-0.604332
C	-1.289393	-3.866862	0.019020
C	-1.561431	-4.242095	1.477904
N	-1.023364	-5.391041	1.889025

C	-1.055315	-6.014799	3.208290
C	-2.240547	-7.053060	3.289972
C	-2.296152	-7.751157	4.666091
C	-2.118873	-8.154307	2.209816
C	-3.602686	-6.346762	3.104694
C	0.372392	-6.580679	3.415730
N	1.003038	-6.501255	4.608848
C	0.489883	-5.953324	5.873770
C	0.676017	-4.435509	6.056706
N	1.422250	-3.744029	5.184792
C	1.786709	-2.339094	5.351723
C	0.908659	-1.347228	4.600043
C	-0.395743	-1.678152	4.174988
C	-1.166144	-0.748708	3.452922
C	-0.656923	0.529200	3.142864
C	-1.436713	1.462936	2.334350
C	-2.183425	1.224858	1.199665
C	-2.380268	-0.076330	0.485403
N	-2.783607	2.374884	0.678606
C	-2.505025	3.458889	1.403844
S	-1.476601	3.150972	2.790253
C	0.632441	0.871238	3.606033
C	1.409260	-0.057940	4.325236
O	0.145266	-3.898332	7.025101
C	1.326518	-6.680766	6.936873
C	2.682652	-6.861998	6.272752
O	3.371718	-7.953035	6.842561
C	2.324683	-7.107316	4.806435
O	0.921623	-7.122570	2.451284
O	-2.239576	-3.516487	2.199428
O	2.560240	-4.257146	2.615972
C	1.701164	0.402383	0.416970
C	1.266617	1.678692	0.004435
N	1.560649	2.767090	0.741744
C	1.110740	3.939098	0.310347
N	0.396970	4.150474	-0.787256
C	0.059737	4.289228	-3.790625
C	-0.793427	4.654196	-5.021224
O	-3.346146	7.072435	-4.090808
C	-1.132121	8.660034	-5.273807
C	-0.449563	9.494732	-6.180976
H	-0.755606	7.583109	-8.991650
H	-1.962563	6.120728	-7.402734
H	-3.057616	3.424950	-4.372821
H	-3.847382	4.723276	-3.529927
H	-2.683720	3.228107	-1.918257
H	-2.012158	4.839778	-1.864436
H	-0.884440	2.439521	-3.339000
H	0.453726	-1.362653	-2.207440
H	1.397980	-2.006458	1.990944

H	3.088302	-1.696773	1.560138
H	2.704299	-3.937716	-0.494941
H	3.165158	-6.348136	1.234620
H	4.118368	-5.958151	-0.182590
H	1.132071	-6.563554	-0.104640
H	2.357330	-7.547653	-0.866541
H	0.217510	-6.775775	-2.335345
H	0.854747	-5.666595	-3.526469
H	-1.060247	-4.544701	-2.561324
H	0.382549	-3.716116	-1.986877
H	-2.234216	-3.686172	-0.495014
H	-0.709625	-2.944557	-0.001694
H	-0.452416	-5.871553	1.203549
H	-1.225621	-5.226086	3.941728
H	-2.510374	-7.042656	5.466163
H	-3.089380	-8.499374	4.696953
H	-1.368453	-8.271089	4.907032
H	-2.102767	-7.737263	1.202489
H	-1.212903	-8.748634	2.331502
H	-2.960359	-8.846810	2.252365
H	-3.728499	-5.957336	2.094774
H	-4.436416	-7.027293	3.280675
H	-3.714560	-5.508011	3.793281
H	-0.561413	-6.180177	6.027423
H	1.813457	-4.209644	4.368926
H	2.812479	-2.228944	4.998413
H	1.801207	-2.060521	6.407441
H	-0.822551	-2.647200	4.386196
H	-2.157845	-1.033244	3.132438
H	-2.547222	0.076716	-0.580986
H	-1.507149	-0.718892	0.588550
H	-3.238488	-0.617301	0.883642
H	-2.893229	4.427873	1.124732
H	1.045202	1.845718	3.384922
H	2.398625	0.222998	4.656817
H	0.874519	-7.652664	7.141138
H	1.393681	-6.153630	7.890625
H	3.273177	-5.948814	6.372087
H	4.224868	-8.023838	6.437732
H	3.066762	-6.678055	4.130404
H	2.253132	-8.175673	4.592050
H	2.253517	0.339906	1.339458
H	1.345574	4.803894	0.913516
H	0.981828	3.798900	-4.104458
H	0.358751	5.206988	-3.281682
H	-0.199815	5.301616	-5.663991
H	-1.009115	3.762340	-5.611138
H	-1.251446	8.970946	-4.245094
H	-0.056036	10.428738	-5.808693

conformer_10

F	1.695302	-3.866814	1.050193
C	1.053751	-3.274128	2.123894
F	0.165503	-4.199729	2.637480
F	1.964666	-3.006505	3.129073
O	0.272282	-2.127759	1.747100
C	0.813679	-1.009918	1.155967
C	2.193002	-0.817134	0.921067
C	2.659079	0.376487	0.345341
C	1.771842	1.400712	-0.030208
C	2.303944	2.651747	-0.629721
N	1.794262	3.177519	-1.760023
C	0.739407	2.538233	-2.550012
C	0.940481	2.812256	-4.045705
C	2.435740	2.711124	-4.389015
C	3.013998	1.354051	-3.967047
C	2.540937	0.152372	-4.535596
N	1.615408	0.153770	-5.507068
C	1.205431	-1.033871	-5.970393
C	1.678266	-2.273725	-5.499553
O	1.158716	-3.424132	-6.044242
C	1.491729	-4.710322	-5.486626
C	0.805855	-4.948297	-4.136985
N	-0.267164	-4.200470	-3.871999
C	-1.100336	-4.334199	-2.689886
C	-0.468377	-3.603935	-1.494828
O	-1.251756	-3.737188	-0.295692
C	-2.474676	-2.983788	-0.323973
C	-3.227916	-3.107307	1.007802
O	-2.575411	-2.357765	2.040925
C	-3.281755	-2.425514	3.288606
C	-2.782565	-1.378750	4.282896
N	-1.473995	-1.126488	4.290003
C	-0.814856	-0.203047	5.202438
C	-0.332350	-0.941163	6.485828
C	-1.539626	-1.411648	7.316260
C	0.471300	0.020282	7.377724
C	0.528057	-2.188544	6.208866
C	0.321361	0.459660	4.400732
N	0.276590	1.769518	4.102847
C	-0.540684	2.749568	4.819896
C	-1.981732	2.812564	4.304909
N	-2.257186	2.118434	3.199685
C	-3.569541	2.065106	2.575447
C	-3.394342	1.982098	1.074447
C	-3.672634	0.792658	0.378261
C	-3.486803	0.717339	-1.013345
C	-3.011675	1.827467	-1.738301
C	-2.787526	1.753346	-3.202612
C	-2.145734	0.699654	-3.859137

C	-1.543076	-0.513104	-3.182820
N	-2.086133	0.884401	-5.231792
C	-2.626245	2.007793	-5.545145
S	-3.279629	2.985209	-4.280394
C	-2.761684	3.026134	-1.042193
C	-2.943872	3.099493	0.349971
O	-2.829365	3.470353	4.906707
C	0.155895	4.101156	4.629936
C	1.606744	3.702552	4.383467
O	2.203242	3.356217	5.620684
C	1.421493	2.456757	3.520707
O	1.246180	-0.240432	3.997885
O	-3.575837	-0.809903	5.032340
O	1.231225	-5.796625	-3.352236
C	2.661177	-2.251440	-4.490149
C	3.116350	-1.017321	-3.999916
N	4.064187	-1.005227	-3.060596
C	4.469056	0.195654	-2.628502
N	3.979554	1.371596	-3.039938
C	3.095163	3.937453	-3.718950
C	2.403440	4.341164	-2.403338
O	3.253963	3.186698	-0.057377
C	0.396607	1.210173	0.203643
C	-0.071712	0.019516	0.786069
H	2.934457	-1.555668	1.188429
H	3.719972	0.516229	0.194320
H	-0.231164	2.929259	-2.251607
H	0.744046	1.456506	-2.417556
H	0.578462	3.810660	-4.295133
H	0.345431	2.107605	-4.621343
H	2.563412	2.805801	-5.468259
H	0.454167	-1.040853	-6.750320
H	2.570282	-4.846400	-5.405669
H	1.121106	-5.470254	-6.174710
H	-0.536144	-3.519645	-4.569265
H	-1.233190	-5.388413	-2.441750
H	-2.072582	-3.908639	-2.932479
H	-0.320513	-2.550562	-1.732681
H	0.508984	-4.047578	-1.309843
H	-3.135068	-3.379194	-1.105143
H	-2.265837	-1.925856	-0.526392
H	-3.303424	-4.165541	1.293922
H	-4.238778	-2.702199	0.862417
H	-3.152406	-3.415706	3.727142
H	-4.346603	-2.252693	3.124020
H	-0.899166	-1.567685	3.584444
H	-1.536968	0.541022	5.526165
H	-2.078460	-2.203497	6.797245
H	-1.205449	-1.806774	8.276105
H	-2.218750	-0.579347	7.503763

H	1.371695	0.361914	6.866746
H	-0.138071	0.885180	7.640328
H	0.772531	-0.484045	8.296533
H	1.484647	-1.915376	5.767352
H	0.733183	-2.707670	7.145541
H	0.009588	-2.878343	5.543141
H	-0.537997	2.525085	5.887299
H	-1.491082	1.620371	2.765833
H	-4.154418	2.955538	2.810862
H	-4.105213	1.190042	2.944495
H	-4.033299	-0.072145	0.916061
H	-3.724706	-0.203368	-1.525488
H	-2.303807	-1.285240	-3.075362
H	-0.730714	-0.901833	-3.795984
H	-1.142979	-0.244240	-2.205467
H	-2.665325	2.322680	-6.578357
H	-2.413828	3.902316	-1.572503
H	-2.732325	4.022858	0.871200
H	0.036699	4.752679	5.496291
H	-0.230587	4.597390	3.737683
H	2.174768	4.482359	3.872349
H	3.089117	3.019059	5.441574
H	1.175005	2.758092	2.502269
H	2.338418	1.865309	3.503757
H	3.087744	-3.152140	-4.077568
H	5.251334	0.229430	-1.880555
H	3.005599	4.786966	-4.397666
H	4.161452	3.779060	-3.555610
H	3.127443	4.854377	-1.769572
H	1.610470	5.058319	-2.620880
H	-0.305499	1.990227	-0.048064
H	-1.130387	-0.102570	0.962286

conformer_11

F	8.766944	14.597183	-4.183485
C	8.043668	13.551242	-4.643848
F	7.616399	13.854140	-5.888731
F	8.854606	12.472237	-4.693675
O	6.952547	13.332351	-3.765960
C	6.097789	12.306239	-4.052080
C	6.178320	11.439319	-5.145108
C	5.225511	10.427259	-5.312227
C	4.198716	10.269577	-4.377347
C	3.180679	9.215728	-4.596340
N	2.860431	8.352802	-3.539575
C	3.872101	7.934466	-2.564820
C	3.251046	7.424878	-1.265303
C	2.119761	6.400262	-1.471841
C	2.600947	4.986053	-1.786343
C	1.794654	3.896974	-1.449409

N	0.590092	4.018473	-0.833546
C	-0.091302	2.882663	-0.561401
C	0.359946	1.611127	-0.874991
O	-0.463221	0.582432	-0.524350
C	-0.046401	-0.743176	-0.828760
C	1.024335	-1.306475	0.117677
N	1.709677	-2.386575	-0.391207
C	2.754798	-3.069172	0.357583
C	2.230482	-4.287245	1.120199
O	1.893930	-5.313899	0.177089
C	1.506867	-6.525063	0.835077
C	1.075239	-7.562733	-0.204574
O	-0.230873	-7.320170	-0.746104
C	-0.287782	-6.209397	-1.639927
C	-0.838006	-4.940522	-0.979148
N	-1.736914	-5.201211	0.029054
C	-2.289774	-4.180491	0.926324
C	-3.846003	-4.107933	0.806926
C	-4.518097	-5.453715	1.140023
C	-4.231027	-3.720925	-0.639102
C	-4.428505	-3.031478	1.741110
C	-1.783960	-4.564319	2.346900
N	-1.590150	-3.586029	3.302056
C	-1.072424	-3.934082	4.643248
C	-2.082586	-4.602524	5.610981
N	-2.897371	-5.554505	5.046861
C	-3.753500	-6.389940	5.852012
C	-4.776702	-7.078905	4.989374
C	-6.028006	-6.489328	4.765911
C	-6.960208	-7.100570	3.922657
C	-6.655130	-8.307613	3.279984
C	-7.622985	-8.952679	2.393601
C	-8.211954	-10.208605	2.466287
C	-8.011763	-11.230833	3.529382
N	-9.080232	-10.511237	1.424888
C	-9.140188	-9.497410	0.591364
S	-8.179428	-8.137373	0.984535
C	-5.403175	-8.895600	3.502400
C	-4.470448	-8.285619	4.346072
O	-2.077747	-4.388852	6.823559
C	-0.594615	-2.601871	5.242619
C	-0.257216	-1.763643	4.025149
O	1.040203	-2.131304	3.559238
C	-1.341402	-2.171866	3.025584
O	-1.630228	-5.758474	2.643439
O	-0.537363	-3.809758	-1.356463
O	1.254843	-0.832463	1.230067
C	1.595444	1.518838	-1.508250
C	2.338851	2.654115	-1.809879
N	3.521752	2.502677	-2.426835

C	4.198583	3.621160	-2.703119
N	3.797027	4.863941	-2.417758
C	1.129347	6.912782	-2.527468
C	1.821955	7.362897	-3.808489
O	2.641263	9.172490	-5.700673
C	4.096968	11.147609	-3.295302
C	5.050769	12.155569	-3.133470
H	6.961096	11.518927	-5.894458
H	5.283528	9.764532	-6.173491
H	4.554592	8.753198	-2.326724
H	4.488130	7.170052	-3.049667
H	2.826106	8.290724	-0.739134
H	4.033236	7.018163	-0.613146
H	1.592332	6.345835	-0.509299
H	-1.047860	3.025783	-0.064970
H	0.258253	-0.836256	-1.877639
H	-0.934116	-1.370959	-0.702586
H	1.223879	-2.942062	-1.097642
H	3.217003	-2.362845	1.054566
H	3.503619	-3.379928	-0.378307
H	1.341340	-4.032775	1.705285
H	3.014008	-4.658997	1.789580
H	0.686696	-6.319068	1.528031
H	2.368786	-6.907657	1.392504
H	1.020380	-8.541125	0.283989
H	1.801047	-7.638438	-1.022474
H	-0.984624	-6.472574	-2.442867
H	0.685825	-5.999305	-2.095441
H	-1.737601	-6.161188	0.375054
H	-1.863068	-3.221458	0.630298
H	-4.306144	-5.761527	2.167361
H	-5.607557	-5.384191	1.039870
H	-4.181861	-6.253652	0.472257
H	-3.762519	-2.774145	-0.930998
H	-3.922109	-4.485357	-1.360101
H	-5.315703	-3.599895	-0.741437
H	-3.976094	-2.053380	1.546086
H	-5.510027	-2.925665	1.594949
H	-4.274681	-3.281472	2.795557
H	-0.226092	-4.620837	4.514329
H	-2.598238	-5.924807	4.145554
H	-4.239385	-5.783656	6.625503
H	-3.126024	-7.124689	6.369848
H	-6.280485	-5.543275	5.240969
H	-7.926592	-6.624073	3.771671
H	-8.051678	-10.774414	4.523356
H	-8.790553	-11.998605	3.481700
H	-7.041757	-11.721997	3.406589
H	-9.759605	-9.514635	-0.295975
H	-5.135974	-9.826314	3.006033

H	-3.497415	-8.751936	4.487694
H	0.258617	-2.753575	5.911829
H	-1.397638	-2.114057	5.809035
H	-0.256327	-0.690432	4.236356
H	1.237798	-1.544405	2.792789
H	-2.271834	-1.633624	3.230093
H	-1.029758	-2.007235	1.996601
H	2.024372	0.561240	-1.785351
H	5.155063	3.511377	-3.203156
H	0.592259	7.773043	-2.105759
H	0.371818	6.157425	-2.766104
H	2.285023	6.518334	-4.332508
H	1.071328	7.789003	-4.484138
H	3.279321	11.055696	-2.584722
H	4.970966	12.833669	-2.285794

conformer_12

F	5.044973	14.990314	-3.145487
C	4.791810	13.958246	-3.984998
F	3.576348	13.455682	-3.673692
F	4.776610	14.441267	-5.247114
O	5.810165	12.980916	-3.820469
C	5.738427	11.847111	-4.578620
C	4.754999	11.541337	-5.522940
C	4.808440	10.334802	-6.231428
C	5.839541	9.424507	-5.986021
C	5.900162	8.166921	-6.765993
N	5.949627	6.948404	-6.080468
C	6.018052	5.729545	-6.884305
C	6.677085	4.572201	-6.135457
C	6.140505	4.354972	-4.708244
C	4.813074	3.601979	-4.643865
C	4.525173	2.810761	-3.528646
N	5.376321	2.650424	-2.477891
C	4.982801	1.855522	-1.453009
C	3.764473	1.202682	-1.419355
O	3.287689	0.388866	-0.433892
C	4.144069	0.163631	0.687563
C	3.467505	-0.766008	1.701282
N	2.091647	-0.729349	1.679553
C	1.260903	-1.622791	2.472730
C	1.116308	-3.004568	1.828512
O	0.463840	-2.865252	0.557228
C	0.328227	-4.127331	-0.106535
C	-0.347587	-3.927389	-1.466254
O	-1.756749	-3.669086	-1.366210
C	-2.072605	-2.348781	-0.920742
C	-2.576952	-2.313207	0.528250
N	-3.300862	-3.430145	0.885507
C	-3.757048	-3.673990	2.258394

C	-5.225806	-4.209148	2.292613
C	-5.360033	-5.606970	1.661188
C	-6.149534	-3.239855	1.519955
C	-5.743129	-4.271035	3.741401
C	-2.714231	-4.644578	2.894873
N	-2.396970	-4.509008	4.234425
C	-1.395178	-5.407686	4.841055
C	-1.893791	-6.856405	5.026903
N	-3.239166	-6.968212	5.283377
C	-3.875982	-8.217617	5.628171
C	-5.356636	-8.141591	5.364512
C	-6.224513	-7.594511	6.318431
C	-7.593083	-7.483097	6.052651
C	-8.120363	-7.912573	4.827390
C	-9.549776	-7.790695	4.537083
C	-10.207302	-7.126557	3.508747
C	-9.583642	-6.316926	2.425677
N	-11.593494	-7.240767	3.526325
C	-11.963621	-7.977624	4.551588
S	-10.703963	-8.573372	5.544530
C	-7.249918	-8.451380	3.871603
C	-5.881426	-8.562679	4.136182
O	-1.123938	-7.816693	5.069846
C	-1.098661	-4.783029	6.209192
C	-1.307819	-3.298301	5.964157
O	-0.150542	-2.755052	5.319577
C	-2.500393	-3.265959	5.003714
O	-2.213195	-5.557358	2.225064
O	-2.405789	-1.350979	1.274303
O	4.106159	-1.452603	2.499097
C	2.913888	1.388925	-2.508425
C	3.267053	2.192034	-3.584193
N	2.400506	2.334976	-4.602433
C	2.785419	3.126135	-5.610232
N	3.952955	3.775689	-5.681382
C	6.073318	5.692194	-3.955387
C	5.354166	6.775758	-4.750335
O	5.936937	8.259574	-7.993325
C	6.837807	9.729973	-5.057580
C	6.778557	10.935529	-4.354517
H	3.930119	12.214368	-5.742957
H	4.041358	10.110044	-6.970189
H	6.589839	5.924208	-7.799315
H	4.999131	5.485527	-7.201976
H	7.749324	4.798971	-6.055399
H	6.598930	3.652808	-6.728179
H	6.887012	3.722733	-4.207972
H	5.712435	1.774474	-0.652593
H	4.361174	1.105624	1.203941
H	5.066656	-0.327790	0.357639

H	1.664208	-0.296482	0.862570
H	0.282602	-1.139707	2.560087
H	1.702473	-1.719358	3.469582
H	0.509177	-3.648295	2.473966
H	2.099892	-3.465209	1.683380
H	-0.269319	-4.799072	0.517074
H	1.325221	-4.555260	-0.258063
H	-0.251337	-4.854210	-2.041194
H	0.132139	-3.126894	-2.041130
H	-2.891813	-1.981369	-1.548381
H	-1.228969	-1.659723	-1.035735
H	-3.169913	-4.242530	0.283850
H	-3.734834	-2.715186	2.780395
H	-4.780126	-6.355460	2.209849
H	-6.403944	-5.941000	1.665862
H	-5.021819	-5.614358	0.619857
H	-6.072958	-2.221505	1.917544
H	-5.901398	-3.205135	0.453626
H	-7.199094	-3.547475	1.596675
H	-5.661522	-3.295761	4.233581
H	-6.797235	-4.568230	3.774946
H	-5.188676	-4.998105	4.336516
H	-0.507405	-5.415506	4.197156
H	-3.750680	-6.112725	5.466450
H	-3.682445	-8.415350	6.688845
H	-3.417888	-9.036367	5.061257
H	-5.840353	-7.244193	7.275607
H	-8.240502	-7.046366	6.811563
H	-9.078405	-6.966542	1.704480
H	-10.340469	-5.737361	1.887365
H	-8.854558	-5.613040	2.837304
H	-13.001841	-8.201252	4.764824
H	-7.627727	-8.796331	2.910546
H	-5.225792	-8.976499	3.371175
H	-0.084110	-5.027335	6.540295
H	-1.804180	-5.139422	6.969585
H	-1.496198	-2.724126	6.875928
H	0.550050	-2.717817	6.004484
H	-3.447878	-3.302413	5.549499
H	-2.463884	-2.389387	4.353681
H	1.945216	0.893081	-2.517820
H	2.093656	3.252702	-6.437433
H	7.099926	6.031104	-3.761307
H	5.591992	5.573415	-2.977595
H	4.296869	6.524291	-4.896543
H	5.369578	7.705915	-4.179157
H	7.660133	9.040617	-4.879381
H	7.556714	11.164807	-3.627719

conformer_13

F	-2.882050	5.823134	-2.369540
C	-2.642168	6.957440	-1.709911
F	-2.218817	7.907286	-2.545304
F	-3.792360	7.368763	-1.180000
O	-1.724351	6.766399	-0.635101
C	-0.474785	6.231678	-0.873631
C	0.080634	6.025576	-2.144043
C	1.352332	5.471753	-2.275203
C	2.082408	5.094242	-1.141066
C	3.473837	4.517269	-1.297074
N	3.854677	3.481372	-0.495955
C	2.892549	2.450979	-0.050392
C	2.844088	1.365207	-1.153694
C	4.233030	0.732978	-1.448795
C	4.594807	-0.333334	-0.392366
C	4.222524	-1.695999	-0.592800
N	3.591703	-2.132690	-1.721271
C	3.241564	-3.440654	-1.788675
C	3.456494	-4.366963	-0.769066
O	2.983087	-5.648333	-0.965703
C	3.133061	-6.614399	0.087759
C	2.484846	-7.960037	-0.290950
N	1.729826	-8.025836	-1.398213
C	1.047696	-9.229825	-1.900248
C	-0.175160	-9.669580	-1.065798
O	-1.204866	-8.681103	-1.134650
C	-2.238321	-8.811749	-0.151735
C	-1.819718	-8.235518	1.217779
O	-1.453776	-6.868447	1.049010
C	-0.827386	-6.266378	2.190573
C	-0.303149	-4.863197	1.828983
N	-0.743978	-4.327495	0.683211
C	-0.361625	-3.042564	0.080108
C	-0.864680	-2.938331	-1.417219
C	-0.436337	-4.188100	-2.231597
C	-0.255453	-1.693139	-2.109752
C	-2.409045	-2.847899	-1.539000
C	-0.745162	-1.833554	0.999348
N	0.226525	-1.031308	1.512205
C	-0.069719	0.161696	2.349436
C	-0.311957	1.465946	1.539895
N	-0.969957	1.367562	0.376128
C	-1.309858	2.471820	-0.521604
C	-2.695677	3.046505	-0.257797
C	-2.878535	3.988437	0.757374
C	-4.128437	4.568614	0.954899
C	-5.202232	4.220841	0.132480
C	-6.532991	4.860615	0.344352
C	-7.240905	5.166790	1.516406
C	-6.860053	4.881495	2.953664

N	-8.401121	5.775231	1.343744
C	-8.668588	5.971349	0.080614
S	-7.470508	5.405226	-1.025568
C	-5.017073	3.281184	-0.885678
C	-3.767497	2.698628	-1.084013
O	0.007073	2.558883	2.008993
C	1.114331	0.237034	3.351745
C	1.815996	-1.108239	3.249975
O	1.120415	-2.035129	4.070152
C	1.614821	-1.438453	1.765515
O	-1.940789	-1.565699	1.156060
O	0.498007	-4.289936	2.571681
O	2.666041	-8.943446	0.428009
C	4.127664	-3.930874	0.381678
C	4.531020	-2.581547	0.486397
N	5.161860	-2.161172	1.618953
C	5.481072	-0.844524	1.678284
N	5.218123	0.091423	0.737250
C	5.299271	1.856364	-1.624854
C	5.241307	2.977589	-0.553757
O	4.234034	5.028599	-2.126617
C	1.531823	5.320304	0.128350
C	0.266321	5.886065	0.253482
H	-0.452371	6.290931	-3.044455
H	1.762446	5.330711	-3.267302
H	1.917144	2.843139	0.232445
H	3.271230	2.030338	0.883010
H	2.452756	1.827310	-2.061881
H	2.119119	0.592514	-0.892901
H	4.166808	0.247682	-2.424205
H	2.750559	-3.749129	-2.700612
H	2.651752	-6.263178	1.001796
H	4.190676	-6.793518	0.287467
H	1.622518	-7.169603	-1.926464
H	1.750582	-10.061157	-1.992062
H	0.710947	-9.021283	-2.917200
H	0.140754	-9.849292	-0.037488
H	-0.562158	-10.616981	-1.444988
H	-2.567891	-9.848428	-0.057616
H	-3.104560	-8.254205	-0.509935
H	-0.987393	-8.811929	1.624191
H	-2.643340	-8.318477	1.928854
H	0.016553	-6.868320	2.532416
H	-1.541429	-6.169028	3.009381
H	-1.396880	-4.888448	0.153725
H	0.721663	-3.088781	-0.004440
H	-0.939586	-5.094909	-1.892735
H	-0.675651	-4.083172	-3.290855
H	0.633684	-4.371144	-2.162419
H	-0.547246	-0.762507	-1.623006

H	0.833592	-1.730283	-2.125273
H	-0.581964	-1.612988	-3.147788
H	-2.800916	-1.896809	-1.179237
H	-2.733447	-2.923875	-2.578120
H	-2.910855	-3.644750	-0.989162
H	-1.027084	0.040283	2.859866
H	-1.368847	0.464629	0.158081
H	-1.240463	2.129959	-1.556351
H	-0.580403	3.280587	-0.441077
H	-2.049852	4.276873	1.389606
H	-4.254480	5.303810	1.737171
H	-6.017363	4.194834	3.030400
H	-6.578867	5.791302	3.484450
H	-7.677413	4.423637	3.512463
H	-9.570968	6.453085	-0.271517
H	-5.839638	3.000974	-1.528830
H	-3.637670	1.982387	-1.883866
H	0.809415	0.503985	4.364600
H	1.843067	0.989674	3.042408
H	2.872652	-1.099474	3.528351
H	1.022610	-2.871636	3.575632
H	2.285521	-0.790337	1.200868
H	1.888641	-2.468326	1.543775
H	4.345067	-4.586775	1.209514
H	5.984857	-0.501070	2.573844
H	5.153339	2.333307	-2.595754
H	6.301197	1.426745	-1.664500
H	5.483555	2.584326	0.434051
H	5.969923	3.778798	-0.696813
H	2.079574	5.067435	1.027268
H	-0.149466	6.049240	1.237629

conformer_14

F	2.470427	13.636909	-5.258042
C	2.727525	12.369173	-4.940650
F	3.641401	12.370116	-3.967317
F	1.590600	11.818135	-4.509615
O	3.212057	11.724944	-6.115073
C	3.533666	10.402228	-5.960729
C	2.571145	9.422291	-6.189273
C	2.902257	8.076751	-6.048728
C	4.198418	7.700790	-5.668475
C	4.539474	6.229268	-5.546295
N	5.422487	5.823115	-4.587257
C	5.816637	4.400790	-4.533524
C	4.766881	3.647692	-3.678512
C	4.586609	4.277408	-2.273967
C	3.504452	3.549745	-1.455926
C	3.804255	2.332679	-0.774137
N	5.043177	1.757434	-0.789031

C	5.211916	0.598184	-0.104663
C	4.203897	-0.050068	0.607999
O	4.541143	-1.231661	1.238888
C	3.561750	-2.008002	1.958008
C	2.820156	-3.007952	1.044461
N	2.836267	-2.794766	-0.278730
C	2.243244	-3.665525	-1.301592
C	0.702109	-3.678471	-1.352101
O	0.194084	-2.377160	-1.635723
C	-1.175841	-2.374488	-2.034857
C	-1.777312	-0.955330	-1.968833
O	-2.036318	-0.486006	-0.641002
C	-0.888788	-0.195886	0.178414
C	-0.703507	-1.239350	1.298109
N	-1.602923	-2.225353	1.384028
C	-1.556902	-3.388938	2.280887
C	-2.487997	-3.221810	3.549558
C	-3.968026	-2.988732	3.147060
C	-2.046370	-1.991238	4.380478
C	-2.433257	-4.450067	4.492134
C	-1.871437	-4.653601	1.424074
N	-1.297206	-5.851656	1.719624
C	-1.567361	-7.097657	0.952142
C	-2.922309	-7.784923	1.284161
N	-3.996089	-6.994531	1.385000
C	-5.356164	-7.408593	1.706654
C	-5.982330	-6.443950	2.701042
C	-5.716566	-6.581395	4.065634
C	-6.288337	-5.697916	4.977683
C	-7.138204	-4.682464	4.534132
C	-7.735467	-3.733260	5.516594
C	-7.184070	-3.075473	6.626368
C	-5.759485	-3.111085	7.135850
N	-8.015033	-2.310263	7.311849
C	-9.217297	-2.313197	6.802193
S	-9.421406	-3.292496	5.395468
C	-7.418910	-4.560551	3.170719
C	-6.847891	-5.441542	2.255979
O	-3.014837	-9.009424	1.345608
C	-0.316867	-7.981064	1.189272
C	0.735625	-7.044434	1.757321
O	1.352404	-6.371606	0.674751
C	-0.121163	-6.069049	2.577492
O	-2.727144	-4.558972	0.534153
O	0.242809	-1.138596	2.080277
O	2.250980	-3.982250	1.536886
C	2.933523	0.536432	0.626039
C	2.709545	1.744378	-0.068291
N	1.466548	2.301953	-0.047204
C	1.313918	3.456087	-0.740958

N	2.265986	4.107774	-1.447577
C	4.410476	5.820003	-2.368470
C	5.491851	6.473633	-3.260871
O	4.019341	5.438714	-6.337657
C	5.170193	8.696753	-5.481047
C	4.835623	10.041313	-5.623180
H	1.570994	9.708599	-6.479324
H	2.146975	7.324097	-6.235434
H	6.800169	4.348802	-4.063305
H	5.975728	3.982087	-5.530334
H	5.113741	2.618133	-3.580540
H	3.815590	3.617759	-4.213769
H	5.507432	4.117524	-1.709872
H	6.203439	0.169830	-0.133543
H	2.854424	-1.398957	2.519061
H	4.104129	-2.586099	2.705757
H	3.307102	-1.957671	-0.589693
H	2.615809	-4.686760	-1.192350
H	2.606084	-3.321094	-2.270994
H	0.293801	-4.023215	-0.402226
H	0.386964	-4.393929	-2.114599
H	-1.770725	-3.031281	-1.398621
H	-1.253649	-2.762448	-3.051681
H	-2.730177	-0.957222	-2.498982
H	-1.141144	-0.245029	-2.499783
H	-1.037729	0.778674	0.642795
H	0.032693	-0.137569	-0.402656
H	-2.331550	-2.260929	0.683863
H	-0.527793	-3.461528	2.623016
H	-4.370844	-3.819235	2.567226
H	-4.611829	-2.885765	4.021904
H	-4.094505	-2.080667	2.556901
H	-0.993071	-2.051215	4.658061
H	-2.188107	-1.057221	3.835995
H	-2.619815	-1.898308	5.303898
H	-1.417242	-4.650940	4.832857
H	-3.040872	-4.296935	5.384473
H	-2.820487	-5.352378	4.017099
H	-1.698395	-6.858508	-0.104255
H	-3.854310	-6.020304	1.136012
H	-5.389305	-8.422019	2.116920
H	-5.949499	-7.453976	0.791221
H	-5.055759	-7.361244	4.416720
H	-6.077041	-5.804926	6.031489
H	-5.358123	-2.109598	7.294755
H	-5.683670	-3.644869	8.083214
H	-5.086251	-3.602563	6.435687
H	-10.039792	-1.750142	7.215947
H	-8.071559	-3.775337	2.818318
H	-7.066488	-5.329348	1.203619

H	0.006732	-8.519326	0.297547
H	-0.512499	-8.738252	1.951425
H	1.506089	-7.542029	2.350598
H	1.701919	-5.522806	1.006439
H	-0.424460	-6.592801	3.485261
H	0.463788	-5.197748	2.865555
H	2.102951	0.105528	1.154997
H	0.328616	3.903346	-0.732014
H	4.496407	6.258024	-1.373196
H	3.424178	6.085602	-2.753822
H	5.446071	7.561497	-3.284324
H	6.485667	6.273126	-2.855933
H	6.192510	8.436533	-5.242194
H	5.583581	10.807372	-5.480859

conformer_15

F	-2.153370	4.030754	3.428912
C	-1.159723	4.696546	4.057556
F	-1.719089	5.493957	4.997744
F	-0.346374	3.818375	4.685199
O	-0.435088	5.510764	3.147212
C	0.164443	4.901753	2.081888
C	0.263649	3.526059	1.859936
C	0.920477	3.041425	0.722142
C	1.462908	3.932808	-0.209825
C	2.208262	3.437600	-1.393094
N	1.624435	2.468088	-2.215100
C	0.170618	2.355220	-2.390420
C	-0.247979	0.925489	-2.718055
C	0.535592	0.396491	-3.927108
C	0.133718	-1.007101	-4.355173
C	0.283688	-2.116046	-3.518924
N	0.742549	-2.050919	-2.238748
C	0.886358	-3.207261	-1.547903
C	0.587031	-4.450341	-2.072561
O	0.746928	-5.663757	-1.469707
C	1.142683	-5.651596	-0.099760
C	1.346667	-7.082202	0.413038
N	1.896473	-7.135878	1.675130
C	2.355726	-8.367991	2.294171
C	3.794891	-8.731405	1.903279
O	4.721747	-7.779838	2.447343
C	5.142591	-6.778709	1.506309
C	5.124363	-5.409150	2.188871
O	3.755791	-5.003822	2.350046
C	3.643840	-3.791999	3.099954
C	2.162531	-3.448128	3.294841
N	1.934578	-2.262512	3.960384
C	0.572293	-1.752365	4.164097
C	0.472052	-0.774381	5.380138

C	1.311976	0.504920	5.204101
C	0.956471	-1.497124	6.656920
C	-0.994825	-0.359956	5.608229
C	0.082852	-1.131741	2.821588
N	-1.105105	-1.575034	2.283213
C	-1.641508	-1.006523	1.043969
C	-2.448033	0.283747	1.328864
N	-2.755436	1.019469	0.205883
C	-3.659968	2.149948	0.262948
C	-3.368424	3.143684	-0.830396
C	-2.774987	4.375383	-0.528087
C	-2.489762	5.298350	-1.539325
C	-2.790286	5.010654	-2.876775
C	-2.482377	5.983472	-3.929674
C	-1.302428	6.658871	-4.221948
C	0.004810	6.530494	-3.520201
N	-1.377705	7.540741	-5.295338
C	-2.593778	7.526502	-5.796167
S	-3.709368	6.479985	-5.031932
C	-3.382164	3.775586	-3.178428
C	-3.671594	2.853324	-2.166594
O	-2.815938	0.606017	2.458758
C	-2.555303	-2.100933	0.502007
C	-3.115163	-2.745851	1.770475
O	-3.535966	-4.073589	1.491063
C	-1.931959	-2.685926	2.744297
O	0.758159	-0.279274	2.233663
O	1.249534	-4.174137	2.899653
O	1.069928	-8.089790	-0.236665
C	0.095086	-4.485267	-3.375970
C	-0.072219	-3.330247	-4.127379
N	-0.545110	-3.438928	-5.381132
C	-0.665264	-2.304486	-6.078160
N	-0.342956	-1.086816	-5.629503
C	2.048007	0.531694	-3.696427
C	2.420263	1.966353	-3.335320
O	3.339536	3.887556	-1.580429
C	1.383644	5.308226	0.016772
C	0.732111	5.786011	1.156211
H	-0.145699	2.792933	2.550436
H	1.012668	1.966768	0.576083
H	-0.105954	3.029358	-3.209797
H	-0.368518	2.699785	-1.508745
H	-1.324276	0.892084	-2.922268
H	-0.073579	0.303543	-1.833781
H	0.287894	1.059352	-4.770606
H	1.271695	-3.071486	-0.541838
H	0.361755	-5.182905	0.509629
H	2.098602	-5.126235	0.010508
H	2.228982	-6.263916	2.093084

H 1.678677 -9.180766 2.011558
H 2.288384 -8.211569 3.375802
H 3.917793 -8.840059 0.819525
H 4.040551 -9.696949 2.358188
H 4.497771 -6.759800 0.620853
H 6.161758 -7.030884 1.198002
H 5.638072 -4.670843 1.564417
H 5.604647 -5.468137 3.171865
H 4.129049 -2.976363 2.553694
H 4.100812 -3.918241 4.087179
H 2.692735 -1.585898 3.954003
H -0.041171 -2.629100 4.395015
H 0.959620 1.111087 4.364123
H 1.250656 1.137207 6.098128
H 2.370631 0.280546 5.041783
H 0.390997 -2.420262 6.827053
H 2.018189 -1.759649 6.594625
H 0.829816 -0.864059 7.542927
H -1.636116 -1.235133 5.758087
H -1.092833 0.274149 6.497213
H -1.388554 0.209810 4.761296
H -0.829559 -0.766418 0.349163
H -2.605944 0.598835 -0.704408
H -3.599389 2.626869 1.247998
H -4.681574 1.766520 0.157149
H -2.532752 4.630789 0.501902
H -2.040924 6.250986 -1.263268
H 0.224359 5.485903 -3.282844
H 0.820074 6.907280 -4.146250
H -0.004615 7.108696 -2.591351
H -2.883714 8.138123 -6.641802
H -3.621876 3.511741 -4.207386
H -4.135814 1.904773 -2.432908
H -1.975426 -2.837200 -0.068887
H -3.352805 -1.737584 -0.153827
H -3.966576 -2.168755 2.149671
H -3.903280 -4.435539 2.325347
H -2.265864 -2.506701 3.770029
H -1.341756 -3.607311 2.723736
H -0.155254 -5.445280 -3.823920
H -1.050256 -2.378197 -7.090612
H 2.600232 0.224944 -4.593131
H 2.375562 -0.127934 -2.884249
H 3.487274 2.008600 -3.090067
H 2.254260 2.637905 -4.186468
H 1.828718 6.011555 -0.683433
H 0.672104 6.860716 1.321636

conformer_16
F -1.249478 8.581861 -6.247568

C	-0.552686	7.778350	-7.081347
F	-1.087107	7.896784	-8.319937
F	0.733844	8.188070	-7.141037
O	-0.641151	6.418646	-6.678448
C	-0.149741	6.081193	-5.449467
C	-0.275291	4.722331	-5.130476
C	0.182118	4.228818	-3.906483
C	0.783819	5.099394	-2.997492
C	1.240495	4.576466	-1.691935
N	2.583461	4.728659	-1.337150
C	3.662764	4.864018	-2.321961
C	4.235729	3.484511	-2.651515
C	4.658897	2.737226	-1.368331
C	5.193844	1.336707	-1.633276
C	4.409203	0.341118	-2.221467
N	3.119648	0.522491	-2.617676
C	2.471649	-0.516510	-3.196282
C	3.048504	-1.755861	-3.397460
O	2.472511	-2.852132	-3.970495
C	1.188476	-2.663859	-4.564156
C	0.715607	-3.958601	-5.236460
N	-0.576248	-3.892161	-5.715335
C	-1.263316	-5.036052	-6.299514
C	-1.935152	-5.913044	-5.239263
O	-3.005373	-5.173991	-4.629207
C	-3.692296	-5.962023	-3.646508
C	-4.874086	-5.161295	-3.089643
O	-4.477118	-3.963758	-2.404201
C	-3.921437	-4.212563	-1.115117
C	-3.806020	-2.926554	-0.279521
N	-3.392850	-3.152271	1.018707
C	-3.099008	-2.046747	1.943277
C	-3.395909	-2.443201	3.428998
C	-3.265295	-1.221750	4.357476
C	-2.454825	-3.547784	3.945187
C	-4.850720	-2.952299	3.548419
C	-1.616364	-1.626989	1.689025
N	-1.261604	-0.301210	1.854764
C	0.134918	0.122938	1.668822
C	1.074160	-0.448538	2.751054
N	0.631184	-0.278033	4.041650
C	1.401654	-0.649432	5.206487
C	0.492019	-1.129719	6.307061
C	0.253220	-2.498364	6.483916
C	-0.619806	-2.945261	7.480683
C	-1.275451	-2.033243	8.317238
C	-2.193201	-2.510664	9.352698
C	-3.334386	-3.297213	9.253076
C	-3.940041	-3.839086	8.005358
N	-3.959822	-3.582358	10.462565

C	-3.295911	-3.017099	11.447892
S	-1.905312	-2.124503	11.004364
C	-1.043690	-0.663528	8.133125
C	-0.169796	-0.215639	7.137207
O	2.192386	-0.889132	2.482341
C	0.088263	1.652261	1.718220
C	-1.280368	1.972162	1.140075
O	-1.220130	1.915639	-0.287397
C	-2.164712	0.840328	1.677511
O	-0.760692	-2.475884	1.407535
O	-4.070779	-1.804223	-0.708316
O	1.412451	-4.967425	-5.345235
C	4.362108	-1.921316	-2.960503
C	5.075525	-0.884838	-2.373024
N	6.345927	-1.106564	-1.991139
C	6.996083	-0.076873	-1.437881
N	6.483164	1.142041	-1.237762
C	3.553046	2.742423	-0.293162
C	3.026389	4.158197	-0.068935
O	0.401439	4.034614	-0.971067
C	0.899505	6.460250	-3.296124
C	0.437805	6.948153	-4.524353
H	-0.737473	4.036883	-5.839574
H	0.070972	3.172433	-3.672078
H	4.434893	5.508732	-1.886244
H	3.319822	5.341540	-3.241473
H	5.095308	3.592722	-3.324149
H	3.476513	2.920471	-3.203387
H	5.495082	3.316000	-0.946580
H	1.450704	-0.290114	-3.488667
H	1.235367	-1.888599	-5.338360
H	0.455715	-2.402186	-3.791538
H	-1.151135	-3.090641	-5.466000
H	-0.541047	-5.629051	-6.870083
H	-2.011658	-4.630055	-6.988130
H	-1.215530	-6.213723	-4.469539
H	-2.347332	-6.807910	-5.718742
H	-2.988554	-6.229650	-2.852168
H	-4.068330	-6.877412	-4.116993
H	-5.490375	-5.781307	-2.428955
H	-5.505733	-4.835157	-3.923022
H	-2.915626	-4.630273	-1.225417
H	-4.557020	-4.912937	-0.560840
H	-2.907381	-4.029053	1.189918
H	-3.763344	-1.222658	1.669460
H	-3.919237	-0.405587	4.032143
H	-3.545112	-1.473287	5.386680
H	-2.240188	-0.846975	4.390461
H	-2.530814	-4.460260	3.345270
H	-1.409541	-3.223851	3.936163

H	-2.699915	-3.820313	4.978211
H	-5.005152	-3.878122	2.983779
H	-5.111911	-3.164159	4.591888
H	-5.560918	-2.206413	3.173908
H	0.467651	-0.234627	0.686252
H	-0.249235	0.200958	4.193935
H	1.959899	0.235350	5.533312
H	2.139362	-1.417116	4.947267
H	0.743546	-3.229695	5.842738
H	-0.775806	-4.016327	7.599006
H	-3.324792	-4.648746	7.601287
H	-4.940619	-4.238525	8.199293
H	-4.034341	-3.055857	7.247560
H	-3.601576	-3.104843	12.483383
H	-1.548168	0.072323	8.757349
H	-0.013412	0.855051	7.011955
H	0.912494	2.084581	1.145631
H	0.154085	2.027536	2.745822
H	-1.655500	2.958965	1.426028
H	-0.663019	2.682906	-0.564951
H	-2.563063	1.093859	2.663851
H	-2.975609	0.597107	0.987007
H	4.849074	-2.885528	-3.094436
H	8.022672	-0.243842	-1.126309
H	3.939548	2.338605	0.650482
H	2.719646	2.097064	-0.593245
H	2.205657	4.149108	0.655476
H	3.812900	4.804795	0.337604
H	1.344897	7.146122	-2.578010
H	0.553162	8.012092	-4.715459

conformer_17

F	6.928457	13.755523	0.836539
C	6.564758	13.083446	1.951224
F	6.960768	13.808268	3.024348
F	5.218762	12.970361	1.997597
O	7.190328	11.808792	2.010471
C	6.920443	10.915762	1.012950
C	7.579099	9.686258	1.144750
C	7.400635	8.673611	0.199267
C	6.543839	8.885516	-0.883817
C	6.366945	7.838379	-1.916631
N	5.938670	6.566579	-1.522407
C	5.798728	5.551616	-2.564609
C	5.963287	4.133335	-2.020783
C	5.144631	3.844738	-0.748316
C	3.670435	3.539707	-1.006780
C	2.982111	2.688912	-0.138004
N	3.554195	2.091301	0.943182
C	2.782446	1.282085	1.708835

C	1.447591	1.033403	1.448777
O	0.602463	0.227910	2.153070
C	1.144332	-0.438131	3.294688
C	0.058312	-1.320770	3.920503
N	0.536308	-2.322448	4.736855
C	-0.343881	-3.284084	5.384759
C	-0.819515	-4.400935	4.447727
O	0.279727	-5.262779	4.110408
C	-0.172539	-6.408767	3.372525
C	1.007527	-7.333809	3.057861
O	1.799721	-6.894949	1.943465
C	2.610921	-5.754605	2.223448
C	2.021043	-4.450370	1.674525
N	1.307609	-4.610501	0.509951
C	0.524974	-3.542834	-0.126985
C	1.117076	-3.148046	-1.517932
C	1.100792	-4.325810	-2.510621
C	2.579757	-2.679794	-1.342397
C	0.336996	-1.975771	-2.140888
C	-0.940311	-4.071624	-0.180973
N	-1.987267	-3.178104	-0.100004
C	-3.374335	-3.660091	-0.161278
C	-3.780339	-4.122726	-1.576652
N	-4.945859	-4.856732	-1.607364
C	-5.426052	-5.457979	-2.831223
C	-6.837394	-5.955575	-2.669972
C	-7.919107	-5.075351	-2.802618
C	-9.230506	-5.530058	-2.633201
C	-9.486073	-6.870853	-2.318301
C	-10.862588	-7.339741	-2.153762
C	-11.935803	-7.305243	-3.035521
C	-11.928126	-6.784504	-4.430736
N	-13.124960	-7.825812	-2.535721
C	-12.940612	-8.242984	-1.301408
S	-11.364115	-8.043432	-0.666513
C	-8.402760	-7.748351	-2.177126
C	-7.090775	-7.294611	-2.346969
O	-3.152675	-3.828588	-2.594340
C	-4.236978	-2.465395	0.263587
C	-3.301015	-1.657678	1.148601
O	-3.288227	-2.243529	2.453773
C	-1.945323	-1.826900	0.456280
O	-1.162668	-5.280517	-0.336780
O	2.218942	-3.358076	2.201436
O	-1.146957	-1.147606	3.728242
C	0.888370	1.665579	0.339030
C	1.633656	2.503715	-0.478383
N	1.035583	3.083722	-1.533272
C	1.795520	3.887794	-2.285407
N	3.089862	4.151240	-2.072066

C	5.321382	4.981458	0.269671
C	5.090210	6.357635	-0.343441
O	6.642319	8.133594	-3.079921
C	5.896926	10.114606	-1.035141
C	6.080104	11.125320	-0.083498
H	8.243992	9.512093	1.989649
H	7.931516	7.730816	0.311190
H	6.552710	5.716995	-3.343173
H	4.823982	5.698476	-3.040787
H	7.024472	3.997175	-1.769886
H	5.735663	3.404142	-2.807630
H	5.584564	2.934589	-0.317735
H	3.307492	0.840334	2.550757
H	1.442953	0.295505	4.052618
H	1.996894	-1.057821	3.006817
H	1.518088	-2.578116	4.655931
H	-1.210620	-2.742723	5.778901
H	0.220484	-3.706505	6.222624
H	-1.242968	-3.988032	3.525998
H	-1.588375	-4.987254	4.963784
H	-0.654384	-6.074375	2.447846
H	-0.896410	-6.954287	3.988083
H	0.611302	-8.313577	2.771258
H	1.653101	-7.477272	3.931863
H	3.569821	-5.904093	1.715579
H	2.811594	-5.648203	3.294877
H	1.095943	-5.570240	0.237080
H	0.570921	-2.673671	0.532696
H	0.079950	-4.660842	-2.721872
H	1.551100	-4.037919	-3.467968
H	1.666573	-5.183185	-2.130984
H	2.646066	-1.854806	-0.623978
H	3.226008	-3.489737	-0.987358
H	2.999175	-2.326455	-2.291582
H	0.319455	-1.111656	-1.468459
H	0.799098	-1.648492	-3.079825
H	-0.694992	-2.252938	-2.375204
H	-3.477008	-4.495443	0.542652
H	-5.295785	-5.243397	-0.735427
H	-4.748879	-6.279453	-3.093514
H	-5.367560	-4.726406	-3.645978
H	-7.746973	-4.025529	-3.037308
H	-10.049796	-4.820612	-2.739375
H	-11.040438	-7.127063	-4.971741
H	-12.809123	-7.131459	-4.980201
H	-11.938147	-5.690261	-4.428418
H	-13.732601	-8.687971	-0.711365
H	-8.567667	-8.798238	-1.939376
H	-6.267866	-7.998176	-2.226617
H	-5.142226	-2.796216	0.783104

H -4.536104 -1.869091 -0.607289
H -3.601832 -0.610783 1.245350
H -2.611711 -1.747361 2.974035
H -1.851493 -1.129902 -0.381493
H -1.111577 -1.707847 1.145099
H -0.160888 1.499364 0.103679
H 1.323527 4.366316 -3.138045
H 6.349592 4.943825 0.653831
H 4.658795 4.847802 1.132841
H 4.049004 6.477924 -0.665569
H 5.263136 7.121156 0.417405
H 5.246257 10.291564 -1.889435
H 5.550307 12.061621 -0.240085

conformer_18
F -5.975771 8.941005 -5.159386
C -5.559258 10.114398 -4.633834
F -4.847033 10.800262 -5.555246
F -6.655632 10.846076 -4.323337
O -4.802824 9.907510 -3.448662
C -3.647335 9.185506 -3.543943
C -3.118157 8.616057 -4.704972
C -1.916443 7.899149 -4.654382
C -1.248298 7.738308 -3.437862
C 0.039253 7.006677 -3.406863
N 0.182793 5.927935 -2.527831
C 1.472468 5.240277 -2.516411
C 1.754565 4.554960 -1.180804
C 0.587579 3.704451 -0.647460
C 0.460210 2.328823 -1.298725
C -0.068568 1.267029 -0.561402
N -0.459663 1.375419 0.736644
C -0.959919 0.273178 1.345597
C -1.107751 -0.949476 0.714937
O -1.611937 -2.101337 1.250429
C -2.041162 -2.027308 2.609213
C -2.615117 -3.381727 3.024608
N -3.895829 -3.603419 2.576294
C -4.632591 -4.831199 2.832300
C -4.240319 -5.975944 1.893566
O -4.296445 -5.519029 0.536219
C -4.312651 -6.604185 -0.399924
C -3.890630 -6.081750 -1.777163
O -2.468674 -6.065302 -1.979051
C -1.757585 -5.151815 -1.146533
C -0.930847 -5.860012 -0.059047
N 0.056013 -5.079207 0.497936
C 0.995884 -5.568038 1.517406
C 2.397310 -5.910462 0.906650
C 3.365853 -6.408356 1.996448

C	3.037365	-4.697177	0.206351
C	2.256478	-7.042727	-0.134322
C	1.059741	-4.465959	2.612220
N	1.177821	-4.841233	3.934385
C	1.290062	-3.822932	4.987737
C	2.664223	-3.119829	4.924851
N	2.593128	-1.763713	4.702003
C	3.759436	-0.935714	4.484603
C	3.919847	-0.604045	3.022734
C	4.654447	-1.445025	2.177443
C	4.784495	-1.148193	0.816731
C	4.180729	-0.006820	0.273726
C	4.312322	0.288808	-1.153561
C	3.970044	-0.470416	-2.265550
C	3.332898	-1.815520	-2.267271
N	4.256452	0.119076	-3.492523
C	4.803535	1.299383	-3.297706
S	5.015896	1.771550	-1.667223
C	3.440542	0.829949	1.118993
C	3.305736	0.531608	2.478386
O	3.729961	-3.728704	5.028823
C	1.139987	-4.591069	6.305554
C	0.335379	-5.822205	5.917094
O	-1.062136	-5.516318	5.933212
C	0.829348	-6.142618	4.504335
O	1.049107	-3.269515	2.298977
O	-1.106054	-7.034530	0.264632
O	-1.995761	-4.187367	3.719708
C	-0.700327	-1.026693	-0.616006
C	-0.170434	0.069237	-1.284090
N	0.204238	-0.069828	-2.566932
C	0.701270	1.018264	-3.166564
N	0.837895	2.221917	-2.598419
C	-0.726994	4.495016	-0.730502
C	-0.957285	5.104477	-2.108775
O	0.941124	7.410706	-4.141572
C	-1.760189	8.319911	-2.275281
C	-2.959467	9.033819	-2.332844
H	-3.605249	8.708221	-5.672613
H	-1.509161	7.466725	-5.566360
H	2.274952	5.960258	-2.715799
H	1.477792	4.531956	-3.351087
H	1.956111	5.342469	-0.441341
H	2.671232	3.959870	-1.254698
H	0.812196	3.533007	0.414332
H	-1.240900	0.436651	2.381739
H	-2.824732	-1.269902	2.734985
H	-1.198641	-1.801033	3.273102
H	-4.250670	-3.004157	1.834853
H	-5.689670	-4.583073	2.688565

H -4.481907 -5.131141 3.874552
H -4.926762 -6.817395 2.041907
H -3.218440 -6.308731 2.103866
H -5.341045 -6.977699 -0.445768
H -3.649913 -7.411155 -0.071489
H -4.289006 -5.079173 -1.970429
H -4.287894 -6.755967 -2.542854
H -2.408137 -4.398976 -0.690910
H -1.051944 -4.626156 -1.799867
H 0.096449 -4.087229 0.274675
H 0.572223 -6.481294 1.939567
H 2.956338 -7.278224 2.520475
H 4.326345 -6.711025 1.562727
H 3.582230 -5.630738 2.735354
H 2.405008 -4.320428 -0.604047
H 3.215191 -3.876915 0.907076
H 4.005976 -4.961733 -0.233773
H 1.660476 -6.729157 -0.997783
H 3.236045 -7.352625 -0.517143
H 1.779812 -7.926092 0.305110
H 0.471843 -3.104395 4.863358
H 1.699979 -1.361527 4.436450
H 4.661091 -1.426384 4.867592
H 3.620493 -0.017431 5.066153
H 5.128986 -2.341793 2.573604
H 5.368694 -1.817688 0.187504
H 4.084758 -2.590095 -2.088652
H 2.563496 -1.887788 -1.492705
H 2.856009 -2.018620 -3.231469
H 5.108513 1.942396 -4.114321
H 2.953332 1.721039 0.729203
H 2.716501 1.195617 3.109388
H 0.644365 -3.976093 7.063854
H 2.115147 -4.898665 6.701444
H 0.491526 -6.656698 6.606325
H -1.278085 -5.012707 5.112515
H 1.745711 -6.739071 4.536643
H 0.062827 -6.647602 3.913261
H -0.800436 -1.966692 -1.152606
H 1.017775 0.916929 -4.200299
H -0.686694 5.310226 0.004349
H -1.584434 3.868657 -0.457735
H -1.093809 4.325812 -2.868653
H -1.884667 5.680082 -2.093256
H -1.233171 8.225055 -1.328583
H -3.355816 9.479792 -1.421607

conformer_19
F -5.663449 1.632601 -2.901690
C -5.880072 2.415111 -1.821545

F	-7.087496	3.009378	-1.970522
F	-5.924507	1.652054	-0.706647
O	-4.887874	3.425932	-1.712509
C	-3.592019	3.034107	-1.530659
C	-2.683957	4.091516	-1.387212
C	-1.323905	3.844269	-1.191472
C	-0.864578	2.527979	-1.148983
C	0.562116	2.239722	-0.897561
N	1.511226	2.660119	-1.830491
C	1.191874	2.965948	-3.227521
C	1.375185	1.711132	-4.079932
C	2.784762	1.110968	-3.887430
C	2.989314	-0.178681	-4.671829
C	2.245289	-1.330661	-4.405027
N	1.277053	-1.402312	-3.452517
C	0.631916	-2.578947	-3.278990
C	0.907325	-3.715528	-4.015874
O	0.322311	-4.942952	-3.886607
C	-0.712879	-5.048528	-2.910998
C	-1.266390	-6.476568	-2.838829
N	-2.132799	-6.669068	-1.782087
C	-2.634826	-7.980844	-1.397335
C	-1.617556	-8.760180	-0.558310
O	-1.373669	-8.048190	0.665862
C	-0.469491	-8.769163	1.515750
C	-0.102812	-7.906281	2.725142
O	0.777065	-6.849305	2.306709
C	1.235942	-6.068177	3.406045
C	0.292285	-4.944526	3.877275
N	0.806101	-4.200419	4.921355
C	0.143687	-2.982237	5.409162
C	0.508061	-2.660376	6.895243
C	0.165818	-3.878395	7.782800
C	-0.324881	-1.468947	7.405990
C	1.998495	-2.325127	7.092465
C	0.485580	-1.833479	4.411801
N	-0.538238	-1.058433	3.916064
C	-0.281581	0.035831	2.972310
C	0.230100	1.300150	3.703719
N	0.676962	2.293499	2.864904
C	1.307132	3.490566	3.371628
C	1.372872	4.560971	2.316021
C	2.476919	4.650184	1.458743
C	2.523962	5.627078	0.459806
C	1.466783	6.531595	0.296862
C	1.505503	7.554757	-0.747943
C	1.434156	8.938808	-0.654435
C	1.325859	9.744217	0.593435
N	1.477904	9.613420	-1.870162
C	1.580160	8.745288	-2.853644

S	1.628427	7.095599	-2.401071
C	0.363517	6.442416	1.155602
C	0.312583	5.460782	2.149840
O	0.215685	1.424601	4.928955
C	-1.633846	0.291127	2.310780
C	-2.632592	-0.057759	3.412024
O	-3.899195	-0.399225	2.868765
C	-1.970808	-1.248557	4.110372
O	1.652317	-1.637535	4.049288
O	-0.813054	-4.727896	3.383920
O	-0.971026	-7.369794	-3.631769
C	1.899500	-3.612460	-4.990184
C	2.589123	-2.426603	-5.211606
N	3.536876	-2.391368	-6.165587
C	4.178578	-1.229251	-6.333966
N	3.954431	-0.113269	-5.630872
C	3.170818	0.961062	-2.399598
C	2.897218	2.251454	-1.629726
O	0.837037	1.631685	0.138100
C	-1.760359	1.464446	-1.281910
C	-3.122590	1.718638	-1.477392
H	-3.036189	5.121286	-1.422425
H	-0.634318	4.674844	-1.073220
H	1.869373	3.760483	-3.560883
H	0.172848	3.339257	-3.341768
H	1.212399	1.955489	-5.136701
H	0.599020	0.989222	-3.804252
H	3.485552	1.848600	-4.307944
H	-0.123507	-2.552124	-2.499516
H	-1.547663	-4.387328	-3.173050
H	-0.315893	-4.801051	-1.918699
H	-2.193059	-5.942579	-1.072475
H	-2.884540	-8.544289	-2.302188
H	-3.549426	-7.806303	-0.821272
H	-0.673952	-8.874419	-1.103716
H	-2.021414	-9.751620	-0.324535
H	0.434772	-9.023076	0.950896
H	-0.965050	-9.686211	1.851955
H	0.413685	-8.529007	3.463905
H	-1.003115	-7.471104	3.171534
H	2.159051	-5.580830	3.071408
H	1.492399	-6.707970	4.258691
H	1.813416	-4.250395	5.048815
H	-0.930587	-3.187824	5.360919
H	0.783217	-4.747954	7.532638
H	0.333929	-3.655677	8.842968
H	-0.885059	-4.167355	7.668175
H	-0.116805	-0.557294	6.838199
H	-1.397920	-1.676871	7.337203
H	-0.102404	-1.253044	8.457682

H	2.282878	-1.412588	6.559239
H	2.223889	-2.157509	8.152588
H	2.648405	-3.136532	6.750321
H	0.476324	-0.273097	2.243432
H	0.832206	2.061369	1.879687
H	2.313589	3.222403	3.714115
H	0.760187	3.850250	4.251166
H	3.309060	3.955021	1.559980
H	3.398245	5.674385	-0.187269
H	2.018770	9.377523	1.357293
H	1.565967	10.794682	0.400532
H	0.307196	9.695561	0.990273
H	1.631079	9.045051	-3.893403
H	-0.478385	7.124297	1.047697
H	-0.564283	5.401743	2.793148
H	-1.772751	-0.379586	1.453255
H	-1.772420	1.314851	1.949682
H	-2.751896	0.777894	4.111564
H	-4.227081	0.395831	2.398438
H	-2.217272	-1.278516	5.174155
H	-2.264374	-2.202757	3.659488
H	2.145560	-4.484704	-5.592750
H	4.944639	-1.189055	-7.102413
H	4.231332	0.695632	-2.310528
H	2.605784	0.148643	-1.929264
H	3.107760	2.105913	-0.565034
H	3.545278	3.061121	-1.984903
H	-1.404039	0.437189	-1.236173
H	-3.781969	0.860671	-1.581685

conformer_20

F	-2.169838	7.785664	-8.369993
C	-2.515864	8.634197	-7.376599
F	-1.578027	9.599580	-7.253162
F	-3.683454	9.227280	-7.721158
O	-2.704952	7.941033	-6.150629
C	-1.640160	7.265690	-5.625551
C	-1.910681	6.610212	-4.417065
C	-0.917754	5.878298	-3.761809
C	0.356759	5.788556	-4.326597
C	1.432897	5.044993	-3.632431
N	1.240870	3.687905	-3.347232
C	2.332670	2.987551	-2.673399
C	1.822344	1.816462	-1.841331
C	0.957954	0.842623	-2.653433
C	1.812396	-0.077238	-3.522212
C	2.299927	-1.272522	-2.988992
N	2.033530	-1.696076	-1.723941
C	2.553989	-2.882929	-1.324371
C	3.343272	-3.679974	-2.131250

O	3.920244	-4.874979	-1.817510
C	3.538207	-5.518119	-0.604737
C	2.160732	-6.196795	-0.640227
N	1.842888	-6.746668	-1.861526
C	0.544415	-7.328452	-2.167347
C	-0.503462	-6.268641	-2.526569
O	-0.070197	-5.553763	-3.692511
C	-1.055225	-4.646093	-4.211350
C	-1.271529	-3.415402	-3.322945
O	-2.258284	-3.708087	-2.323635
C	-2.386017	-2.660647	-1.362973
C	-1.341605	-2.711887	-0.236284
N	-1.447100	-1.690142	0.686808
C	-0.625783	-1.724485	1.903104
C	-0.376444	-0.302836	2.501403
C	0.527919	-0.400956	3.745991
C	-1.678168	0.417490	2.896889
C	0.355666	0.566282	1.455942
C	-1.336476	-2.691450	2.900446
N	-0.562050	-3.548564	3.663224
C	-1.184681	-4.453325	4.653655
C	-1.592200	-3.747139	5.973383
N	-2.530746	-2.753871	5.826411
C	-3.034061	-1.956183	6.921924
C	-2.339087	-0.619810	6.995763
C	-1.053741	-0.514577	7.544422
C	-0.407495	0.723712	7.615120
C	-1.032915	1.883544	7.139501
C	-0.368933	3.185421	7.222519
C	-0.029373	4.093225	6.226816
C	-0.239324	3.933329	4.761813
N	0.582090	5.258981	6.677009
C	0.695985	5.221687	7.987146
S	0.091207	3.817879	8.755563
C	-2.312777	1.776518	6.580701
C	-2.959332	0.537658	6.508663
O	-1.180111	-4.098349	7.079875
C	-0.121646	-5.532312	4.918943
C	0.663064	-5.581161	3.621443
O	-0.066768	-6.360401	2.669618
C	0.714292	-4.108610	3.208367
O	-2.563677	-2.643883	3.056960
O	-0.480028	-3.585391	-0.154270
O	1.441834	-6.284052	0.355089
C	3.606025	-3.212586	-3.418689
C	3.092623	-2.008990	-3.881417
N	3.375002	-1.618974	-5.136416
C	2.857446	-0.450869	-5.532031
N	2.087598	0.346593	-4.782779
C	-0.130568	1.610098	-3.425408

C	0.380461	2.837272	-4.178601
O	2.442140	5.673429	-3.311768
C	0.643268	6.453828	-5.521220
C	-0.356921	7.185570	-6.172815
H	-2.904158	6.671212	-3.974742
H	-1.142663	5.386427	-2.818087
H	2.867746	3.680633	-2.014330
H	3.045183	2.657835	-3.438270
H	1.209390	2.221117	-1.025043
H	2.668033	1.299817	-1.372285
H	0.415657	0.201262	-1.945347
H	2.294804	-3.151361	-0.305243
H	3.601371	-4.834266	0.248834
H	4.270845	-6.312606	-0.421167
H	2.422956	-6.479848	-2.654333
H	0.205703	-7.910055	-1.303648
H	0.701815	-8.005511	-3.013262
H	-0.624475	-5.576209	-1.692570
H	-1.460703	-6.759886	-2.732298
H	-1.990225	-5.187183	-4.394624
H	-0.662662	-4.311242	-5.177099
H	-1.651319	-2.589423	-3.934208
H	-0.330620	-3.119214	-2.850183
H	-3.369597	-2.777551	-0.895224
H	-2.354837	-1.679908	-1.851421
H	-2.355712	-1.239459	0.754699
H	0.347403	-2.129552	1.616781
H	1.465621	-0.917855	3.513729
H	0.786916	0.593010	4.127565
H	0.037109	-0.940281	4.561672
H	-2.340636	0.563420	2.037733
H	-2.231830	-0.137251	3.658892
H	-1.466511	1.410090	3.309568
H	-0.262720	0.730730	0.567041
H	0.606276	1.551967	1.864997
H	1.290452	0.094425	1.132766
H	-2.080464	-4.903273	4.207035
H	-2.835090	-2.512694	4.883328
H	-2.916894	-2.489712	7.871847
H	-4.109001	-1.822675	6.757161
H	-0.545898	-1.400242	7.924154
H	0.591941	0.769616	8.044944
H	-1.306719	3.938736	4.522062
H	0.234651	4.750075	4.208021
H	0.197344	2.994086	4.410710
H	1.144198	6.026509	8.556954
H	-2.828498	2.659224	6.206250
H	-3.955307	0.486769	6.070709
H	-0.588168	-6.488170	5.178765
H	0.551367	-5.241852	5.734534

H	1.655759	-6.024548	3.739367
H	0.449566	-6.330935	1.827946
H	1.507684	-3.575529	3.741969
H	0.847277	-4.009570	2.130996
H	4.228517	-3.808216	-4.083974
H	3.080314	-0.122458	-6.542559
H	-0.874322	1.957278	-2.694777
H	-0.661634	0.944332	-4.116368
H	0.963991	2.557930	-5.061904
H	-0.479380	3.393944	-4.557503
H	1.641445	6.404292	-5.952140
H	-0.089184	7.680195	-7.103144

conformer_21

F	2.306462	5.142170	-3.206844
C	1.632179	5.725468	-2.189709
F	2.218137	5.401507	-1.015766
F	1.720741	7.066242	-2.352649
O	0.263321	5.349993	-2.204525
C	-0.040023	4.025633	-2.063036
C	-1.412706	3.744957	-2.068688
C	-1.875224	2.433236	-1.943228
C	-0.954873	1.390191	-1.821618
C	-1.423207	0.000051	-1.637363
N	-2.207396	-0.580811	-2.634673
C	-2.656945	-1.956199	-2.443106
C	-1.678527	-2.921377	-3.107879
C	-1.485724	-2.557958	-4.593420
C	-0.521600	-3.495609	-5.304816
C	0.832674	-3.572107	-4.966256
N	1.421335	-2.831425	-3.986000
C	2.751402	-2.987372	-3.770976
C	3.538831	-3.869999	-4.484359
O	4.876906	-4.094938	-4.350712
C	5.573556	-3.451483	-3.288371
C	5.340247	-4.039961	-1.890123
N	5.160799	-5.403835	-1.871793
C	4.862621	-6.147077	-0.656586
C	3.410107	-5.975065	-0.198026
O	2.531282	-6.510699	-1.196802
C	1.154865	-6.542394	-0.786611
C	0.509740	-5.153372	-0.760412
O	0.808455	-4.499365	0.480067
C	0.321721	-3.157418	0.492784
C	0.553742	-2.476445	1.849608
N	0.249163	-1.130901	1.855890
C	0.258404	-0.346739	3.098270
C	0.599070	1.160022	2.841639
C	0.778853	1.918972	4.170912
C	-0.492234	1.881214	2.034404

C	1.929337	1.265484	2.063948
C	-1.131929	-0.556858	3.767468
N	-1.195913	-0.699705	5.137677
C	-2.479486	-0.911526	5.825857
C	-3.163876	0.442804	6.146926
N	-3.457518	1.197324	5.034268
C	-4.202078	2.435409	5.083373
C	-3.628380	3.444945	4.123809
C	-2.688319	4.385290	4.562822
C	-2.136196	5.311430	3.671091
C	-2.496536	5.310439	2.316388
C	-1.904602	6.283384	1.388578
C	-0.583430	6.682544	1.205523
C	0.622350	6.174766	1.917391
N	-0.390994	7.665473	0.239281
C	-1.546253	7.997781	-0.292160
S	-2.915926	7.176487	0.314526
C	-3.428879	4.357576	1.878526
C	-3.990704	3.436958	2.771225
O	-3.475326	0.789745	7.285692
C	-2.105053	-1.694340	7.084044
C	-0.705310	-1.182862	7.411504
O	0.011275	-2.115902	8.207064
C	-0.080854	-1.017042	6.024770
O	-2.172615	-0.553625	3.097059
O	0.976320	-3.066453	2.843967
O	5.357603	-3.350109	-0.871230
C	2.905551	-4.628119	-5.468516
C	1.550607	-4.498354	-5.738243
N	1.011723	-5.254299	-6.710847
C	-0.295112	-5.093865	-6.942632
N	-1.095424	-4.248353	-6.285232
C	-1.139317	-1.066963	-4.786807
C	-2.136604	-0.175348	-4.043021
O	-1.106352	-0.575997	-0.596171
C	0.415666	1.657967	-1.795833
C	0.871648	2.975355	-1.921157
H	-2.133266	4.555050	-2.168574
H	-2.944480	2.235050	-1.935258
H	-3.655687	-2.050151	-2.885313
H	-2.748168	-2.185813	-1.376153
H	-2.049545	-3.948929	-3.012633
H	-0.724435	-2.877939	-2.572241
H	-2.467369	-2.702683	-5.070636
H	3.144878	-2.349260	-2.985816
H	5.371839	-2.374096	-3.280747
H	6.643986	-3.564763	-3.496272
H	4.990820	-5.868842	-2.761361
H	5.542612	-5.808337	0.132160
H	5.069810	-7.199179	-0.877503

H	3.194917	-4.913402	-0.048310
H	3.263036	-6.512805	0.744928
H	1.070896	-7.049920	0.180877
H	0.638223	-7.151730	-1.535274
H	-0.578112	-5.255313	-0.837921
H	0.885920	-4.549421	-1.592260
H	-0.756830	-3.159807	0.299773
H	0.841926	-2.579006	-0.278854
H	-0.347870	-0.800694	1.090409
H	1.037130	-0.775255	3.736779
H	1.585825	1.483019	4.769141
H	1.038670	2.969449	3.992904
H	-0.137243	1.912578	4.770094
H	-0.690693	1.383108	1.085831
H	-1.431886	1.927750	2.588969
H	-0.199660	2.910207	1.803067
H	1.852993	0.821701	1.065581
H	2.228601	2.311695	1.930415
H	2.738771	0.755046	2.598107
H	-3.166576	-1.493698	5.200420
H	-3.301251	0.775269	4.119432
H	-4.214631	2.837776	6.102537
H	-5.240963	2.207506	4.818511
H	-2.380082	4.407765	5.607298
H	-1.427500	6.041544	4.056824
H	0.602728	5.085214	2.000164
H	1.534770	6.450030	1.378676
H	0.682734	6.604937	2.921413
H	-1.636363	8.746952	-1.069403
H	-3.723979	4.309516	0.831451
H	-4.706862	2.706455	2.397467
H	-2.065693	-2.769476	6.864288
H	-2.798267	-1.567739	7.921059
H	-0.747711	-0.218697	7.931435
H	-0.482025	-2.199645	9.050758
H	0.666566	-0.221608	6.011991
H	0.395139	-1.941736	5.679223
H	3.491230	-5.336990	-6.051263
H	-0.741653	-5.697905	-7.726402
H	-1.143415	-0.813621	-5.853846
H	-0.131652	-0.848898	-4.415253
H	-1.837992	0.868892	-4.153000
H	-3.140486	-0.277406	-4.471356
H	1.132077	0.847620	-1.677851
H	1.946398	3.136807	-1.901314

conformer_22

F	-7.092444	8.583849	-0.315015
C	-6.454684	9.111507	-1.383403
F	-6.241373	8.149786	-2.308713

F	-7.263752	10.048207	-1.932637
O	-5.236819	9.734625	-0.999117
C	-4.273487	8.957146	-0.422080
C	-4.359595	7.587521	-0.159419
C	-3.287571	6.916667	0.441382
C	-2.120257	7.614187	0.769116
C	-0.994608	6.920828	1.436349
N	-0.416562	5.812217	0.808606
C	-0.418392	5.650912	-0.652439
C	-0.352781	4.182608	-1.061306
C	0.836150	3.483763	-0.386308
C	1.004559	2.033452	-0.813080
C	0.038091	1.058412	-0.554774
N	-1.131953	1.294821	0.097828
C	-1.985556	0.259075	0.285547
C	-1.734486	-1.024849	-0.159341
O	-2.533115	-2.122291	-0.022949
C	-3.727793	-1.954284	0.737229
C	-4.509020	-3.272943	0.794138
N	-5.429045	-3.322561	1.819364
C	-6.204506	-4.513802	2.135689
C	-5.379325	-5.575974	2.869989
O	-4.879579	-5.030818	4.099431
C	-4.261842	-6.041500	4.912088
C	-3.286295	-5.373967	5.881550
O	-2.089973	-5.025046	5.164836
C	-1.194122	-4.263027	5.978810
C	0.228943	-4.272875	5.403705
N	0.483254	-5.347237	4.580569
C	1.745317	-5.521800	3.857073
C	2.114115	-7.028650	3.666495
C	1.080736	-7.803741	2.827363
C	2.214518	-7.707655	5.051150
C	3.489697	-7.159631	2.984609
C	1.629629	-4.730511	2.520180
N	2.614633	-3.818244	2.209222
C	2.558952	-3.021394	0.978879
C	3.060337	-3.826208	-0.245865
N	2.969021	-3.149755	-1.440748
C	3.298868	-3.778683	-2.700113
C	3.502883	-2.745769	-3.775780
C	4.748198	-2.124029	-3.934931
C	4.929566	-1.136131	-4.907675
C	3.869026	-0.748036	-5.736262
C	4.062854	0.298637	-6.739384
C	4.449530	1.624609	-6.591156
C	4.742823	2.330240	-5.312964
N	4.556224	2.341874	-7.778055
C	4.251701	1.562928	-8.793995
S	3.826654	-0.048991	-8.406725

C	2.621534	-1.363492	-5.570015
C	2.439219	-2.351192	-4.597333
O	3.524468	-4.963756	-0.163253
C	3.465643	-1.826501	1.269155
C	4.533035	-2.416230	2.189297
O	5.143868	-1.407242	2.979983
C	3.739229	-3.408338	3.042938
O	0.658048	-4.883393	1.770284
O	1.074871	-3.429413	5.695353
O	-4.348684	-4.198624	-0.000930
C	-0.534904	-1.236626	-0.834729
C	0.383968	-0.216269	-1.031462
N	1.541235	-0.507943	-1.649797
C	2.380403	0.514826	-1.855565
N	2.173175	1.776147	-1.465032
C	0.776532	3.663775	1.136872
C	0.681462	5.141396	1.506249
O	-0.639189	7.341596	2.537576
C	-2.033013	8.985756	0.528010
C	-3.106076	9.648816	-0.072466
H	-5.243702	7.002964	-0.401068
H	-3.370742	5.852283	0.653291
H	0.455445	6.193694	-1.034185
H	-1.293852	6.114350	-1.110803
H	-0.267859	4.109135	-2.152373
H	-1.297811	3.701643	-0.784520
H	1.740644	4.011435	-0.726385
H	-2.893784	0.528537	0.816630
H	-4.383083	-1.213948	0.263295
H	-3.476215	-1.652597	1.761068
H	-5.387796	-2.606839	2.540861
H	-6.604479	-4.929539	1.204990
H	-7.037964	-4.182009	2.763663
H	-4.531729	-5.899917	2.255911
H	-6.016079	-6.441421	3.086524
H	-3.726210	-6.760627	4.281395
H	-5.054492	-6.555457	5.465128
H	-3.018700	-6.076319	6.678199
H	-3.728892	-4.468946	6.312442
H	-1.138678	-4.681655	6.989952
H	-1.548907	-3.228308	6.017017
H	-0.354032	-5.782470	4.195564
H	2.519149	-5.063828	4.480315
H	1.025298	-7.426650	1.801521
H	1.348769	-8.865069	2.761645
H	0.078520	-7.751984	3.264339
H	2.934127	-7.188547	5.694393
H	1.248433	-7.718175	5.567511
H	2.544959	-8.748751	4.958866
H	4.269469	-6.654780	3.564651

H	3.784238	-8.211208	2.887406
H	3.483613	-6.731450	1.977837
H	1.527438	-2.711125	0.784317
H	2.396713	-2.306190	-1.486611
H	2.479787	-4.458648	-2.962243
H	4.198338	-4.394487	-2.582706
H	5.586692	-2.403174	-3.298322
H	5.911136	-0.676632	-5.013407
H	5.711448	2.011986	-4.915674
H	4.777328	3.413690	-5.465454
H	3.970537	2.121892	-4.565867
H	4.265599	1.909973	-9.820114
H	1.773320	-1.072021	-6.187541
H	1.455381	-2.803238	-4.479434
H	2.907104	-1.041985	1.796027
H	3.909198	-1.365702	0.381389
H	5.303489	-2.940050	1.611396
H	5.598604	-0.800451	2.358174
H	4.344992	-4.274379	3.321994
H	3.352481	-2.944253	3.956713
H	-0.305975	-2.233471	-1.206359
H	3.309448	0.301373	-2.374815
H	1.663641	3.224080	1.608597
H	-0.092998	3.144296	1.555800
H	0.550030	5.232114	2.590286
H	1.608127	5.667173	1.245560
H	-1.137762	9.540479	0.799978
H	-3.028239	10.718055	-0.264562

conformer_23

F	0.511119	7.906765	3.902497
C	0.123047	7.937350	2.608496
F	-1.132845	8.441288	2.560875
F	0.931380	8.763674	1.908619
O	0.108116	6.631866	2.045962
C	1.290473	5.951722	1.974178
C	2.530153	6.392860	2.444253
C	3.665676	5.586071	2.304293
C	3.565292	4.341418	1.678838
C	4.767277	3.484706	1.571377
N	5.179176	3.061498	0.311236
C	4.799022	3.702201	-0.952205
C	4.374895	2.657665	-1.979069
C	5.455396	1.572171	-2.145489
C	5.067247	0.484604	-3.139927
C	3.960417	-0.341466	-2.934145
N	3.127720	-0.227845	-1.868060
C	2.091765	-1.090080	-1.767157
C	1.846734	-2.099146	-2.677997
O	0.852484	-3.033620	-2.619650

C	-0.033777	-2.939761	-1.505301
C	-1.081485	-4.055591	-1.533139
N	-1.878318	-4.088664	-0.406403
C	-2.821834	-5.170116	-0.150472
C	-2.157872	-6.343171	0.578280
O	-1.863801	-5.931201	1.920356
C	-1.065452	-6.897887	2.619568
C	-0.894310	-6.429318	4.065956
O	-0.172071	-5.189923	4.068146
C	-0.190032	-4.559563	5.353173
C	0.209421	-3.086233	5.207445
N	0.973301	-2.833767	4.087180
C	1.170020	-1.482162	3.559575
C	2.567988	-1.295468	2.893465
C	2.681061	0.112777	2.278446
C	2.861007	-2.338497	1.800593
C	3.662421	-1.423731	3.976627
C	-0.033816	-1.222166	2.601866
N	-0.783646	-0.074153	2.760463
C	-1.944253	0.182084	1.895686
C	-1.566975	0.434718	0.419233
N	-2.648130	0.455568	-0.432941
C	-2.515951	0.786800	-1.833661
C	-3.708069	0.293971	-2.608981
C	-3.765607	-1.033013	-3.054392
C	-4.885829	-1.503131	-3.746007
C	-5.973307	-0.658000	-4.001123
C	-7.148399	-1.163087	-4.711713
C	-7.991941	-2.226195	-4.413770
C	-7.910816	-3.126366	-3.229701
N	-9.013098	-2.442405	-5.333634
C	-8.931865	-1.554162	-6.300766
S	-7.654676	-0.422048	-6.179335
C	-5.919104	0.666450	-3.546175
C	-4.798778	1.137103	-2.853872
O	-0.413770	0.620890	0.034383
C	-2.601111	1.445176	2.471070
C	-2.128554	1.485489	3.916585
O	-2.992544	0.684085	4.730259
C	-0.718523	0.895562	3.853235
O	-0.337896	-2.049393	1.730136
O	-0.114436	-2.219126	6.016534
O	-1.206291	-4.850926	-2.463624
C	2.710637	-2.188232	-3.768774
C	3.781295	-1.315086	-3.928807
N	4.582165	-1.448426	-5.001304
C	5.606186	-0.591226	-5.097713
N	5.895133	0.372787	-4.215449
C	5.895577	0.988551	-0.789359
C	6.265148	2.091132	0.198518

O	5.327292	3.160033	2.618442
C	2.326960	3.882998	1.221346
C	1.197454	4.691669	1.367600
H	2.658903	7.356729	2.930412
H	4.624575	5.936187	2.681866
H	5.677645	4.253129	-1.310687
H	4.006514	4.441032	-0.817372
H	4.180189	3.145071	-2.942111
H	3.425180	2.223289	-1.650942
H	6.338052	2.079568	-2.563782
H	1.469479	-0.921893	-0.894664
H	-0.569499	-1.984259	-1.526144
H	0.533736	-3.055631	-0.576145
H	-1.594677	-3.530234	0.399339
H	-3.238779	-5.510062	-1.104279
H	-3.625867	-4.744059	0.458353
H	-1.236262	-6.646006	0.068236
H	-2.846873	-7.193394	0.618741
H	-0.090007	-6.967152	2.126028
H	-1.564272	-7.872431	2.598739
H	-0.334594	-7.169946	4.645862
H	-1.882182	-6.276792	4.515182
H	0.518541	-5.060711	6.019191
H	-1.199886	-4.584959	5.776537
H	0.923221	-3.587426	3.399850
H	1.117358	-0.797654	4.407886
H	2.475685	0.888141	3.024645
H	3.688142	0.292812	1.885334
H	1.981510	0.248016	1.448174
H	2.873362	-3.356904	2.202059
H	2.118542	-2.302471	1.001805
H	3.840606	-2.160660	1.341487
H	3.664749	-2.420331	4.431196
H	4.659354	-1.254846	3.553523
H	3.515415	-0.690297	4.777518
H	-2.612623	-0.685593	1.956668
H	-3.585458	0.466370	-0.042020
H	-1.591351	0.354518	-2.233735
H	-2.419079	1.875868	-1.914554
H	-2.937690	-1.713541	-2.864605
H	-4.896149	-2.536982	-4.087846
H	-7.725859	-2.555143	-2.314567
H	-8.846598	-3.678485	-3.095562
H	-7.103637	-3.853676	-3.359656
H	-9.626650	-1.530783	-7.131636
H	-6.753922	1.344751	-3.714817
H	-4.788680	2.168525	-2.503297
H	-3.691462	1.401274	2.378429
H	-2.248074	2.340786	1.944450
H	-2.135910	2.496739	4.332235

H	-2.810760	-0.255574	4.522755
H	0.019509	1.652271	3.570329
H	-0.439942	0.422838	4.795989
H	2.548894	-2.965541	-4.513178
H	6.257507	-0.688128	-5.961087
H	6.751111	0.316141	-0.927051
H	5.093014	0.385816	-0.348640
H	6.493197	1.645064	1.172456
H	7.160766	2.628190	-0.134775
H	2.233086	2.905033	0.754847
H	0.236183	4.332317	1.002925

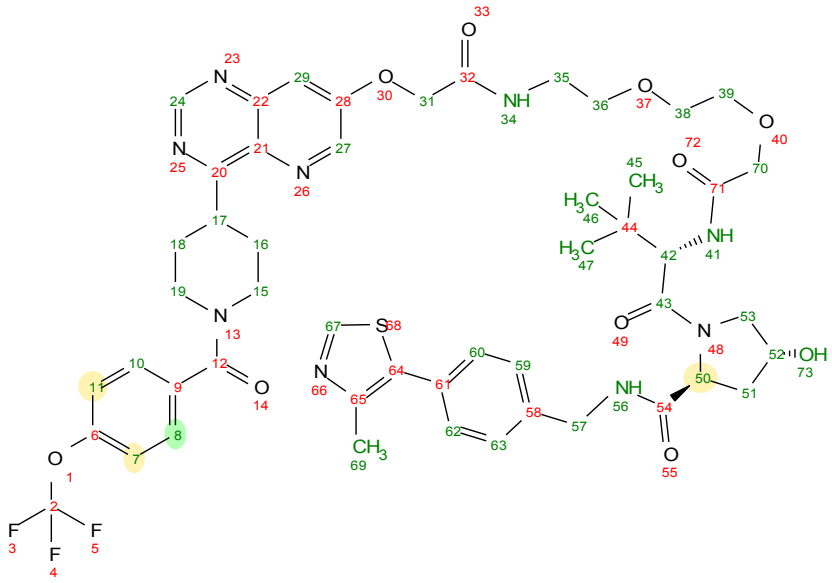
conformer_24

F	-1.141690	10.387720	-0.922399
C	-2.033321	9.653086	-1.623490
F	-2.319948	8.517036	-0.949275
F	-3.174335	10.373580	-1.733625
O	-1.549929	9.368191	-2.928902
C	-0.421033	8.607452	-3.040884
C	-0.052965	8.310474	-4.359958
C	1.077352	7.535883	-4.631450
C	1.842370	7.043423	-3.573848
C	3.045516	6.229452	-3.863800
N	3.132491	4.943370	-3.320602
C	4.323284	4.155878	-3.636141
C	4.626268	3.097342	-2.574374
C	3.403998	2.256983	-2.155813
C	3.016762	1.158149	-3.144451
C	2.219889	0.096806	-2.709469
N	1.793284	-0.045375	-1.424852
C	0.984566	-1.091847	-1.134505
C	0.576087	-2.021299	-2.072422
O	-0.269406	-3.073543	-1.880970
C	-0.803292	-3.239679	-0.568865
C	-1.833276	-4.373685	-0.572253
N	-2.151525	-4.836360	0.686207
C	-3.019446	-5.984241	0.898582
C	-2.291237	-7.313138	0.679584
O	-1.253988	-7.449529	1.661689
C	-0.575014	-8.707055	1.530226
C	0.558514	-8.767034	2.552244
O	1.636824	-7.916372	2.125397
C	2.648649	-7.819817	3.128670
C	2.416955	-6.658638	4.104039
N	1.915817	-5.523147	3.507958
C	1.515186	-4.327200	4.258056
C	2.458358	-3.116633	3.946199
C	3.917303	-3.490248	4.292418
C	2.083626	-1.893193	4.802894
C	2.408990	-2.700267	2.462363

C	0.030230	-4.062437	3.882477
N	-0.841067	-3.655451	4.865862
C	-2.236946	-3.335789	4.555196
C	-2.389302	-1.850397	4.155346
N	-3.541171	-1.570809	3.457191
C	-3.919470	-0.228815	3.075643
C	-3.410885	0.146657	1.707152
C	-2.165559	0.770453	1.557029
C	-1.724434	1.186416	0.297022
C	-2.514468	0.980998	-0.841527
C	-2.073953	1.489509	-2.142736
C	-1.700734	2.773821	-2.523009
C	-1.714573	3.998463	-1.674405
N	-1.279898	2.898780	-3.842510
C	-1.373754	1.734891	-4.447579
S	-1.953866	0.437034	-3.496479
C	-3.740007	0.317063	-0.696223
C	-4.181863	-0.100768	0.564472
O	-1.588575	-0.980782	4.500366
C	-2.990359	-3.616869	5.853137
C	-1.958443	-3.294279	6.933757
O	-2.247708	-3.985541	8.140795
C	-0.643953	-3.768344	6.306918
O	-0.353225	-4.167867	2.709713
O	2.693190	-6.731808	5.300302
O	-2.348181	-4.824912	-1.595398
C	1.056592	-1.867106	-3.372182
C	1.881718	-0.809213	-3.725336
N	2.292131	-0.700015	-5.000950
C	3.061774	0.353641	-5.294436
N	3.441554	1.298965	-4.427450
C	2.220126	3.188224	-1.849380
C	1.940456	4.153774	-2.993659
O	3.928852	6.740704	-4.552041
C	1.499529	7.354227	-2.253564
C	0.365023	8.130108	-1.988881
H	-0.651578	8.684134	-5.189693
H	1.348627	7.315801	-5.661503
H	5.190158	4.820996	-3.726448
H	4.169331	3.710481	-4.624439
H	4.991326	3.620731	-1.679693
H	5.448119	2.454947	-2.912578
H	3.691579	1.748926	-1.224648
H	0.673033	-1.131444	-0.095182
H	-1.326979	-2.333547	-0.242356
H	0.005939	-3.496833	0.122867
H	-1.509573	-4.605176	1.450848
H	-3.874145	-5.909699	0.218370
H	-3.378545	-5.913081	1.930443
H	-1.849134	-7.353801	-0.322105

H	-3.003341	-8.138376	0.791794
H	-0.176092	-8.798189	0.513854
H	-1.290050	-9.513754	1.724261
H	0.935291	-9.793184	2.622017
H	0.199125	-8.435743	3.533284
H	3.599285	-7.625313	2.620805
H	2.748347	-8.758195	3.685896
H	1.570157	-5.621906	2.553850
H	1.582366	-4.563367	5.323887
H	4.294838	-4.292560	3.649397
H	4.587362	-2.632271	4.162760
H	4.002992	-3.821948	5.333249
H	1.073185	-1.538314	4.582459
H	2.141855	-2.124889	5.871479
H	2.765706	-1.055601	4.614513
H	1.421164	-2.321215	2.181691
H	3.128296	-1.898738	2.256033
H	2.654552	-3.535287	1.797940
H	-2.601554	-3.964931	3.735909
H	-4.119180	-2.331595	3.113221
H	-3.555436	0.486563	3.822686
H	-5.014197	-0.178476	3.097587
H	-1.538078	0.959163	2.427426
H	-0.757614	1.681411	0.218495
H	-1.626425	4.899134	-2.290728
H	-2.648660	4.070728	-1.108593
H	-0.877150	3.986811	-0.970586
H	-1.106074	1.595404	-5.487883
H	-4.381725	0.142356	-1.558618
H	-5.149199	-0.594275	0.649217
H	-3.273666	-4.675659	5.909460
H	-3.905227	-3.028113	5.974930
H	-1.921121	-2.217278	7.134286
H	-3.117848	-3.655466	8.450546
H	0.200325	-3.154676	6.629349
H	-0.425131	-4.813554	6.553748
H	0.760690	-2.582375	-4.137308
H	3.402386	0.452710	-6.320512
H	2.458547	3.771375	-0.949852
H	1.312334	2.620639	-1.620141
H	1.642824	3.619673	-3.903657
H	1.098276	4.791638	-2.722592
H	2.109641	6.994599	-1.427234
H	0.134560	8.341059	-0.947689

8. NMR Spectra of PROTAC 1



Structure and numbering of PROTAC **1**

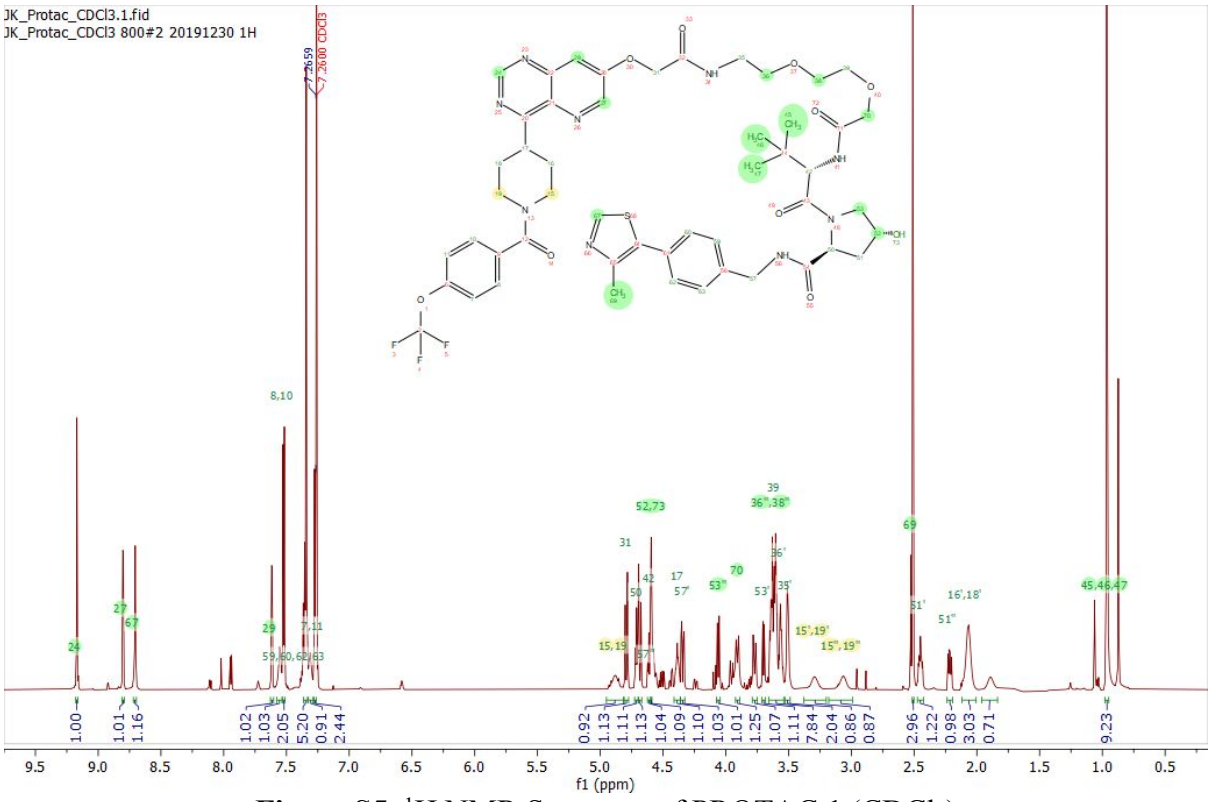


Figure S5. ^{1}H NMR Spectrum of PROTAC **1** ($CDCl_3$)

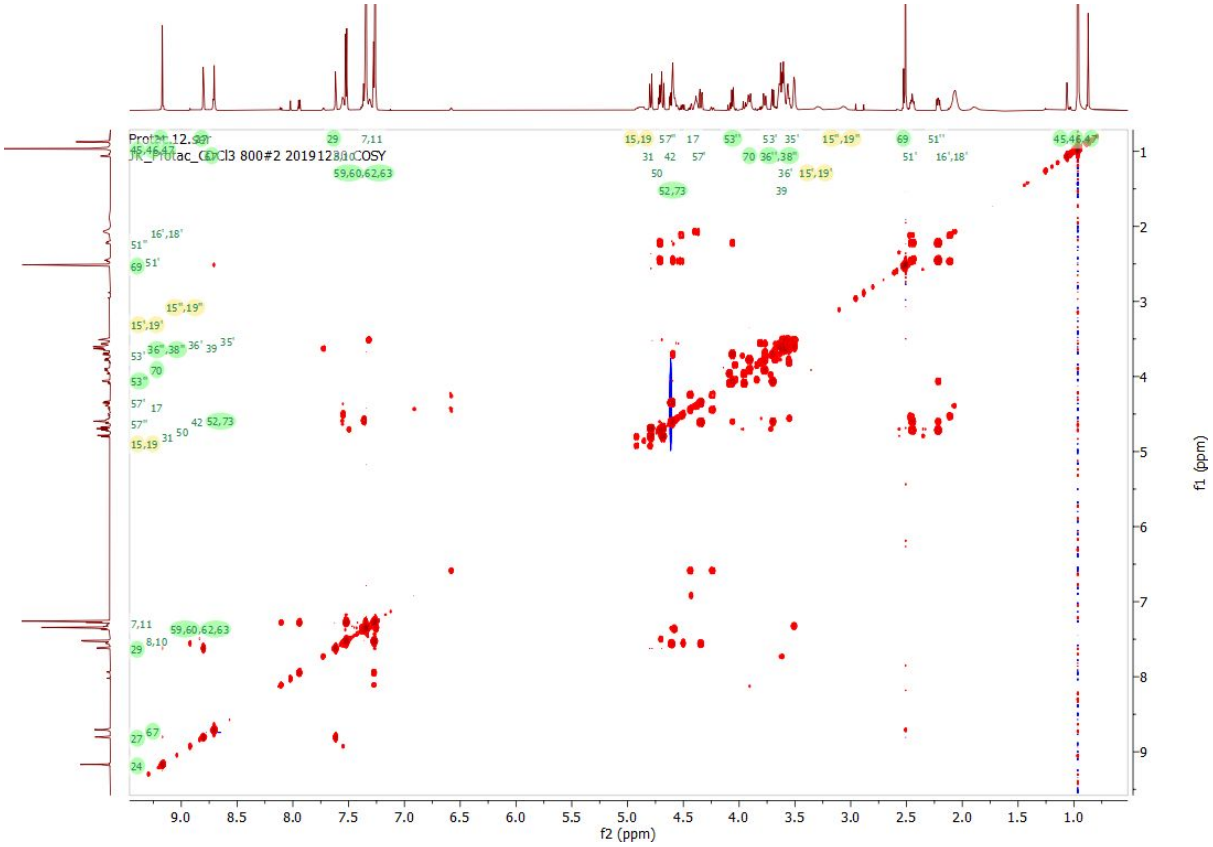


Figure S6. COSY Spectrum of PROTAC **1** ($CDCl_3$)

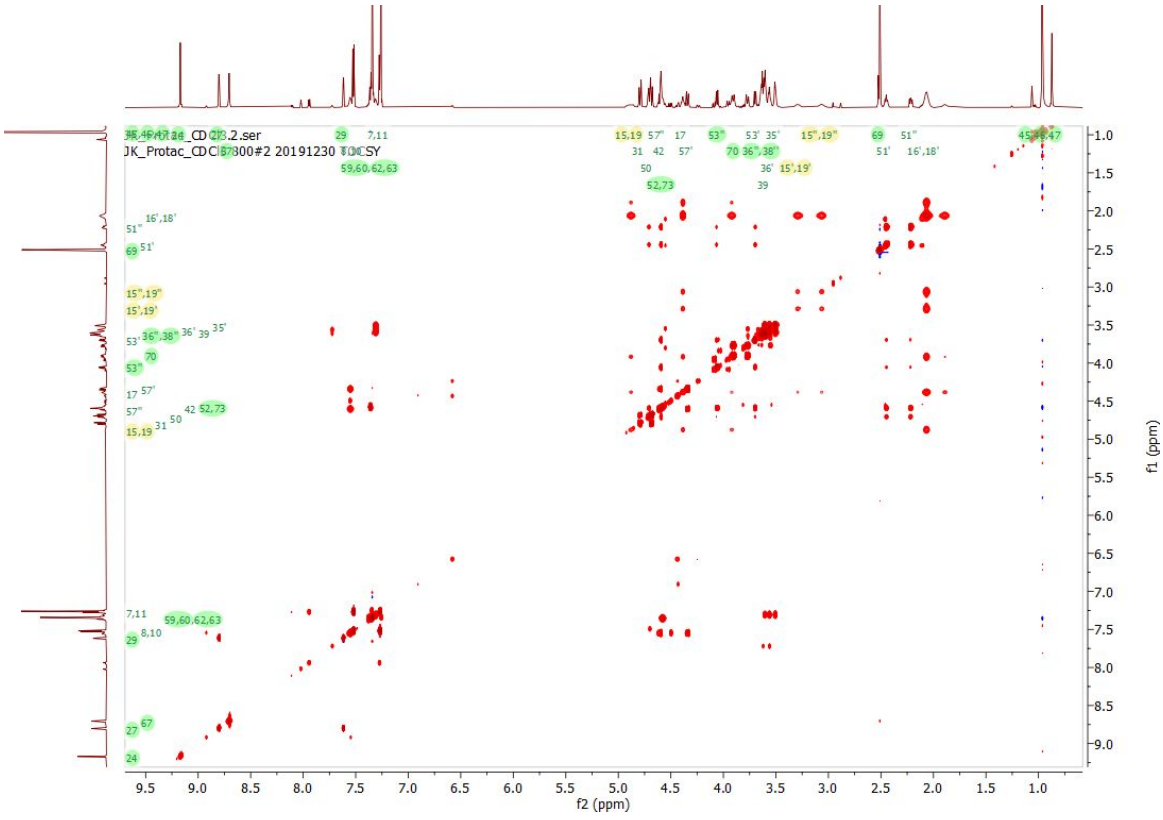


Figure S7. TOCSY Spectrum of PROTAC **1** ($CDCl_3$)

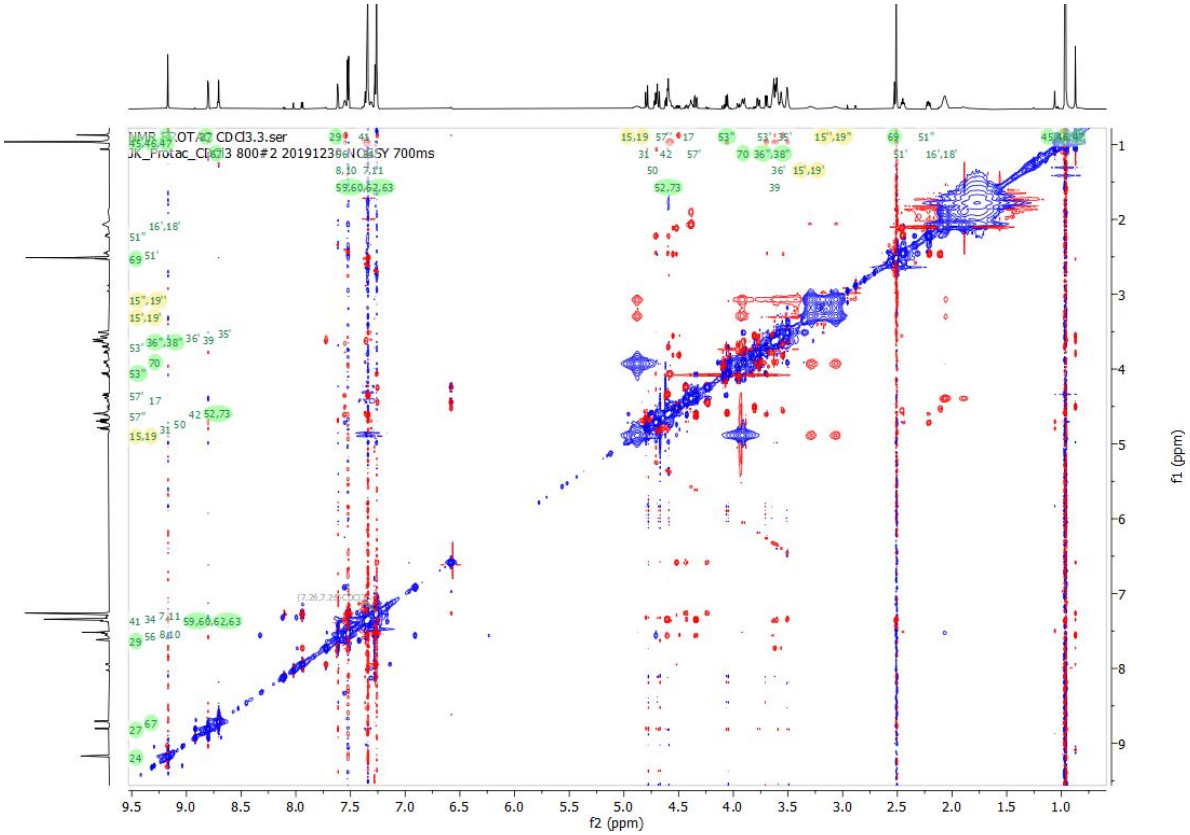


Figure S8. NOESY Spectrum of PROTAC **1** ($CDCl_3$)

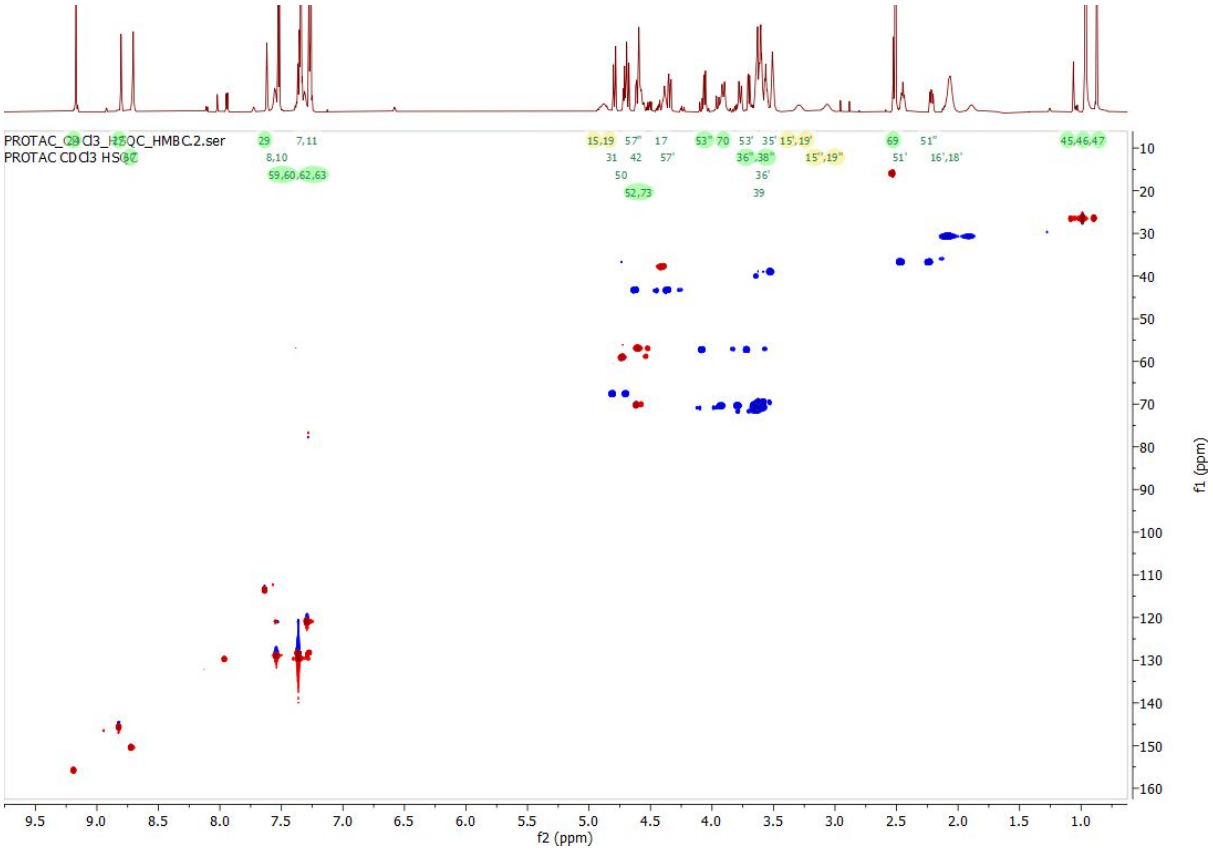


Figure S9. HSQC Spectrum of PROTAC **1** ($CDCl_3$)

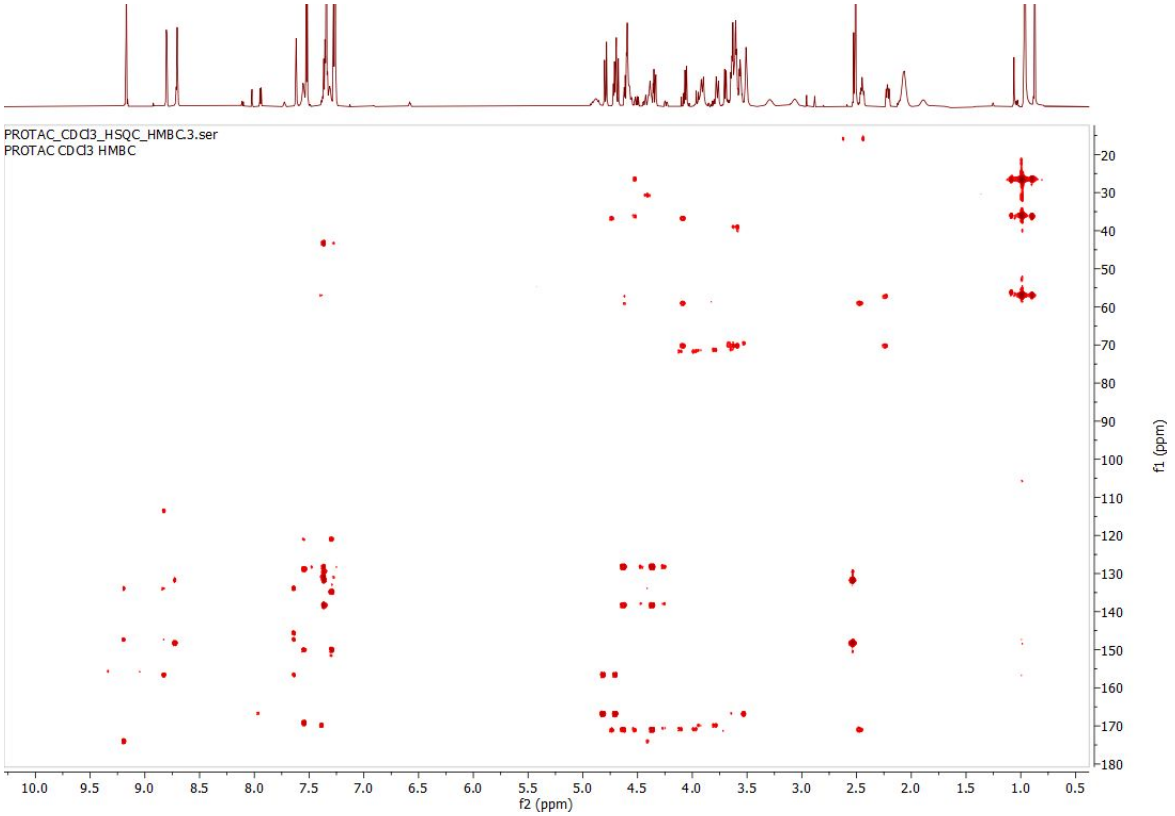


Figure S10. HMBC Spectrum of PROTAC **1** ($CDCl_3$)

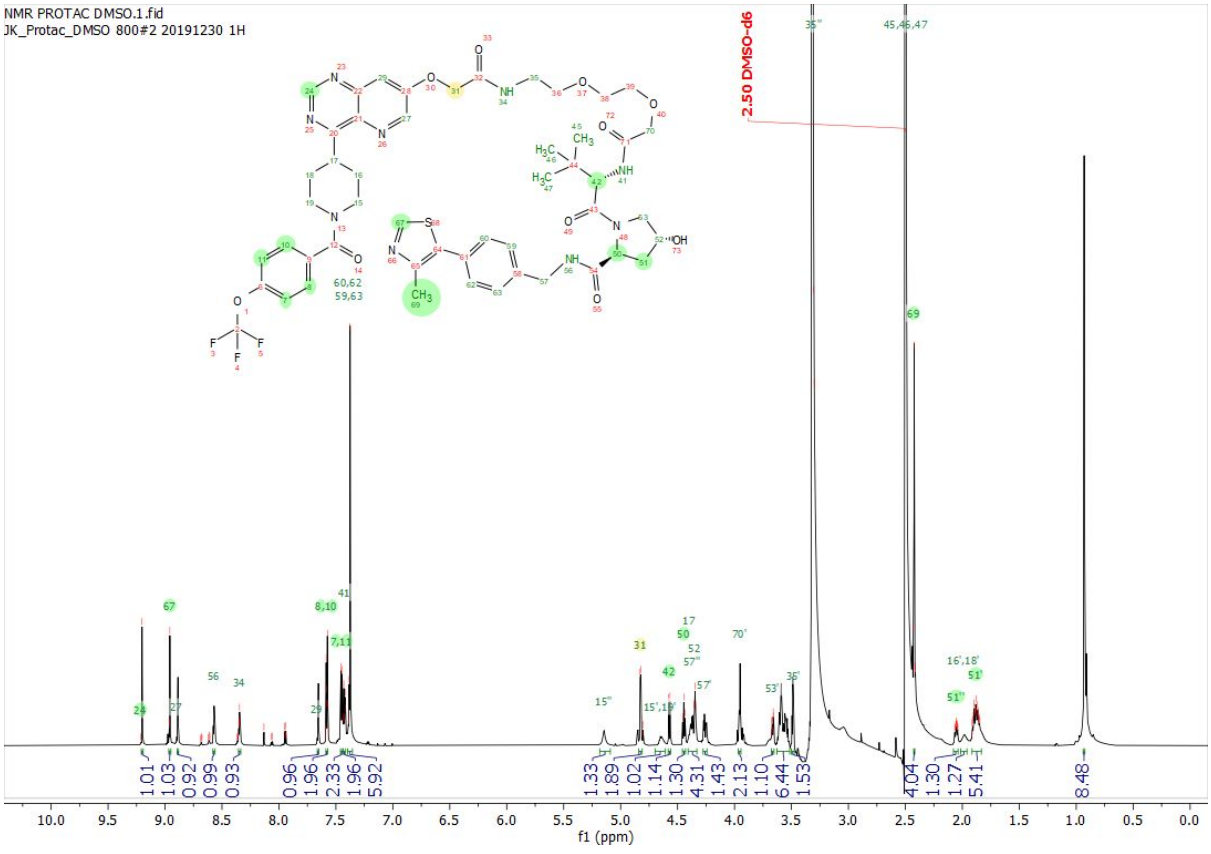


Figure S11. ^{1}H NMR Spectrum of PROTAC **1** (DMSO-d_6)

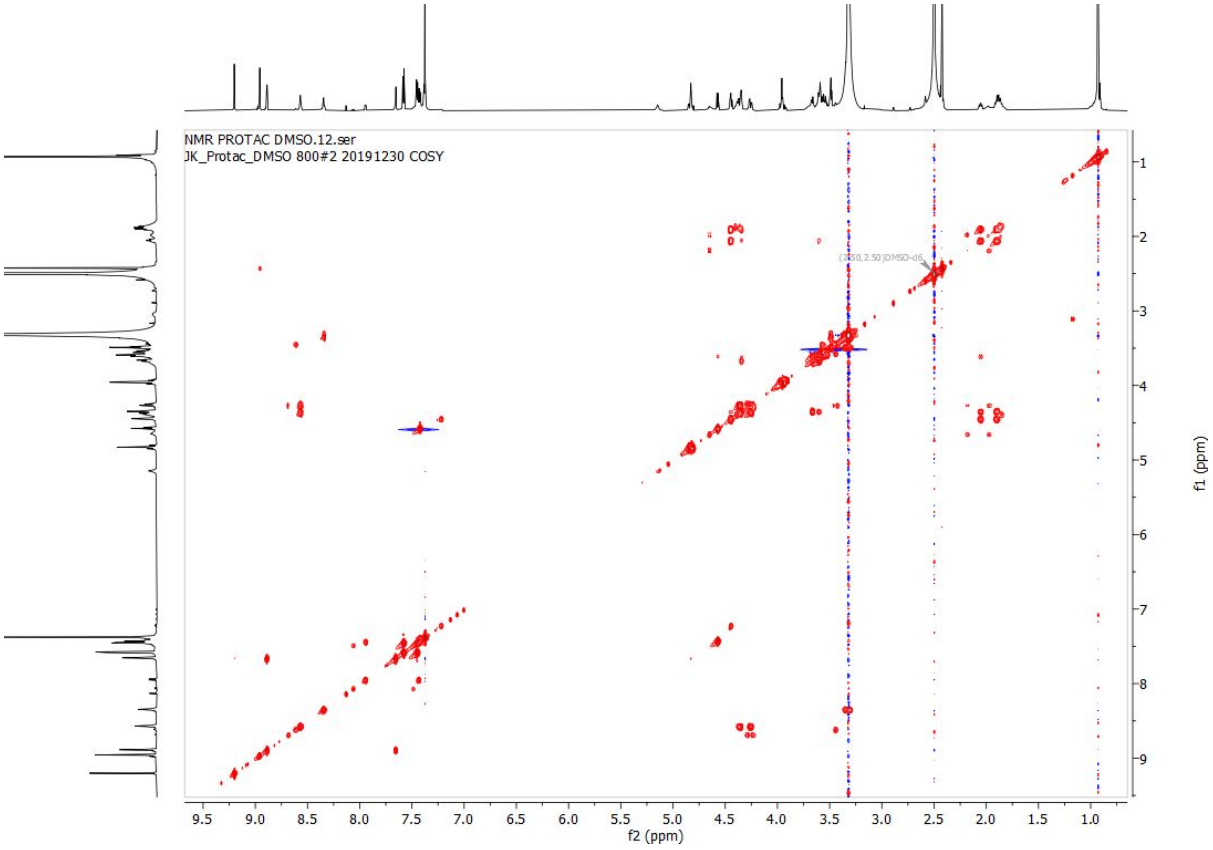


Figure S12. COSY Spectrum of PROTAC **1** (DMSO-d_6)

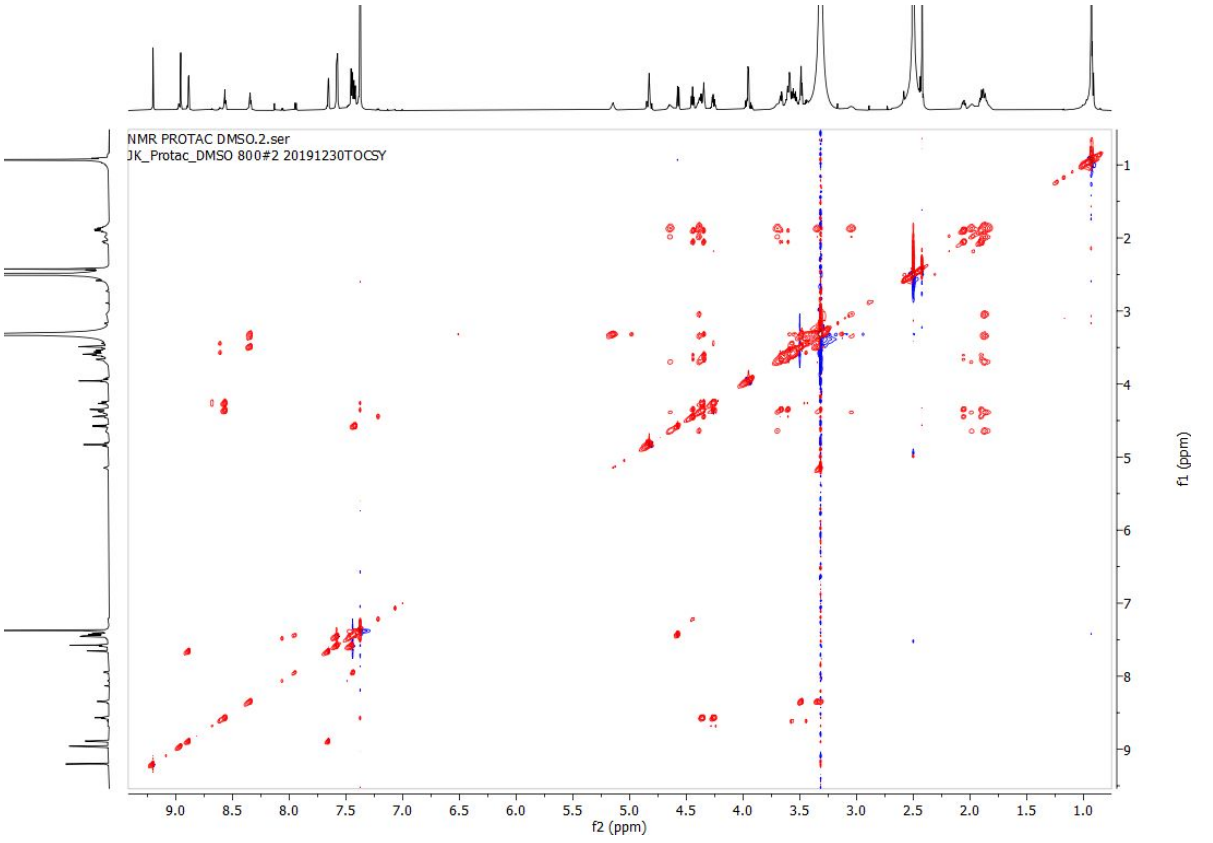


Figure S13. TOCSY Spectrum of PROTAC **1** (DMSO-d_6)

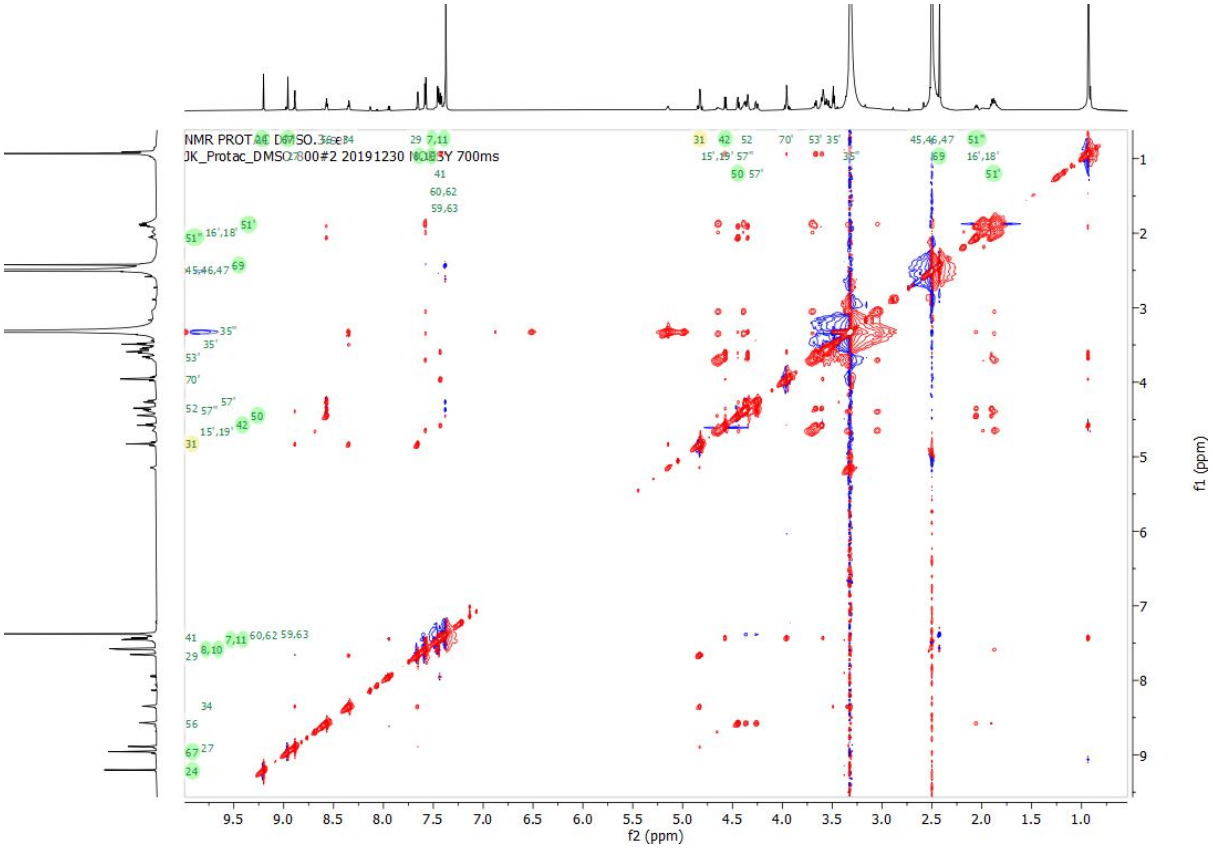


Figure S14. NOESY Spectrum of PROTAC **1** (DMSO-d_6)

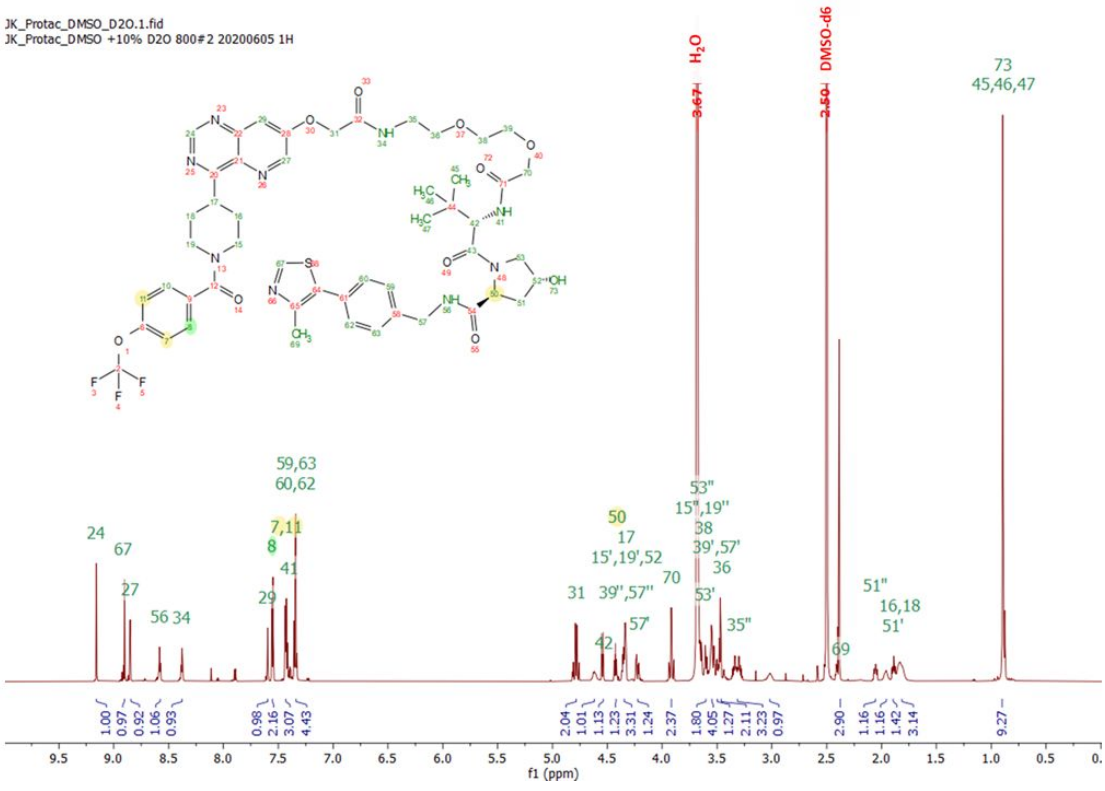


Figure S15. ^{1}H NMR Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

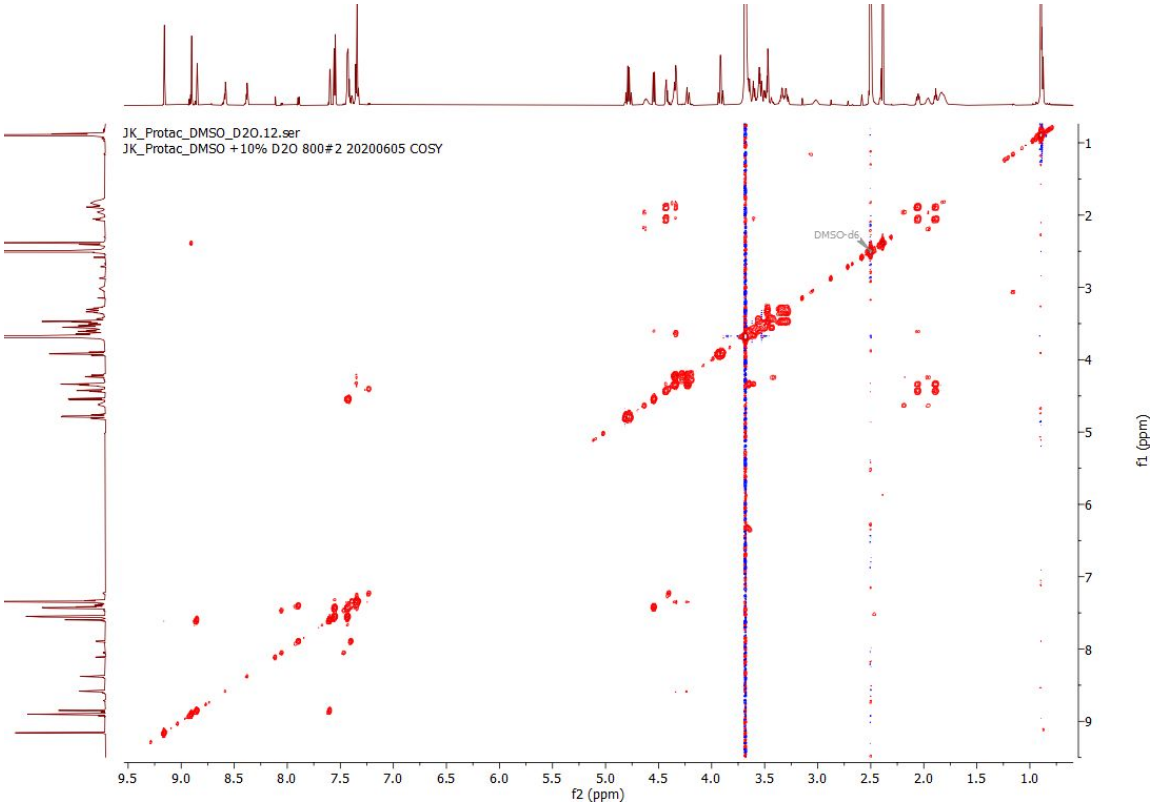


Figure S16. COSY Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

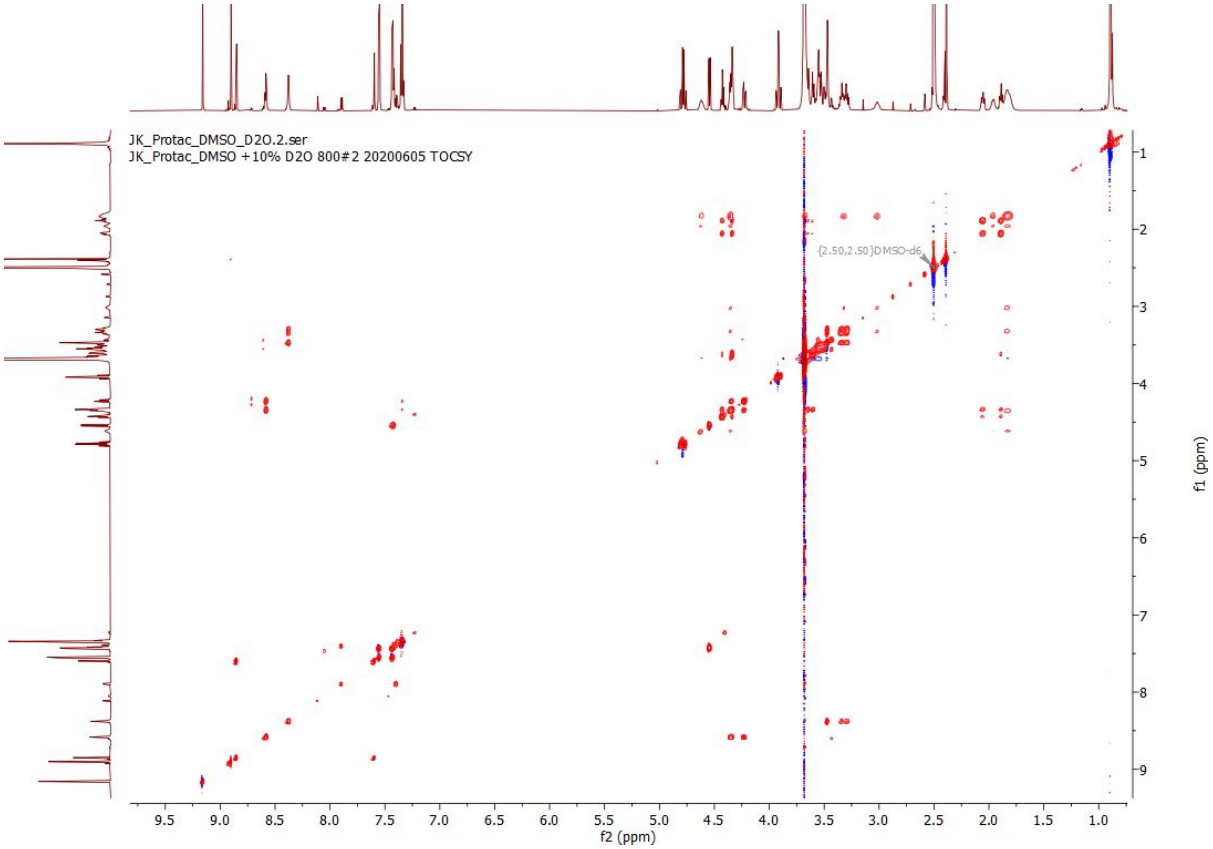


Figure S17. TOCSY Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

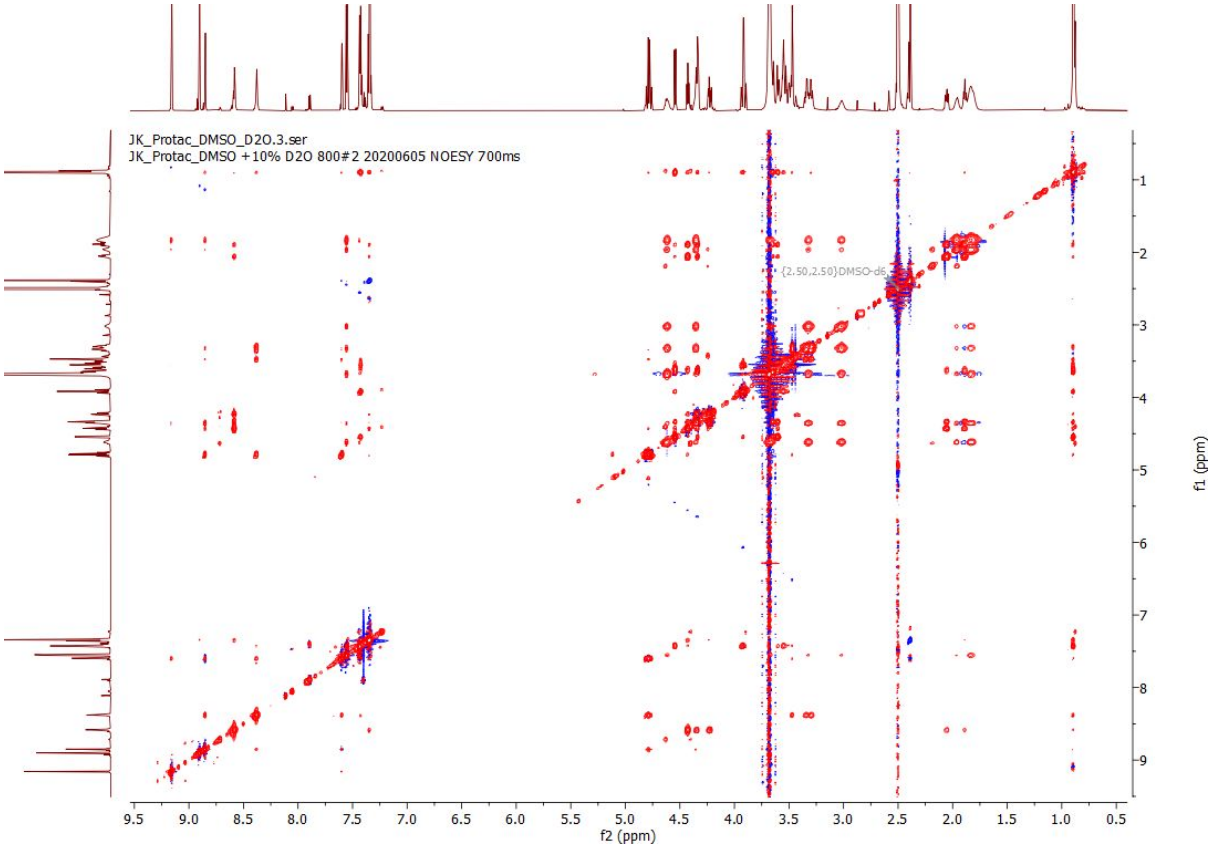


Figure S18. NOESY Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

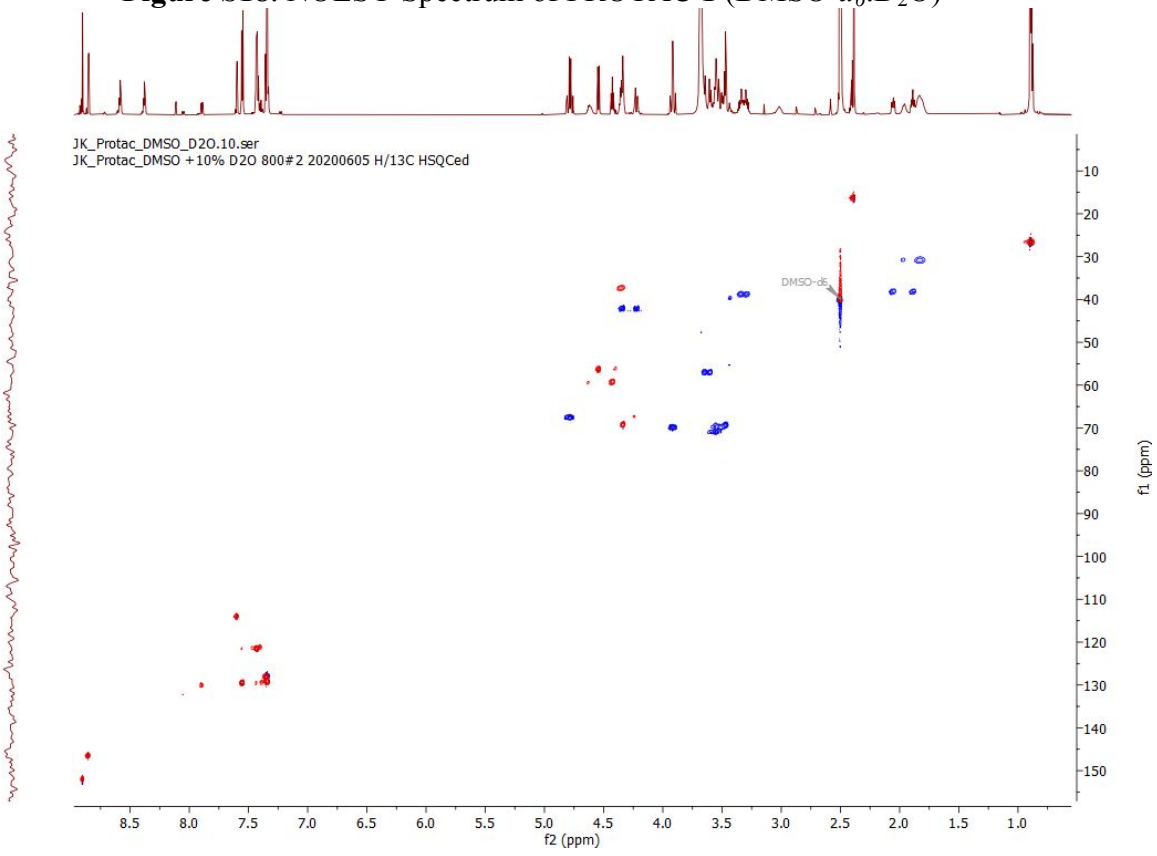


Figure S19. HSQC Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

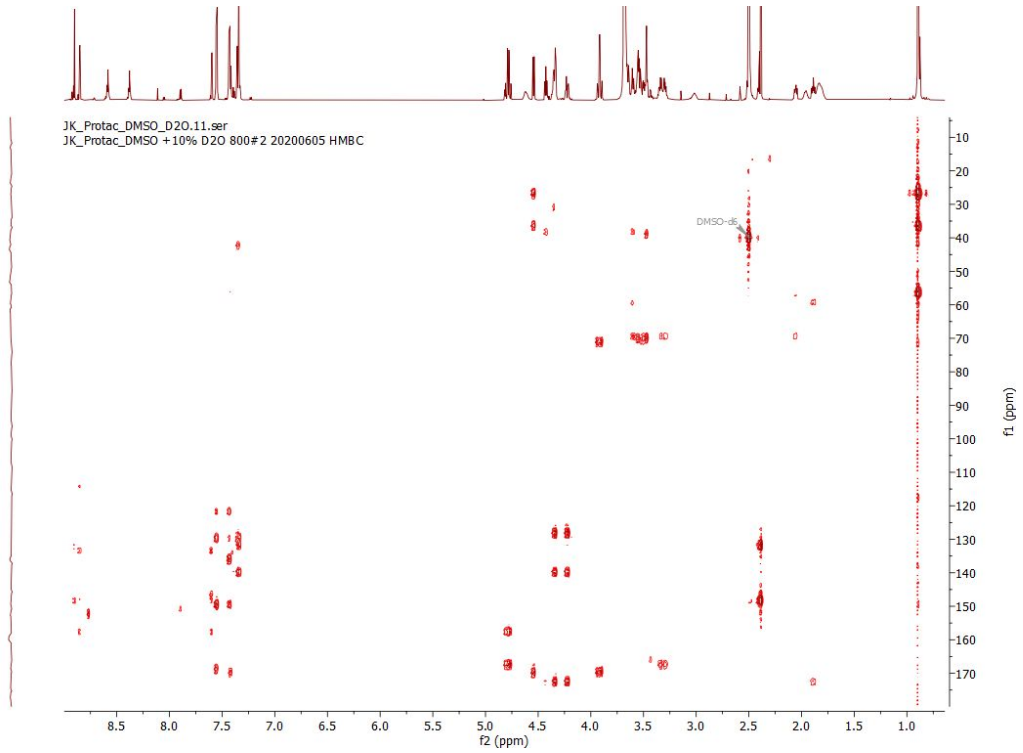


Figure S20. HMBC Spectrum of PROTAC **1** (DMSO-d_6:D_2O)

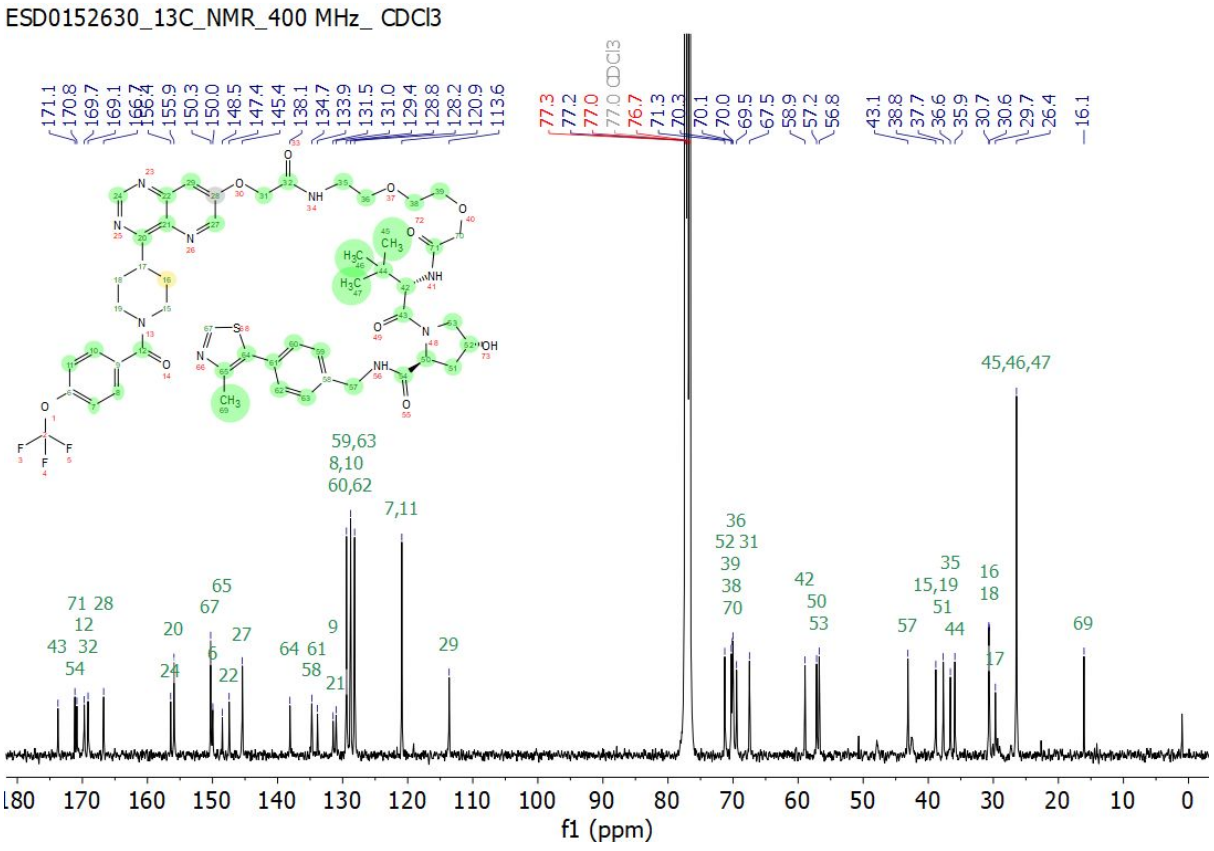


Figure S21. ^{13}C NMR Spectrum of PROTAC **1** ($CDCl_3$)

9. References

1) Nguyen, D; Wortmann, L.; Lemos, C.; Boemer, U.; Suelzle, D.; Holton; S. J.; Lechner; C. The identification and use of ERK5 inhibitors. WO2019/170543 A1, September, 12th, 2019. Also see: Nguyen, D.; Lemos, C.; Wortmann, L.; Eis, K.; Holton,S. J.; Boemer, U.; Moosmayer, D.; Eberspaecher, U.; Weiske, J.; Lechner, C.; Prechtl; S.; Suelzle, D.; Siegel, F.; Prinz, F.; Lesche, R.; Nicke, B.; Nowak-Reppel, K.; Himmel, H.; Mumberg, D.; von Nussbaum, F.; Nising, C. F.; Bauser. M, Haegebarth, A. Discovery and characterization of the potent and highly selective (Piperidin-4-yl)pyrido[3,2-*d*]pyrimidine based *in vitro* probe BAY-885 for the kinase ERK5. *J. Med. Chem*. **2019**, *62*, 928−940.
2) Chan, K.-H.; Zengerle, M.; Testa, A.; Ciulli., A. Impact of target warhead and linkage vector on inducing protein degradation: Comparison of Bromodomain and extra-terminal (BET) degraders derived from triazolodiazepine (JQ1) and tetrahydroquinoline (I-BET726) BET inhibitor scaffolds. *J. Med. Chem*. **2019**, *61*, 504−513. Yang, B.; Kettle, J. G.; Haylow, T. G. C.; Rasmusson, T. G.; Nissink, J. W. M.; Fallan, C.; Lamont, G. M. Compounds and their use in treating cancer. US2019194190 A1, June 27th, **2019**.
3) Cicero, D. O.; Barbato, G.; Bazzo, R., NMR Analysis of Molecular Flexibility in Solution: A New Method for the Study of Complex Distributions of Rapidly Exchanging Conformations. Application to a 13-Residue Peptide with an 8-Residue Loop. *J. Am. Chem. Soc.* **1995**, *117* , 1027-1033.
4) Nevins, N.; Cicero, D.; Snyder, J. P., A Test of the Single-Conformation Hypothesis in the Analysis of NMR Data for Small Polar Molecules: A Force Field Comparison. *J. Org. Chem.* **1999**, *64* , 3979-3986.
5) Maple, H. J.; Clayden, N.; Baron, A.; Stacey, C.; Felix, R. Developing degraders: principles and perspectives on design and chemical space. *Med. Chem. Comm.,* **2019**, *10*, 1755-1764.
6) MOE Molecular Operating Environment, Chemical Computing Group ULC, 1010 Sherbooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7., **2016**.
7) Team, R. RStudio Team. R Studio: Integrated Development for R. RStudio, PBC, Boston, MA **2020**.
8) Danelius, E.; Poongavanam, V.; Peintner, S.; Wieske, L. H. E.; Erdelyi, M.; Kihlberg, J. Solution Conformations Explain the Chameleonic Behaviour of Macrocyclic Drugs. *Chem. Eur. J.* **2020**, *26*, 5231-5244.
9) Sander, T.; Freyss, J.; von Korff, M.; Rufener, C. DataWarrior: an open-source program for chemistry aware data visualization and analysis. *J. Chem. Inf. Model.* **2015**, *55*, 460-73.
10) Maestro Schrödinger Release 2019, Schrödinger, LLC, New York, NY, **2019**.