Emission Wavelength Prediction of a Full-Color-Tunable Fluorescent Core Skeleton, 9-Aryl-1,2-dihydropyrrolo[3,4-*b*]indolizin-3-one (Seoul-Fluor)

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The geometry of the molecules was optimized using the Materials Studio® 4.2 program (Accelrys Software Inc.). Truncated structure was used to reduce the calculation time. A generalized gradient approximation (GAA) for the exchange-correlation function of Perdew, Burke, and Ernzerhof (PBE) was used with the double numerical basis set with polarization (DNP) as implemented in DMol3. The TD-DFT (Time Dependent Density Functional Theory) calculation of energy gap (S_1-S_0) of the molecules was executed with the optimized Cartesian coordinates using Gaussian 03 (Gaussian, Inc.) program in the Seoul National University Computer Center. A Becke's three-parameter exchange functional with the Lee, Yang, and Parr correlation (B3LYP) functional was used with the 6-31G* basis set. The followings are the input parameters and coordinates for the calculation.

Input parameters

<Geometry Optimization>

```
# Task parameters

Calculate                    optimize

Opt_energy_convergence       2.0000e-005

Opt_gradient_convergence     4.0000e-003 A

Opt_displacement_convergence 5.0000e-003 A
```

```
Opt_iterations                50
Opt_max_displacement          0.3000 A
Symmetry                      on

# Electronic parameters
Spin_polarization             restricted
Charge                        0
Basis                         dnp
Pseudopotential               none
Functional                    pbe
Aux_density                   octupole
Integration_grid              medium
Occupation                    fermi
Cutoff_Global                 3.3000 angstrom
Scf_density_convergence       1.0000e-005
Scf_charge_mixing             0.2000
Scf_iterations                50
Scf_diis                      6 pulay

# Print options
Print                         eigval_last_it

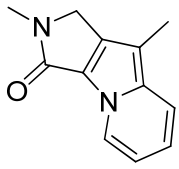
# Calculated properties
Plot                          homo
Plot                          lumo
Plot                          density
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Plot	potential
Mulliken_analysis	population
Hirshfeld_analysis	charge
Frequency_analysis	on
Grid	msbox 3 0.2500 0.2500 0.2500 3.0000

<Energy gap calculation>

B3LYP/6-31+G* TD

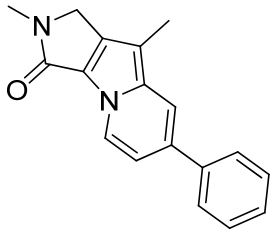
Input Coordinates



A1

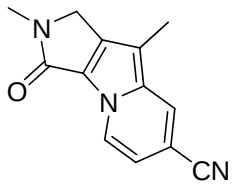
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C	-0.47791	-0.33058	0.00005
C	-0.63882	0.95196	0.00135
N	0.85734	-0.63867	-0.00055
C	1.5453	0.57298	0.00025
C	0.65896	1.58685	0.00155
O	-1.88217	-2.22507	-0.00165
C	-4.10112	-0.25162	0.00015
C	1.48921	-1.8689	-0.00205
C	2.83416	-1.87838	-0.00275
C	3.62345	-0.57169	-0.00175
C	2.98525	0.61133	-0.00025
C	0.94159	3.05489	0.00275
H	-2.34355	1.98383	-0.88745
H	-2.34332	1.98199	0.89285
H	-4.27616	-1.31516	-0.00085
H	-4.55368	0.20151	-0.88935
H	-4.55397	0.19995	0.89035
H	0.91571	-2.79168	-0.00265
H	3.35911	-2.81265	-0.00395
H	4.69418	-0.60183	-0.00225

H	3.52376	1.55206	0.00045
H	0.02985	3.61513	0.00355
H	1.53911	3.30602	-0.88715
H	1.53985	3.30447	0.89255



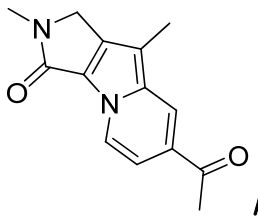
A3

N	-3.0406	0.6831	1.0235
C	-2.4083	0.3441	-0.1816
C	-1.0368	0.0924	0.2253
C	-0.8417	0.2547	1.5894
C	-2.1609	0.6391	2.1952
C	0.5027	0.0149	1.9065
C	1.1274	-0.3076	0.6768
N	0.1525	-0.2456	-0.3571
C	0.4725	-0.4804	-1.6707
C	1.7628	-0.7862	-2.0041
C	2.7885	-0.8807	-1.0099
C	2.4442	-0.6417	0.3151
O	-2.9452	0.288	-1.2933
C	-4.4539	0.9472	1.1089
C	1.1837	0.077	3.2363
H	-2.1333	1.6215	2.7022
H	-2.5248	-0.1015	2.9303
H	-0.3562	-0.4159	-2.3722
H	1.9941	-0.9987	-3.0459
C	4.1714	-1.2156	-1.4008
H	3.2014	-0.673	1.0976
H	-4.9675	0.2128	1.7539
H	-4.856	0.8725	0.0907
H	-4.6544	1.9584	1.5016
H	2.0832	0.7124	3.2024
H	1.5002	-0.9174	3.5891
H	0.5128	0.499	3.9966
C	4.7028	-0.7487	-2.6177
C	6.0033	-1.0713	-3.0012
C	6.8033	-1.8678	-2.1777
C	6.2915	-2.336	-0.9638
C	4.9902	-2.0138	-0.5808
H	4.0953	-0.1067	-3.2564
H	6.3974	-0.6967	-3.9467
H	7.8185	-2.1256	-2.4802
H	6.9049	-2.9658	-0.3186
H	4.5834	-2.4132	0.3494



A4

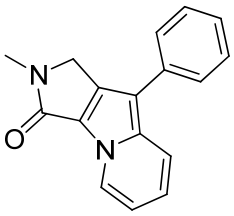
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C	-0.9844	0.0852	0.1547
C	-0.776	0.2442	1.5179
C	-2.0936	0.6049	2.1415
C	0.5733	0.0208	1.8189
C	1.1856	-0.2885	0.5792
N	0.1949	-0.2364	-0.4461
C	0.4915	-0.4765	-1.7675
C	1.7699	-0.7973	-2.124
C	2.7964	-0.8836	-1.1278
C	2.4934	-0.6238	0.2061
O	-2.9115	0.2628	-1.3413
C	-4.4016	0.9028	1.085
H	-2.0748	1.5807	2.6599
H	-2.4396	-0.1514	2.8686
H	-0.3475	-0.3968	-2.4549
H	2.0052	-0.9906	-3.1674
H	3.2652	-0.6796	0.9711
H	-4.9064	0.137	1.6999
H	-4.8147	0.8751	0.0694
H	-4.5961	1.8938	1.528
C	4.1217	-1.2373	-1.5077
N	5.2028	-1.5413	-1.8395
C	1.265	0.065	3.1444
H	2.2004	0.6432	3.0953
H	1.521	-0.9429	3.5081
H	0.6247	0.5378	3.9018



A5

N	-2.8575	1.0018	1.0541
C	-2.365	0.4477	-0.1344
C	-1.0816	-0.109	0.2701
C	-0.8051	0.1022	1.6163
C	-1.9633	0.8518	2.2068
C	0.4483	-0.4323	1.9287
C	0.9345	-0.985	0.712
N	-0.0433	-0.7719	-0.3058

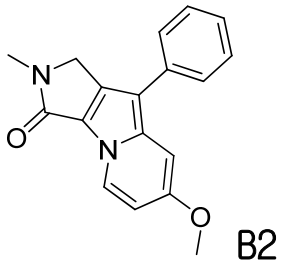
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C	1.3044	-1.8474	-1.9278
C	2.3176	-2.0838	-0.9481
C	2.111	-1.6459	0.3552
O	-2.9261	0.4613	-1.2338
C	-4.1123	1.7066	1.1256
C	1.1685	-0.4646	3.2387
H	-1.6686	1.839	2.6063
H	-2.4651	0.3	3.0214
H	-0.6719	-0.9851	-2.2856
H	1.4335	-2.1766	-2.957
H	2.8849	-1.8331	1.1006
H	-4.7923	1.2419	1.8586
H	-4.5694	1.6616	0.1293
H	-3.9647	2.7645	1.4042
C	3.5955	-2.7814	-1.2618
C	3.8282	-3.2408	-2.6871
H	3.815	-2.3857	-3.3807
H	3.0394	-3.934	-3.0161
H	4.8007	-3.7405	-2.7432
O	4.4422	-2.9819	-0.3891
H	2.1442	0.0438	3.1831
H	1.3594	-1.4974	3.5714
H	0.5799	0.0317	4.022



B1

N	-2.8831	0.9883	1.0958
C	-2.3323	0.5601	-0.119
C	-1.0098	0.0927	0.2666
C	-0.7699	0.2135	1.6213
C	-2.0032	0.7923	2.2519
C	0.5447	-0.2058	1.9102
C	1.0897	-0.615	0.6592
N	0.1058	-0.4088	-0.3481
C	0.3191	-0.7175	-1.6701
C	1.519	-1.262	-2.0432
C	2.5235	-1.5112	-1.0716
C	2.3064	-1.199	0.2551
O	-2.883	0.5974	-1.2242
C	-4.2372	1.4693	1.2114
C	1.2131	-0.2417	3.2119
H	-1.8118	1.7468	2.7728
H	-2.4725	0.1085	2.9829
H	-0.5171	-0.5081	-2.334
H	1.6832	-1.5038	-3.0919

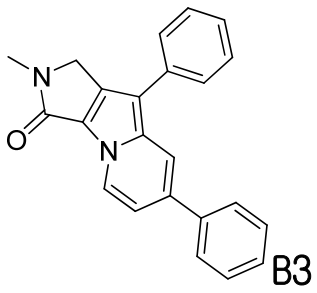
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H	-4.2651	2.4851	1.6376
C	2.5835	0.0441	3.354
C	3.2012	0.0038	4.6026
C	2.4623	-0.3142	5.745
C	1.0977	-0.5844	5.6224
C	0.4815	-0.551	4.3744
H	3.161	0.3351	2.4753
H	4.2659	0.2275	4.686
H	0.5098	-0.8311	6.5078
H	-0.5786	-0.7935	4.2866
H	3.4679	-1.9628	-1.3763
H	2.9424	-0.3418	6.7239



B2

N	-2.8444	1.0646	1.0619
C	-2.3588	0.4917	-0.1224
C	-1.087	-0.077	0.2865
C	-0.8115	0.1175	1.6247
C	-1.9655	0.8717	2.2182
C	0.4751	-0.3782	1.9263
C	0.9651	-0.9153	0.7006
N	-0.0217	-0.7101	-0.3044
C	0.1508	-1.1276	-1.5954
C	1.3044	-1.7757	-1.9555
C	2.3063	-2.032	-0.9778
C	2.1267	-1.6128	0.3299
O	-2.9223	0.5027	-1.2228
C	-4.1459	1.676	1.1574
C	1.1751	-0.3466	3.2105
H	-1.6553	1.8394	2.6527
H	-2.4875	0.3082	3.0128
H	-0.674	-0.9098	-2.2707
H	1.416	-2.0941	-2.9886
H	2.8847	-1.8418	1.0757
H	-4.8125	1.1137	1.8333
H	-4.579	1.6759	0.1492
H	-4.0761	2.7152	1.5174
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C	3.2216	-0.142	4.5217
C	2.497	-0.2744	5.7073

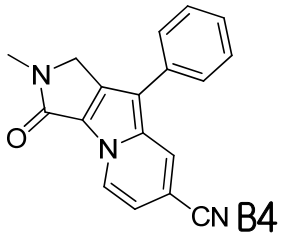
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C	0.4587	-0.4705	4.4165
H	3.1427	-0.0155	2.3763
H	4.303	-0.0004	4.5561
H	0.5326	-0.54	6.5668
H	-0.6208	-0.6276	4.38
H	3.0063	-0.2508	6.6718
O	3.4743	-2.6977	-1.2489
C	3.6855	-3.1431	-2.5887
H	3.6991	-2.299	-3.2969
H	2.9203	-3.8727	-2.8977
H	4.6678	-3.6275	-2.5871



B3

N	-2.9387	1.0141	1.1441
C	-2.39	0.6107	-0.0806
C	-1.0712	0.1236	0.2947
C	-0.8296	0.2191	1.6518
C	-2.0573	0.7938	2.2942
C	0.4871	-0.2003	1.9304
C	1.0282	-0.592	0.6701
N	0.0445	-0.3643	-0.3301
C	0.2757	-0.6325	-1.6565
C	1.4768	-1.1647	-2.0351
C	2.4893	-1.4689	-1.0732
C	2.2385	-1.1763	0.2627
O	-2.9394	0.6808	-1.1843
C	-4.2889	1.5014	1.2712
C	1.1638	-0.2417	3.2269
H	-1.8571	1.7396	2.8285
H	-2.5286	0.1027	3.0176
H	-0.5512	-0.4118	-2.3285
H	1.6356	-1.3966	-3.0869
H	2.9914	-1.3839	1.022
H	-4.9039	0.8392	1.9027
H	-4.7161	1.5341	0.262
H	-4.3083	2.5153	1.7032
C	2.536	0.0424	3.3607
C	3.1615	0.0007	4.6052
C	2.4291	-0.3153	5.7523
C	1.0636	-0.584	5.6384
C	0.4392	-0.5492	4.3944
H	3.1088	0.334	2.4791

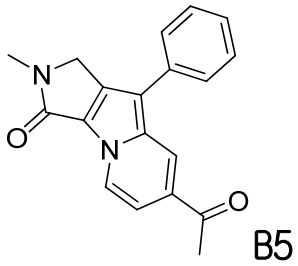
H	4.2259	0.2288	4.6823
H	0.4809	-0.8314	6.5272
H	-0.6225	-0.7881	4.3143
C	3.7603	-2.0926	-1.4928
H	2.9166	-0.3442	6.7279
C	4.3635	-1.7613	-2.7186
C	5.5685	-2.3456	-3.1033
C	6.1975	-3.2767	-2.2753
C	5.606	-3.6214	-1.0588
C	4.4029	-3.0361	-0.6726
H	3.8967	-1.0131	-3.3626
H	6.0244	-2.0637	-4.0541
H	7.1399	-3.735	-2.5799
H	6.0794	-4.3611	-0.4102
H	3.9325	-3.3387	0.2653



B4

N	-3.0272	0.8024	0.8776
C	-2.2939	0.7382	-0.3122
C	-1.0649	0.0663	0.0962
C	-1.0563	-0.2583	1.442
C	-2.3608	0.1855	2.0295
C	0.1871	-0.8192	1.7841
C	0.9336	-0.8444	0.5708
N	0.1312	-0.2762	-0.4616
C	0.575	-0.1431	-1.757
C	1.8264	-0.5788	-2.0849
C	2.6618	-1.1821	-1.0908
C	2.2045	-1.3125	0.2172
O	-2.6439	1.1678	-1.4142
C	-4.3688	1.328	0.9374
H	-2.2322	0.9099	2.8539
H	-2.9644	-0.6545	2.4203
H	-0.134	0.3076	-2.448
H	2.1816	-0.4804	-3.108
H	2.8229	-1.7909	0.9749
H	-5.1083	0.5365	1.1487
H	-4.589	1.7688	-0.0432
H	-4.4553	2.1058	1.7114
C	3.9559	-1.6501	-1.4511
N	5.0175	-2.0369	-1.7572
C	0.6269	-1.2817	3.1014
C	1.9448	-1.0997	3.5575
C	2.3303	-1.5462	4.8209

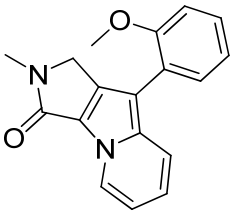
C	1.4098	-2.1793	5.6579
C	0.0945	-2.354	5.2243
C	-0.2916	-1.9114	3.9615
H	2.6609	-0.5638	2.9325
H	3.3558	-1.3859	5.1587
H	1.7143	-2.5262	6.6452
H	-0.6331	-2.85	5.8693
H	-1.3121	-2.0838	3.614



B5

N	-2.801	0.9988	1.1108
C	-2.3134	0.4465	-0.0798
C	-1.0497	-0.1526	0.3306
C	-0.7848	0.0241	1.6788
C	-1.9394	0.7771	2.2746
C	0.4905	-0.4833	1.9785
C	0.9831	-1.0133	0.7466
N	0.0033	-0.7804	-0.2637
C	0.1901	-1.1631	-1.5724
C	1.346	-1.8044	-1.9217
C	2.3393	-2.1081	-0.9418
C	2.1337	-1.7156	0.3758
O	-2.8577	0.4948	-1.1864
C	-4.0777	1.6629	1.1966
C	1.1918	-0.4709	3.2636
H	-1.6284	1.7328	2.7321
H	-2.4738	0.1949	3.047
H	-0.6245	-0.9172	-2.2493
H	1.4774	-2.0922	-2.9626
H	2.8834	-1.9789	1.1198
H	-4.7614	1.1328	1.8797
H	-4.5123	1.6658	0.1896
H	-3.968	2.7021	1.5476
C	3.5943	-2.8448	-1.2677
C	3.8604	-3.1973	-2.7154
H	3.8355	-2.3003	-3.3534
H	3.0943	-3.888	-3.098
H	4.8444	-3.6709	-2.7895
O	4.3999	-3.149	-0.3859
C	2.5848	-0.2842	3.3404
C	3.2396	-0.2825	4.5696
C	2.5176	-0.4463	5.7523
C	1.1318	-0.6121	5.6945

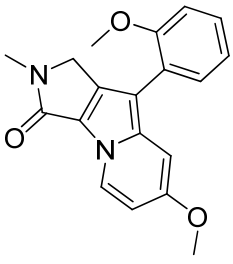
C	0.4771	-0.6279	4.4652
H	3.1527	-0.1088	2.4277
H	4.3201	-0.1373	4.6036
H	3.0287	-0.4406	6.7158
H	0.5591	-0.7459	6.6126
H	-0.6008	-0.7947	4.4273



C1

N	-2.8543	1.2114	0.9856
C	-2.3035	0.6951	-0.1937
C	-1.0292	0.1513	0.2503
C	-0.817	0.3162	1.6066
C	-2.0197	1.0049	2.1739
C	0.4604	-0.1674	1.9473
C	1.0118	-0.6589	0.7305
N	0.0684	-0.4432	-0.311
C	0.3051	-0.8152	-1.6117
C	1.4863	-1.4324	-1.9281
C	2.4494	-1.6925	-0.917
C	2.211	-1.3114	0.3882
O	-2.8207	0.7258	-1.3161
C	-4.176	1.7809	1.0419
C	1.1546	-0.1629	3.2394
H	-1.7762	1.9672	2.6585
H	-2.5376	0.3803	2.9231
H	-0.4944	-0.5851	-2.3124
H	1.6689	-1.7201	-2.9619
H	2.9299	-1.5162	1.1807
H	-4.8741	1.1447	1.6132
H	-4.5387	1.8646	0.0098
H	-4.1598	2.7824	1.5008
C	2.4942	0.2471	3.3285
C	3.1889	0.252	4.5382
C	2.5369	-0.1473	5.702
C	1.2003	-0.5555	5.6537
C	0.5116	-0.5662	4.4374
H	2.9849	0.5965	2.4186
H	4.2266	0.5834	4.5703
H	0.7027	-0.8673	6.5709
O	-0.7962	-0.9706	4.3123
H	3.3773	-2.2027	-1.1744
H	3.0591	-0.1423	6.66
C	-1.4393	-1.4836	5.4766
H	-0.8956	-2.3528	5.8813
H	-2.4367	-1.7968	5.1516

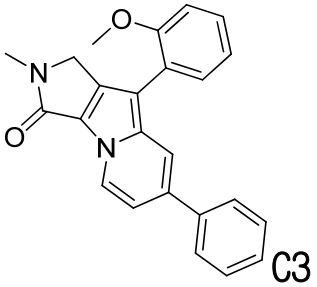
H	-1.5348	-0.7147	6.2604



C2

N	-2.8249	1.2759	0.9762
C	-2.3604	0.6202	-0.1708
C	-1.1384	-0.0147	0.2854
C	-0.8752	0.21	1.622
C	-1.9905	1.054	2.1627
C	0.3571	-0.3819	1.9721
C	0.827	-0.9998	0.7766
N	-0.1167	-0.7529	-0.2577
C	0.0472	-1.2303	-1.5278
C	1.1536	-1.9787	-1.8436
C	2.1149	-2.2716	-0.8353
C	1.9441	-1.7885	0.4517
O	-2.9026	0.6212	-1.2832
C	-4.0869	1.9678	1.0197
C	1.0949	-0.3531	3.2381
H	-1.6387	2.0133	2.5821
H	-2.5548	0.5357	2.9568
H	-0.7432	-0.9709	-2.2289
H	1.2579	-2.342	-2.8629
H	2.673	-2.0385	1.2198
H	-4.8267	1.439	1.6476
H	-4.4652	2.0182	-0.0087
H	-3.9668	2.9916	1.4107
C	2.484	-0.1497	3.2486
C	3.2282	-0.1412	4.4291
C	2.5796	-0.3252	5.6478
C	1.1961	-0.5156	5.6788
C	0.4571	-0.535	4.4916
H	2.9847	0.0306	2.2967
H	4.3061	0.0204	4.3921
H	0.6983	-0.6617	6.6359
O	-0.9034	-0.74	4.4536
H	3.1413	-0.3135	6.5837
C	-1.5519	-1.0482	5.685
H	-1.1107	-1.9412	6.1563
H	-2.5978	-1.2511	5.4278
H	-1.509	-0.202	6.3908
O	3.2316	-3.038	-1.053
C	3.4351	-3.5509	-2.3693

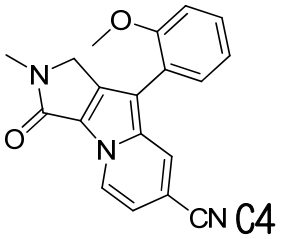
H	4.3663	-4.1259	-2.3214
H	3.5475	-2.7387	-3.1065
H	2.6125	-4.2174	-2.6763



C3

N	-2.798	1.292	0.9794
C	-2.3455	0.6449	-0.1756
C	-1.1364	-0.0262	0.275
C	-0.8705	0.1842	1.6157
C	-1.9706	1.0418	2.165
C	0.3547	-0.4216	1.9552
C	0.8124	-1.0387	0.7525
N	-0.127	-0.7658	-0.2767
C	0.0406	-1.2197	-1.5614
C	1.1479	-1.9589	-1.8752
C	2.1151	-2.2996	-0.8787
C	1.9212	-1.8353	0.4165
O	-2.8808	0.6769	-1.2895
C	-4.0388	2.0213	1.0294
C	1.0999	-0.3983	3.2171
H	-1.6019	1.9896	2.5955
H	-2.5466	0.5248	2.9512
H	-0.7509	-0.9498	-2.2566
H	1.2534	-2.3328	-2.8923
H	2.6459	-2.0644	1.1967
H	-4.7931	1.5081	1.6523
H	-4.4171	2.0961	0.0023
H	-3.8876	3.036	1.4338
C	2.4892	-0.1962	3.2204
C	3.2388	-0.187	4.3976
C	2.5951	-0.3687	5.6194
C	1.2113	-0.5558	5.6573
C	0.4665	-0.575	4.4736
H	2.9851	-0.0143	2.2666
H	4.3162	-0.0261	4.3557
H	0.7173	-0.6978	6.6168
O	-0.8947	-0.7701	4.4429
H	3.1613	-0.3565	6.5523
C	-1.5389	-1.0932	5.6728
H	-1.0874	-1.9843	6.138
H	-2.5816	-1.3068	5.4143
H	-1.506	-0.2524	6.3849
C	3.2916	-3.1178	-1.2275

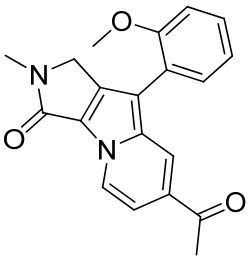
C	3.9207	-2.973	-2.4774
C	5.0456	-3.7292	-2.8066
C	5.5635	-4.6513	-1.8931
C	4.9457	-4.8109	-0.6499
C	3.8224	-4.0528	-0.3196
H	3.5446	-2.232	-3.1834
H	5.5273	-3.5886	-3.7754
H	6.4426	-5.2438	-2.149
H	5.3325	-5.5396	0.0629
H	3.324	-4.2099	0.6382



C4

N	-2.8288	1.2746	0.98
C	-2.388	0.6106	-0.1668
C	-1.1646	-0.0436	0.2829
C	-0.8883	0.1929	1.619
C	-1.9868	1.0549	2.1623
C	0.3384	-0.4058	1.9595
C	0.7893	-1.0361	0.7618
N	-0.166	-0.79	-0.2664
C	-0.0184	-1.2708	-1.5472
C	1.0901	-2.0007	-1.8687
C	2.0774	-2.2821	-0.8703
C	1.907	-1.814	0.4292
O	-2.933	0.6126	-1.2746
C	-4.0652	2.0142	1.0257
C	1.0895	-0.3765	3.2183
H	-1.6192	2.0145	2.566
H	-2.5503	0.5525	2.9661
H	-0.8216	-1.0165	-2.2349
H	1.215	-2.3731	-2.8831
H	2.6388	-2.0474	1.1997
H	-4.8091	1.5257	1.6786
H	-4.4603	2.0543	0.0038
H	-3.8991	3.0412	1.3899
C	2.4787	-0.1762	3.215
C	3.2324	-0.1733	4.3893
C	2.592	-0.3615	5.6118
C	1.2083	-0.5461	5.6554
C	0.4577	-0.5563	4.475
H	2.9726	0.0123	2.2613
H	4.3096	-0.0132	4.3441
H	0.719	-0.6918	6.6166
O	-0.9025	-0.7522	4.4459

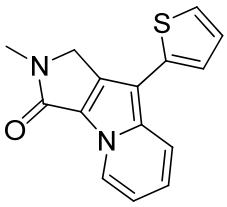
H	3.162	-0.36	6.5424
C	-1.5514	-1.037	5.6855
H	-1.133	-1.9406	6.1562
H	-2.6041	-1.2111	5.4362
H	-1.4759	-0.189	6.3857
C	3.2253	-3.0524	-1.2065
N	4.1795	-3.6715	-1.4914



C5

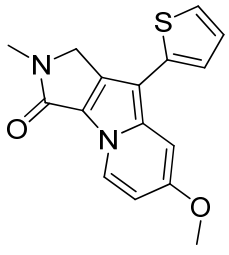
N	-2.8219	1.1993	0.9851
C	-2.3443	0.5595	-0.1611
C	-1.1106	-0.0627	0.3005
C	-0.8501	0.1847	1.6391
C	-1.9692	1.0302	2.1682
C	0.3733	-0.4076	1.9966
C	0.846	-1.0399	0.8045
N	-0.1014	-0.8041	-0.2338
C	0.065	-1.2881	-1.5104
C	1.1791	-2.0224	-1.809
C	2.1545	-2.3069	-0.8044
C	1.965	-1.8154	0.4828
O	-2.8763	0.5548	-1.2761
C	-4.0253	1.993	0.9872
C	1.1026	-0.3759	3.2679
H	-1.6212	2.0077	2.5465
H	-2.5163	0.5321	2.9851
H	-0.7296	-1.0354	-2.2088
H	1.2935	-2.3923	-2.8259
H	2.7039	-2.0578	1.2456
H	-4.7324	1.6433	1.7555
H	-4.4847	1.8847	-0.0033
H	-3.8083	3.0598	1.1647
C	2.4916	-0.1756	3.2879
C	3.2223	-0.1645	4.4762
C	2.5601	-0.3481	5.6873
C	1.177	-0.54	5.7071
C	0.4501	-0.5605	4.513
H	3.0028	0.0001	2.3414
H	4.3004	-0.0051	4.4503
H	0.6714	-0.6868	6.6596
O	-0.9074	-0.7749	4.4598
H	3.1124	-0.3377	6.6283
C	-1.5729	-1.0597	5.6901

H	-1.1518	-1.9552	6.1731
H	-2.6199	-1.2462	5.4254
H	-1.5188	-0.2059	6.386
C	3.37	-3.1246	-1.0702
C	3.5766	-3.6588	-2.4732
O	4.1883	-3.3604	-0.1789
H	3.5907	-2.8399	-3.2082
H	2.7556	-4.3326	-2.7614
H	4.5261	-4.2027	-2.5122



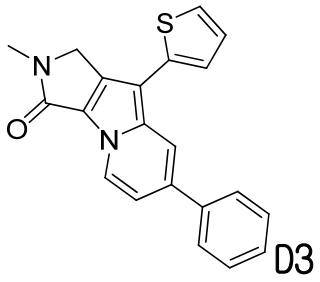
D1

N	-2.8171	1.1194	1.0715
C	-2.2929	0.6246	-0.1273
C	-0.9943	0.0996	0.2723
C	-0.7497	0.2525	1.6195
C	-1.9449	0.9136	2.2327
C	0.5472	-0.2207	1.9243
C	1.0734	-0.6874	0.6851
N	0.0976	-0.4663	-0.3267
C	0.3082	-0.7876	-1.6444
C	1.4973	-1.3565	-2.0131
C	2.4951	-1.6188	-1.039
C	2.2807	-1.2935	0.2853
O	-2.8421	0.6528	-1.2326
C	-4.1439	1.6755	1.1701
C	1.179	-0.2144	3.2256
H	-1.6969	1.8717	2.7207
H	-2.447	0.2806	2.9841
H	-0.5161	-0.562	-2.3154
H	1.6584	-1.6095	-3.0583
H	3.035	-1.5075	1.0387
H	-4.798	1.0551	1.8044
H	-4.5581	1.7039	0.155
H	-4.1214	2.6982	1.5782
H	3.4308	-2.0873	-1.3378
S	2.9065	-0.4	3.4497
C	2.7727	-0.2629	5.1681
C	1.4701	-0.0663	5.5538
C	0.5695	-0.0413	4.459
H	3.6634	-0.3348	5.7826
H	1.1662	0.0508	6.5917
H	-0.5065	0.0833	4.568



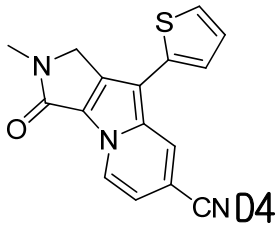
D2

N	-2.87928	1.95679	-0.06943
C	-2.50203	1.18793	-1.17735
C	-1.31213	0.49695	-0.70824
C	-0.97984	0.82097	0.58769
C	-2.01386	1.77549	1.10097
C	0.23668	0.1908	0.94427
C	0.62122	-0.55438	-0.20864
N	-0.35253	-0.33835	-1.22366
C	-0.25315	-0.9054	-2.46267
C	0.81698	-1.70536	-2.76785
C	1.80726	-1.96495	-1.78048
C	1.70006	-1.39488	-0.52151
O	-3.07749	1.15497	-2.27054
C	-4.08495	2.74688	-0.0463
C	0.93437	0.31413	2.2054
H	-1.58316	2.73511	1.4309
H	-2.58604	1.35967	1.94853
H	-1.06054	-0.66893	-3.14996
H	0.8696	-2.14118	-3.76096
H	2.45632	-1.61711	0.22602
H	-4.8933	2.25918	0.52341
H	-4.41666	2.87064	-1.08309
H	-3.89444	3.73613	0.39214
S	2.6389	-0.05276	2.38365
C	2.63345	0.38693	4.05554
C	1.39195	0.81193	4.45688
C	0.43097	0.77287	3.41238
H	3.54494	0.295	4.63596
H	1.16864	1.13054	5.47235
H	-0.61202	1.04783	3.54919
O	2.89593	-2.7691	-1.99275
C	3.04375	-3.3636	-3.28325
H	3.98585	-3.9169	-3.24362
H	3.1047	-2.59966	-4.07315
H	2.21985	-4.05819	-3.50186



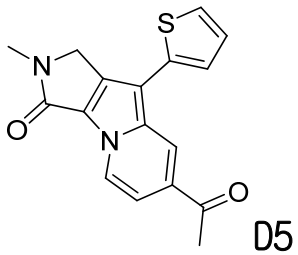
D3

N	-2.7452	1.3626	1.0549
C	-2.3523	0.5879	-0.0423
C	-1.1703	-0.106	0.451
C	-0.8642	0.2237	1.7543
C	-1.9039	1.184	2.2432
C	0.3414	-0.4075	2.1345
C	0.742	-1.1642	0.9924
N	-0.2074	-0.9434	-0.0413
C	-0.0718	-1.5006	-1.2878
C	1.0029	-2.3005	-1.5556
C	1.9764	-2.5921	-0.5495
C	1.8184	-2.0191	0.7062
O	-2.9071	0.5487	-1.1444
C	-3.946	2.1601	1.0533
C	1.019	-0.2742	3.4056
H	-1.4742	2.1435	2.5762
H	-2.4987	0.7789	3.0803
H	-0.863	-1.261	-1.9935
H	1.0838	-2.7511	-2.5425
H	2.5526	-2.2075	1.4861
H	-4.6909	1.7781	1.7705
H	-4.366	2.1128	0.0416
H	-3.7269	3.2102	1.3009
S	2.7288	-0.6023	3.6058
C	2.6936	-0.1551	5.2749
C	1.4383	0.2451	5.659
C	0.492	0.1811	4.6039
H	3.5993	-0.2235	5.8677
H	1.1962	0.5637	6.6709
H	-0.5581	0.4376	4.7256
C	3.1279	-3.466	-0.8542
C	3.7526	-3.4068	-2.1139
C	4.8586	-4.2026	-2.4039
C	5.3596	-5.0864	-1.4459
C	4.744	-5.1639	-0.1939
C	3.6411	-4.3636	0.0993
H	3.3907	-2.6975	-2.8597
H	5.3366	-4.1278	-3.3808
H	6.2239	-5.7112	-1.6716
H	5.1164	-5.8626	0.5565
H	3.1514	-4.4514	1.0696



D4

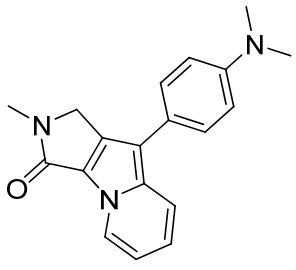
N	-2.9235	1.2425	0.8564
C	-2.2083	0.9706	-0.3111
C	-1.2409	-0.0323	0.123
C	-1.3597	-0.3448	1.4613
C	-2.4872	0.4665	2.0219
C	-0.3795	-1.2984	1.8173
C	0.3543	-1.5399	0.6138
N	-0.2155	-0.7413	-0.4238
C	0.2608	-0.7455	-1.7122
C	1.3315	-1.5271	-2.0328
C	1.9479	-2.3409	-1.0286
C	1.4525	-2.3375	0.2732
O	-2.3882	1.4816	-1.4189
C	-4.0277	2.172	0.8934
H	-2.1665	1.1364	2.8372
H	-3.3094	-0.1611	2.4069
H	-0.266	-0.0953	-2.4054
H	1.7119	-1.5304	-3.0517
H	1.9282	-2.9534	1.0301
H	-4.9819	1.6578	1.0862
H	-4.0776	2.6542	-0.0892
H	-3.8754	2.94	1.6661
C	3.0674	-3.154	-1.3655
N	3.9915	-3.8143	-1.6507
C	-0.1945	-1.8864	3.1249
S	0.9964	-3.1217	3.465
C	0.5287	-3.22	5.1248
C	-0.4961	-2.3512	5.407
C	-0.9056	-1.5967	4.2813
H	1.0368	-3.9172	5.7818
H	-0.9427	-2.2543	6.3943
H	-1.7012	-0.8554	4.3145



D5

N	-2.756	1.3661	1.0816
C	-2.3844	0.61	-0.0332

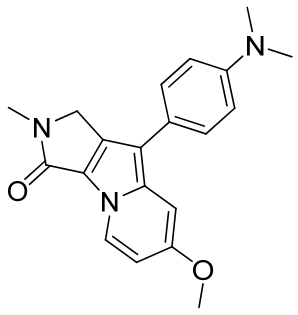
C	-1.1922	-0.0934	0.4295
C	-0.8655	0.2161	1.7363
C	-1.8897	1.1789	2.2517
C	0.3357	-0.43	2.0903
C	0.7132	-1.1774	0.9292
N	-0.2552	-0.9341	-0.0893
C	-0.1481	-1.4802	-1.3464
C	0.9062	-2.2995	-1.6354
C	1.889	-2.609	-0.6454
C	1.7651	-2.0398	0.6195
O	-2.9578	0.5839	-1.1253
C	-3.9433	2.1844	1.1089
C	1.0298	-0.3298	3.3554
H	-1.4475	2.1347	2.5784
H	-2.4695	0.7738	3.0988
H	-0.9414	-1.2115	-2.0393
H	0.9613	-2.7168	-2.6373
H	2.5133	-2.2965	1.3679
H	-4.6736	1.8136	1.846
H	-4.3915	2.1439	0.1094
H	-3.6991	3.2301	1.3503
S	2.7269	-0.7186	3.5352
C	2.7165	-0.2932	5.2079
C	1.4781	0.1404	5.6124
C	0.5227	0.1232	4.5635
H	3.6265	-0.3955	5.7904
H	1.2551	0.4523	6.6303
H	-0.5185	0.4081	4.697
C	3.047	-3.5186	-0.8766
C	3.2839	-4.1305	-2.2439
H	2.6212	-3.7794	-3.0398
H	3.1824	-5.2207	-2.1544
H	4.3247	-3.9326	-2.5282
O	3.8207	-3.7934	0.0437



E1

N	-2.8993	0.9478	1.0918
C	-2.3498	0.5071	-0.119
C	-1.0245	0.0516	0.267
C	-0.7787	0.1958	1.62
C	-2.011	0.7762	2.2466
C	0.5425	-0.2017	1.9106
C	1.0873	-0.6169	0.6614

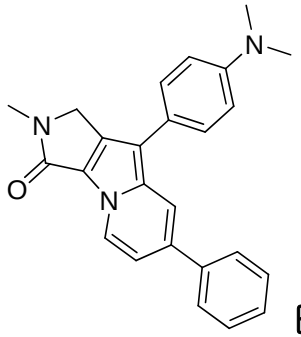
N	0.0963	-0.4377	-0.3458
C	0.3179	-0.7404	-1.6684
C	1.5296	-1.257	-2.0417
C	2.5384	-1.489	-1.0692
C	2.3136	-1.1816	0.2573
O	-2.9058	0.5282	-1.2228
C	-4.2555	1.4214	1.2073
C	1.219	-0.1976	3.207
H	-1.8259	1.7415	2.7512
H	-2.4773	0.1077	2.9948
H	-0.5216	-0.5451	-2.3325
H	1.7003	-1.4916	-3.0909
H	3.0695	-1.3796	1.0161
H	-4.8832	0.7296	1.7934
H	-4.6593	1.4938	0.1896
H	-4.2876	2.416	1.6804
C	2.5886	0.0982	3.3453
C	3.2178	0.1029	4.582
C	2.5077	-0.1912	5.7664
C	1.1326	-0.4713	5.6348
C	0.5125	-0.4698	4.3894
N	3.1346	-0.1383	7.0205
C	2.321	-0.3546	8.2027
C	4.4941	-0.6422	7.1648
H	3.166	0.3743	2.4619
H	4.2694	0.3849	4.6299
H	0.5379	-0.7123	6.5142
H	-0.5478	-0.7213	4.3303
H	1.9573	-1.3972	8.3009
H	1.4559	0.3227	8.1984
H	2.9242	-0.1186	9.0897
H	5.0619	-0.5055	6.2413
H	4.5098	-1.7213	7.4188
H	5.0093	-0.0927	7.9669
H	3.4898	-1.9259	-1.3731



E2

N	-2.9366	1.2032	1.1235
C	-2.512	0.5536	-0.0453
C	-1.2661	-0.0698	0.3593
C	-0.944	0.1747	1.6815
C	-2.0443	1.0089	2.2694

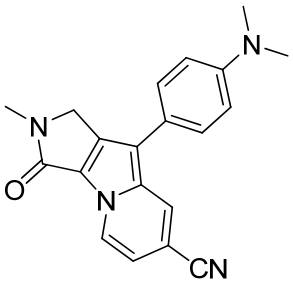
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C	0.7508	-0.9893	0.769
N	-0.2472	-0.78	-0.2248
C	-0.1209	-1.2674	-1.4962
C	0.9847	-2.0038	-1.8426
C	1.9942	-2.2652	-0.8728
C	1.8669	-1.7649	0.4125
O	-3.1041	0.5524	-1.1312
C	-4.1982	1.8909	1.2204
C	1.0613	-0.3207	3.2386
H	-1.6802	1.976	2.6615
H	-2.5804	0.5039	3.0934
H	-0.943	-1.0352	-2.1699
H	1.0564	-2.3748	-2.8615
H	2.6262	-1.9923	1.1582
H	-4.883	1.3907	1.9278
H	-4.6505	1.8836	0.2199
H	-4.0609	2.9363	1.5455
C	2.4609	-0.166	3.2853
C	3.1526	-0.12	4.4877
C	2.4831	-0.2263	5.7257
C	1.0803	-0.3611	5.6841
C	0.3962	-0.4026	4.4721
N	3.1847	-0.1386	6.9393
C	2.4207	-0.1777	8.1725
C	4.4839	-0.7884	7.0564
H	3.0145	-0.03	2.3556
H	4.2297	0.0466	4.4617
H	0.5118	-0.4649	6.6065
H	-0.6863	-0.5443	4.4848
H	1.9442	-1.1621	8.3616
H	1.6382	0.5924	8.1611
H	3.0984	0.0369	9.0099
H	5.0256	-0.7555	6.1065
H	4.3902	-1.8517	7.3576
H	5.0925	-0.2682	7.8117
O	3.112	-3.0188	-1.1284
C	3.2423	-3.5798	-2.4351
H	4.1884	-4.1323	-2.4272
H	3.2859	-2.7968	-3.2095
H	2.4157	-4.2752	-2.6581



E3

N	-2.9014	0.9774	1.0962
C	-2.3486	0.5562	-0.1214
C	-1.0381	0.0604	0.2668
C	-0.7978	0.18	1.624
C	-2.0241	0.7736	2.2529
C	0.5184	-0.2303	1.9145
C	1.0614	-0.6439	0.6614
N	0.0807	-0.4306	-0.3471
C	0.3193	-0.7149	-1.6696
C	1.524	-1.2462	-2.0365
C	2.534	-1.5339	-1.0653
C	2.2747	-1.2298	0.2664
O	-2.8936	0.6176	-1.2287
C	-4.246	1.4808	1.2097
C	1.1939	-0.2487	3.2107
H	-1.8194	1.728	2.7705
H	-2.504	0.1002	2.9878
H	-0.5072	-0.507	-2.3464
H	1.6875	-1.4938	-3.0841
H	3.0244	-1.4252	1.0326
H	-4.8664	0.8379	1.8571
H	-4.6757	1.4906	0.1997
H	-4.2608	2.5052	1.6157
C	2.5643	0.0393	3.3504
C	3.1984	0.0286	4.5852
C	2.4883	-0.2791	5.7674
C	1.1091	-0.5518	5.6354
C	0.4876	-0.532	4.3922
N	3.1089	-0.2787	7.0114
C	2.3241	-0.3851	8.2238
C	4.535	-0.5053	7.1623
C	3.8106	-2.1536	-1.4726
C	4.4212	-1.8267	-2.696
C	5.6276	-2.4135	-3.0728
C	6.2525	-3.3419	-2.2386
C	5.6552	-3.6804	-1.023
C	4.4504	-3.093	-0.645
H	3.1383	0.3325	2.4697
H	4.2482	0.3158	4.6346
H	0.5182	-0.8148	6.512
H	-0.5727	-0.7839	4.3316

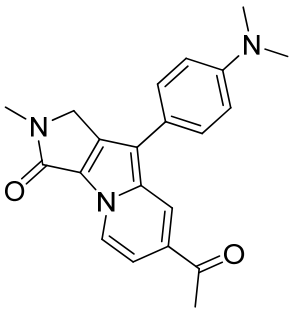
H	1.9578	-1.4132	8.4187
H	1.4561	0.2897	8.1834
H	2.9454	-0.078	9.0766
H	4.9906	-0.7525	6.1976
H	4.7164	-1.3595	7.8377
H	5.053	0.3751	7.5803
H	3.9582	-1.0801	-3.3447
H	6.0885	-2.135	-4.0222
H	7.1956	-3.8025	-2.5376
H	6.1251	-4.4171	-0.3685
H	3.9738	-3.3926	0.2908



E4

N	-2.9341	1.174	1.1044
C	-2.5069	0.5255	-0.059
C	-1.2586	-0.1042	0.3556
C	-0.9474	0.1475	1.6826
C	-2.0471	0.9928	2.2571
C	0.3129	-0.4001	1.9866
C	0.7418	-1.0271	0.7809
N	-0.2506	-0.815	-0.2223
C	-0.1182	-1.2988	-1.5046
C	0.9915	-2.0204	-1.8409
C	2.0019	-2.2872	-0.8608
C	1.8592	-1.7963	0.4334
O	-3.0822	0.5243	-1.1507
C	-4.1683	1.9159	1.1772
C	1.0496	-0.347	3.2476
H	-1.6795	1.9642	2.6332
H	-2.5862	0.4979	3.0845
H	-0.9399	-1.0653	-2.1781
H	1.0958	-2.4024	-2.8543
H	2.6078	-2.0143	1.193
H	-4.8636	1.4708	1.9079
H	-4.6244	1.8892	0.1793
H	-3.9864	2.9673	1.4589
C	2.4493	-0.1959	3.2938
C	3.1417	-0.1535	4.4951
C	2.4714	-0.2522	5.7351
C	1.0655	-0.3837	5.6908
C	0.3825	-0.4247	4.4804
N	3.1574	-0.1676	6.9492

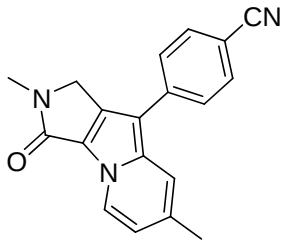
C	2.3967	-0.2649	8.1821
C	4.5184	-0.6763	7.0632
H	3.0055	-0.0631	2.3652
H	4.2195	0.0003	4.462
H	0.4958	-0.4849	6.6124
H	-0.7002	-0.5655	4.4938
H	1.9557	-1.27	8.3459
H	1.5866	0.4766	8.1907
H	3.0663	-0.0441	9.0232
H	5.0728	-0.5386	6.1317
H	4.5366	-1.7541	7.3193
H	5.047	-0.1247	7.8543
C	3.1436	-3.0602	-1.2091
N	4.0909	-3.6855	-1.5022



E5

N	-2.10519	-3.65809	0.08375
C	-3.05308	-2.62922	0.06323
C	-2.23328	-1.42728	-0.02194
C	-0.87454	-1.7058	-0.02674
C	-0.71424	-3.19649	0.03805
C	-0.14398	-0.50489	-0.01539
C	-1.13092	0.52986	-0.02705
N	-2.42244	-0.07953	-0.01676
C	-3.58377	0.65934	-0.01513
C	-3.51093	2.02465	-0.03911
C	-2.24613	2.68905	-0.08087
C	-1.08337	1.92491	-0.08162
O	-4.27953	-2.7635	0.11305
C	-2.46723	-5.04784	0.20656
C	1.30578	-0.33398	0.0216
H	-0.15674	-3.52159	0.93517
H	-0.19832	-3.61859	-0.84259
H	-4.50219	0.07765	0.00447
H	-4.44207	2.58708	-0.03198
H	-0.12683	2.44174	-0.13753
H	-2.07296	-5.64232	-0.63319
H	-3.56313	-5.10056	0.20019
H	-2.09394	-5.47921	1.15024
C	1.92601	0.73367	0.69715
C	3.3059	0.88702	0.71938
C	4.15683	-0.0441	0.08167

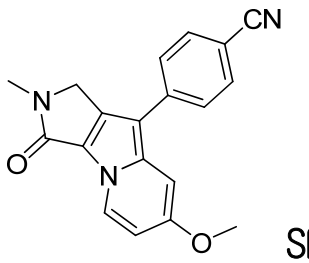
C	3.53825	-1.12235	-0.59179
C	2.15632	-1.25795	-0.61123
N	5.5398	0.08822	0.12909
C	6.36578	-0.79997	-0.66792
C	6.11321	1.35748	0.54577
H	1.31493	1.4507	1.24694
H	3.72352	1.73528	1.25904
H	4.14145	-1.85576	-1.12535
H	1.72168	-2.08972	-1.16912
H	6.22333	-0.66739	-1.75838
H	6.15444	-1.85044	-0.4194
H	7.42011	-0.61259	-0.43239
H	5.82015	1.60121	1.57872
H	5.80625	2.19781	-0.10496
H	7.20626	1.2806	0.52344
C	-2.11487	4.16874	-0.13811
C	-3.38541	4.99629	-0.17534
H	-3.99794	4.73402	-1.05199
H	-3.11742	6.0572	-0.22161
H	-4.00305	4.81209	0.71678
O	-1.00807	4.71372	-0.15629



SF01

C	0.3164	-0.38142	1.65846
C	1.04242	-1.54695	1.98616
C	1.3343	-1.87211	3.30595
C	0.89819	-1.04557	4.3572
C	0.16133	0.1139	4.04897
C	-0.11907	0.43087	2.72763
C	1.18359	-1.3705	5.71504
N	1.39977	-1.61522	6.84023
N	-3.00511	1.86611	-0.88956
C	-2.27093	1.5595	-2.04123
C	-1.10051	0.87362	-1.51006
C	-1.12484	0.75194	-0.13786
C	-2.378	1.41625	0.35495
C	-0.01144	-0.0096	0.28993
C	0.70947	-0.32484	-0.90164
N	0.00314	0.22556	-2.00347
C	0.43973	0.10021	-3.29637
C	1.60676	-0.57315	-3.54575
C	2.3821	-1.11935	-2.48711
C	1.92441	-0.97306	-1.18665
O	-2.58751	1.8253	-3.20427

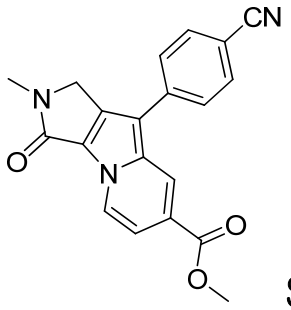
C	-4.24732	2.59652	-0.9254
H	-2.18081	2.2773	1.0191
H	-3.03534	0.71918	0.90543
H	-0.19479	0.56549	-4.04859
H	1.94463	-0.66752	-4.57716
H	2.51701	-1.35344	-0.35512
H	-5.06258	2.02153	-0.45682
H	-4.49154	2.77092	-1.98092
H	-4.16276	3.56836	-0.41038
C	3.67332	-1.83602	-2.78117
H	3.9754	-1.69824	-3.82808
H	3.57662	-2.91868	-2.60315
H	4.4904	-1.47288	-2.14039
H	1.34357	-2.23657	1.19894
H	1.88841	-2.78111	3.53563
H	-0.17456	0.76495	4.85568
H	-0.66385	1.34872	2.51186



SF02

N	-3.08754	1.93911	-0.7601
C	-2.34637	1.58636	-1.89502
C	-1.20413	0.88318	-1.33198
C	-1.2384	0.80656	0.04159
C	-2.47945	1.51488	0.50293
C	-0.14145	0.03848	0.50369
C	0.58911	-0.31886	-0.6705
N	-0.10213	0.2056	-1.79634
C	0.34407	0.04095	-3.07747
C	1.50838	-0.6446	-3.31299
C	2.26082	-1.1489	-2.21746
C	1.80184	-0.98012	-0.91951
O	-2.64081	1.83527	-3.06841
C	-4.30279	2.7109	-0.82677
H	-2.26207	2.39464	1.13533
H	-3.15731	0.85639	1.07408
H	-0.28222	0.48434	-3.84911
H	1.83875	-0.76755	-4.3411
H	2.40675	-1.34896	-0.09449
H	-5.13796	2.18378	-0.33882
H	-4.53967	2.85298	-1.88895
H	-4.18331	3.69967	-0.35148
O	3.45359	-1.80344	-2.35742
C	3.96432	-1.97958	-3.68107

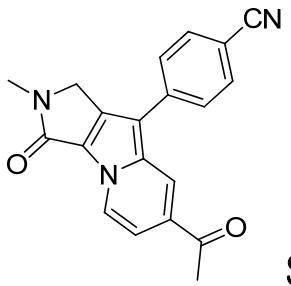
H	4.91555	-2.50679	-3.55955
H	4.14335	-1.01119	-4.17509
H	3.28494	-2.59096	-4.29597
C	0.16739	-0.30807	1.88174
C	0.897	-1.46427	2.23536
C	1.1732	-1.76679	3.56346
C	0.72106	-0.92664	4.59653
C	-0.01905	0.22418	4.26236
C	-0.28526	0.51846	2.93313
C	0.99307	-1.23166	5.96124
N	1.19795	-1.46366	7.09086
H	1.21613	-2.16167	1.4629
H	1.73195	-2.66805	3.81395
H	-0.36554	0.8869	5.05451
H	-0.83379	1.42913	2.69599



SF03

C	-0.11416	-0.14274	2.02243
C	0.6127	-1.30456	2.35675
C	0.90672	-1.61821	3.67914
C	0.47223	-0.78123	4.72225
C	-0.26316	0.37671	4.40679
C	-0.5441	0.68323	3.08258
C	0.74924	-1.0992	6.08412
N	0.95101	-1.33622	7.21273
N	-3.39262	2.15655	-0.53792
C	-2.69277	1.79259	-1.69171
C	-1.5444	1.06275	-1.16092
C	-1.55208	0.98096	0.21772
C	-2.76828	1.70963	0.71004
C	-0.44997	0.21233	0.64977
C	0.25267	-0.14104	-0.54493
N	-0.46552	0.38819	-1.65389
C	-0.05448	0.22138	-2.95652
C	1.10093	-0.46375	-3.21154
C	1.88181	-0.97363	-2.13587
C	1.45403	-0.8019	-0.82707
O	-3.01172	2.04546	-2.85572
C	-4.6018	2.94252	-0.56919
H	-2.51761	2.57932	1.34431
H	-3.44985	1.06325	1.29024
H	-0.70469	0.66726	-3.70678

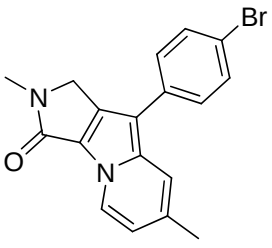
H	1.4261	-0.60023	-4.23966
H	2.08248	-1.17647	-0.02134
H	-5.43547	2.40985	-0.08565
H	-4.84964	3.11876	-1.62343
H	-4.46279	3.91294	-0.06441
C	3.16905	-1.67836	-2.34762
O	3.46439	-1.80733	-3.6741
O	3.89159	-2.0991	-1.45502
C	4.7139	-2.48099	-3.93759
H	4.79186	-2.53487	-5.02754
H	4.70695	-3.48561	-3.49642
H	5.55107	-1.91122	-3.51427
H	0.91746	-1.99902	1.57565
H	1.4619	-2.52477	3.91489
H	-0.59628	1.0356	5.20798
H	-1.08671	1.60118	2.86174



SF04

C	0.09043	-0.26225	1.93033
C	0.81086	-1.43513	2.23743
C	1.11761	-1.77373	3.55016
C	0.69704	-0.95137	4.61144
C	-0.03369	0.216	4.32225
C	-0.32857	0.54722	3.00678
C	0.99801	-1.28814	5.96376
N	1.23123	-1.55102	7.08114
N	-3.24656	1.96804	-0.61727
C	-2.51925	1.65852	-1.77017
C	-1.3421	0.97542	-1.24087
C	-1.36298	0.86236	0.13664
C	-2.61782	1.52351	0.62906
C	-0.24739	0.11364	0.56373
C	0.47525	-0.20118	-0.62969
N	-0.24375	0.33538	-1.73641
C	0.1833	0.19463	-3.03622
C	1.35315	-0.46922	-3.28712
C	2.13698	-0.9887	-2.21629
C	1.68778	-0.8362	-0.90984
O	-2.84051	1.91257	-2.93329
C	-4.50506	2.67244	-0.65347
H	-2.42076	2.3876	1.28895
H	-3.27363	0.8281	1.18181
H	-0.46744	0.63828	-3.78729

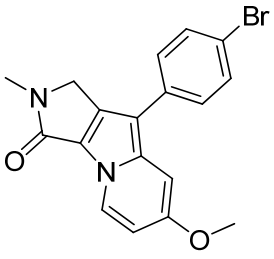
H	1.67247	-0.5753	-4.3218
H	2.31598	-1.21776	-0.10617
H	-5.30336	2.08483	-0.17232
H	-4.76019	2.83054	-1.7089
H	-4.43566	3.65108	-0.15007
C	3.43986	-1.6855	-2.42902
C	3.93269	-1.86388	-3.8486
O	4.09156	-2.10827	-1.47339
H	4.05726	-0.89138	-4.34947
H	3.21347	-2.44512	-4.44612
H	4.89484	-2.38665	-3.82689
H	1.10354	-2.1159	1.43948
H	1.67203	-2.68567	3.76452
H	-0.35647	0.86187	5.13829
H	-0.87015	1.47032	2.8049



SF05

C	-4.67599	1.73365	0.29923
N	-3.39814	1.067	0.25098
C	-3.27305	-0.32556	0.19569
C	-1.83628	-0.52233	0.06323
C	-1.13274	0.66294	0.02244
C	-2.12556	1.78503	0.12812
N	-0.95495	-1.57163	0.03689
C	0.35579	-1.03075	-0.02557
C	0.25355	0.39104	-0.01649
C	-1.19301	-2.92367	0.05365
C	-0.13724	-3.7909	-0.00758
C	1.20434	-3.31404	-0.10791
C	1.42214	-1.94828	-0.11911
O	-4.19644	-1.1447	0.24938
C	1.34755	1.36351	-0.05304
C	2.59889	1.12233	0.54949
C	3.62654	2.0627	0.50034
C	3.4077	3.2815	-0.13933
C	2.17854	3.5651	-0.73201
C	1.16494	2.61098	-0.68386
Br	4.81754	4.58751	-0.20279
C	2.33833	-4.29522	-0.22348
H	-5.44782	0.95354	0.33104
H	-4.84055	2.3616	-0.59181
H	-4.76624	2.36703	1.19696
H	-2.13998	2.43763	-0.76152

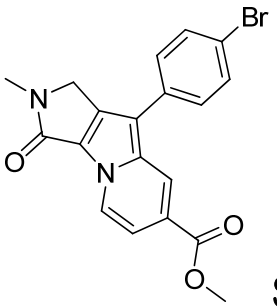
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H	-2.24074	-3.21226	0.10639
H	-0.33692	-4.86139	0.01134
H	2.43447	-1.55834	-0.21851
H	2.76389	0.19313	1.0963
H	4.58706	1.86224	0.97296
H	2.02079	4.51854	-1.23434
H	0.21711	2.82508	-1.17938
H	2.34754	-4.77015	-1.21664
H	2.24367	-5.10291	0.51724
H	3.30896	-3.80608	-0.07562



SF06

C	0.28753	-0.25952	2.05416
C	0.8688	-1.49114	2.41745
C	1.21997	-1.7702	3.73829
C	0.98722	-0.80951	4.72141
C	0.40503	0.41618	4.40334
C	0.06677	0.68393	3.07735
Br	1.47047	-1.18293	6.54564
N	-3.14111	1.82369	-0.5295
C	-2.43088	1.46226	-1.68055
C	-1.25103	0.79868	-1.14536
C	-1.23469	0.7592	0.23181
C	-2.47851	1.44175	0.72233
C	-0.10298	0.03907	0.67629
C	0.59198	-0.33721	-0.50917
N	-0.14733	0.13777	-1.62811
C	0.26228	-0.07189	-2.91641
C	1.43142	-0.74447	-3.1624
C	2.2274	-1.20146	-2.07279
C	1.80567	-0.99404	-0.76916
O	-2.77088	1.68166	-2.84815
C	-4.38607	2.54898	-0.57357
H	-2.26886	2.3375	1.33306
H	-3.11573	0.77194	1.32646
H	-0.39267	0.33021	-3.68662
H	1.72891	-0.90118	-4.1957
H	2.43086	-1.32893	0.05531
H	-5.22579	1.94513	-0.1931
H	-4.57922	2.80163	-1.62339
H	-4.32772	3.47863	0.01439
O	3.42131	-1.85228	-2.22969

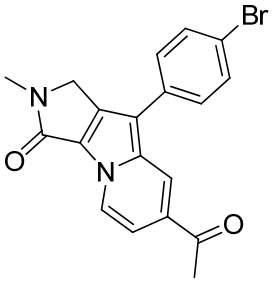
C	3.9118	-2.04043	-3.55821
H	4.87269	-2.55319	-3.44564
H	4.07278	-1.07773	-4.06818
H	3.23186	-2.66877	-4.15553
H	1.0178	-2.26097	1.65998
H	1.66248	-2.72862	4.00562
H	0.23723	1.15932	5.18091
H	-0.35879	1.65694	2.82742



SF07

C	-4.99872	1.95474	-0.01048
N	-3.71686	1.29365	0.04348
C	-3.58941	-0.09644	0.11651
C	-2.14266	-0.29501	0.09335
C	-1.44127	0.89333	0.01311
C	-2.44024	2.01119	-0.03744
N	-1.26709	-1.33549	0.21346
C	0.04413	-0.78912	0.2044
C	-0.05986	0.62994	0.10048
C	-1.50171	-2.68525	0.34749
C	-0.44287	-3.54143	0.44665
C	0.89708	-3.05452	0.36376
C	1.12061	-1.69062	0.24791
O	-4.5092	-0.91529	0.18609
C	1.04916	1.58862	0.10813
C	2.16296	1.41194	0.95258
C	3.21483	2.32477	0.97169
C	3.15721	3.44483	0.14356
C	2.06495	3.66073	-0.69546
C	1.02337	2.73469	-0.70921
Br	4.60019	4.71468	0.16348
C	1.99858	-4.0453	0.56643
O	1.90327	-4.94036	1.38595
O	3.15882	-3.93871	-0.15456
C	3.22502	-3.20196	-1.39313
H	-5.76837	1.17774	0.07604
H	-5.1392	2.49206	-0.96269
H	-5.11455	2.66926	0.81903
H	-2.38572	2.59954	-0.96972
H	-2.32423	2.71595	0.80316
H	-2.54863	-2.98048	0.36311

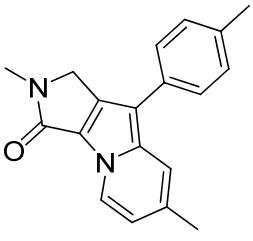
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H	2.12955	-1.28339	0.20601
H	2.18761	0.56355	1.63654
H	4.06513	2.1774	1.63622
H	2.03654	4.53731	-1.34094
H	0.18534	2.89021	-1.38985
H	2.23675	-3.08697	-1.85471
H	3.87868	-3.7871	-2.05293
H	3.6719	-2.21342	-1.22788



SF08

C	-4.77648	1.98192	0.76002
N	-3.49514	1.34224	0.58124
C	-3.35024	-0.04418	0.48804
C	-1.92153	-0.20898	0.23107
C	-1.24667	0.99744	0.16615
C	-2.24784	2.09288	0.39621
N	-1.03593	-1.23554	0.09068
C	0.25911	-0.66193	-0.07154
C	0.12955	0.75981	-0.00358
C	-1.24547	-2.59544	0.07736
C	-0.18437	-3.43441	-0.11217
C	1.13124	-2.91432	-0.31535
C	1.32399	-1.53838	-0.29847
O	-4.24559	-0.88488	0.60167
C	1.20609	1.74922	-0.08868
C	2.47429	1.53097	0.48368
C	3.48125	2.49146	0.40145
C	3.2228	3.69766	-0.24761
C	1.97598	3.95261	-0.81802
C	0.98082	2.98164	-0.73169
Br	4.6031	5.02981	-0.35414
C	2.31513	-3.79084	-0.55439
C	2.11551	-5.29101	-0.53907
O	3.42942	-3.30649	-0.75473
H	-5.53372	1.18884	0.80665
H	-5.00834	2.65197	-0.08348
H	-4.80925	2.56448	1.69355
H	-2.34114	2.78604	-0.45696
H	-2.01011	2.69597	1.28971
H	-2.27748	-2.90876	0.21742
H	-0.37019	-4.50581	-0.11793

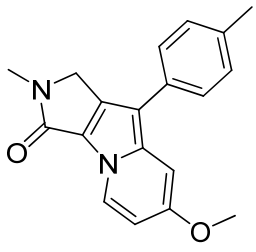
H	2.32695	-1.15271	-0.47464
H	2.66717	0.60526	1.0282
H	4.45522	2.31417	0.85423
H	1.79505	4.89788	-1.3282
H	0.0163	3.16822	-1.2053
H	3.08268	-5.7769	-0.69987
H	1.41677	-5.60421	-1.32992
H	1.69107	-5.6257	0.41844



SF09

C	-5.06194	1.35762	0.28437
N	-3.78188	0.70363	0.18892
C	-3.64044	-0.69033	0.15477
C	-2.20175	-0.87177	0.04209
C	-1.50953	0.32307	0.01984
C	-2.51372	1.43379	0.11639
N	-1.30977	-1.91074	0.00242
C	-0.00564	-1.35216	-0.04219
C	-0.12306	0.0666	-0.0127
C	-1.52595	-3.26642	0.00108
C	-0.45614	-4.11711	-0.06788
C	0.87745	-3.61912	-0.16065
C	1.07441	-2.25041	-0.14536
O	-4.55708	-1.51679	0.21194
C	0.97372	1.03649	-0.01255
C	2.17796	0.80187	0.67518
C	3.20848	1.73883	0.66422
C	3.07902	2.95674	-0.0155
C	1.87045	3.20258	-0.68289
C	0.84142	2.2663	-0.68463
C	4.19897	3.96296	-0.03607
C	2.02704	-4.57848	-0.29591
H	-5.82439	0.57081	0.33594
H	-5.25828	1.99141	-0.59666
H	-5.12796	1.98406	1.18947
H	-2.50416	2.10815	-0.75996
H	-2.36142	2.06369	1.0115
H	-2.56884	-3.57236	0.04608
H	-0.64046	-5.19123	-0.0639
H	2.08005	-1.83866	-0.2278
H	2.29417	-0.11541	1.25279
H	4.12932	1.53033	1.21254
H	1.73587	4.14611	-1.21677

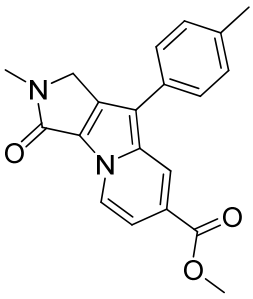
H	-0.07291	2.46998	-1.24313
H	4.78828	3.8855	-0.96417
H	4.88968	3.8098	0.80524
H	3.81664	4.99219	0.01877
H	2.02691	-5.06072	-1.28755
H	1.96548	-5.38353	0.45221
H	2.99002	-4.06728	-0.16945



SF10

C	0.15505	-0.21912	1.58028
C	0.77498	-1.44208	1.89575
C	1.10506	-1.76784	3.21062
C	0.82577	-0.89545	4.27077
C	0.19087	0.31467	3.96194
C	-0.13401	0.65027	2.64877
C	1.21891	-1.23423	5.68355
N	-3.21495	1.97723	-0.97934
C	-2.49574	1.63702	-2.13404
C	-1.32892	0.95439	-1.60527
C	-1.32667	0.87808	-0.22732
C	-2.57007	1.55832	0.26805
C	-0.2083	0.1347	0.20925
C	0.49628	-0.21345	-0.97807
N	-0.22645	0.29616	-2.09279
C	0.19265	0.11367	-3.38178
C	1.35822	-0.56503	-3.63268
C	2.14046	-1.05081	-2.54786
C	1.70753	-0.87294	-1.24414
O	-2.82864	1.88398	-3.29894
C	-4.44093	2.73302	-1.01891
H	-2.35821	2.43682	0.90409
H	-3.22053	0.88049	0.84813
H	-0.45349	0.53967	-4.14638
H	1.66524	-0.69859	-4.66675
H	2.32347	-1.22612	-0.41938
H	-5.29294	2.14949	-0.62976
H	-4.63293	2.98326	-2.07036
H	-4.35773	3.66404	-0.43493
O	3.33617	-1.70226	-2.70964
C	3.82013	-1.87381	-4.04226
H	3.98857	-0.90424	-4.53829
H	3.13086	-2.48448	-4.64696
H	4.77454	-2.40054	-3.94263

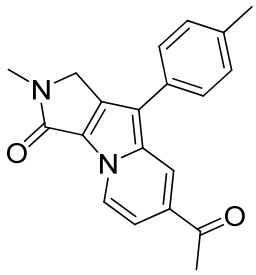
H	0.96047	-2.17028	1.10447
H	1.57911	-2.73013	3.41827
H	-0.04248	1.01696	4.76626
H	-0.59998	1.61547	2.44196
H	2.22685	-0.85353	5.91752
H	1.2362	-2.3214	5.84617
H	0.5256	-0.79137	6.41264



SF11

C	-5.2538	1.73856	-0.52216
N	-4.01099	1.05139	-0.27232
C	-3.92794	-0.34103	-0.15116
C	-2.50167	-0.56781	0.05236
C	-1.76717	0.60577	0.03017
C	-2.72115	1.74233	-0.18578
N	-1.65533	-1.63062	0.18552
C	-0.33272	-1.11145	0.24918
C	-0.39694	0.30707	0.13983
C	-1.92039	-2.97818	0.29945
C	-0.88711	-3.85	0.48834
C	0.46004	-3.38193	0.5611
C	0.71473	-2.02332	0.44918
O	-4.86841	-1.13624	-0.21702
C	0.73961	1.23053	0.1151
C	1.91984	0.93327	-0.58945
C	2.9875	1.82827	-0.60887
C	2.92336	3.05404	0.06486
C	1.74215	3.35555	0.75858
C	0.67354	2.46448	0.78574
C	4.06826	4.03027	0.02303
C	1.51542	-4.37	0.92835
O	1.30518	-5.27742	1.71196
O	2.77887	-4.24008	0.4048
C	3.01716	-3.52733	-0.82345
H	-6.05206	0.98701	-0.49518
H	-5.25552	2.22686	-1.51172
H	-5.44921	2.50258	0.24796
H	-2.5075	2.30199	-1.11337
H	-2.72633	2.47083	0.6444
H	-2.97083	-3.25355	0.23905
H	-1.08967	-4.91215	0.60986

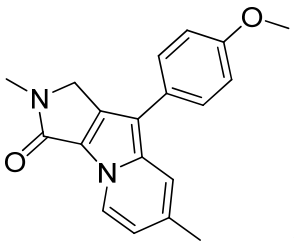
H	1.7214	-1.62396	0.55921
H	1.98478	0.0052	-1.15997
H	3.89016	1.573	-1.16839
H	1.66619	4.30097	1.30106
H	-0.22208	2.70989	1.35953
H	3.92951	4.77316	-0.78036
H	5.02346	3.52052	-0.16258
H	4.15558	4.58588	0.967
H	2.11593	-3.47609	-1.44826
H	3.80102	-4.08795	-1.34729
H	3.38313	-2.51026	-0.61829



SF12

C	-5.12039	1.76681	0.27119
N	-3.84559	1.09784	0.19742
C	-3.72462	-0.29547	0.1534
C	-2.28515	-0.49676	0.03915
C	-1.57732	0.69432	0.02253
C	-2.57035	1.81583	0.11467
N	-1.416	-1.54491	0.01033
C	-0.09747	-1.00247	-0.02408
C	-0.19831	0.42257	0.00508
C	-1.65374	-2.89982	0.00574
C	-0.59766	-3.76633	-0.05104
C	0.74276	-3.27869	-0.12819
C	0.9631	-1.90623	-0.11796
O	-4.64953	-1.11127	0.2036
C	0.90998	1.3781	0.00439
C	2.11712	1.12394	0.67958
C	3.15811	2.04811	0.6593
C	3.03758	3.26862	-0.01816
C	1.82562	3.53318	-0.67153
C	0.78509	2.61043	-0.6639
C	4.17473	4.25345	-0.05972
C	1.92612	-4.17814	-0.2246
C	1.69005	-5.67544	-0.2017
O	3.06684	-3.72147	-0.31739
H	-5.89479	0.98993	0.27562
H	-5.27771	2.42802	-0.59723
H	-5.20848	2.36528	1.19232
H	-2.55996	2.48351	-0.76651
H	-2.40737	2.44955	1.00498

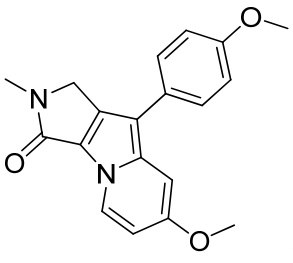
H	-2.70156	-3.18973	0.03991
H	-0.80672	-4.83422	-0.05035
H	1.98785	-1.54471	-0.19305
H	2.23105	0.20309	1.25137
H	4.08283	1.82353	1.19464
H	1.6983	4.47851	-1.20367
H	-0.13137	2.82746	-1.21407
H	4.76696	4.13421	-0.98144
H	4.85953	4.11156	0.78835
H	3.81223	5.29057	-0.03985
H	2.65802	-6.18636	-0.2442
H	1.07279	-5.9892	-1.05846
H	1.15742	-5.9772	0.71354



SF13

C	-5.08965	1.26031	-0.33738
N	-3.82475	0.58115	-0.22409
C	-3.71573	-0.81544	-0.17654
C	-2.28226	-1.02925	-0.0525
C	-1.56201	0.15011	-0.04709
C	-2.54114	1.28403	-0.15031
N	-1.41328	-2.08715	-0.02515
C	-0.09574	-1.55725	0.00717
C	-0.18206	-0.13698	-0.02403
C	-1.66032	-3.43735	-0.0094
C	-0.60943	-4.31148	0.04789
C	0.73752	-3.84403	0.11284
C	0.96507	-2.4797	0.09883
O	-4.65287	-1.61846	-0.23574
C	0.93313	0.81161	-0.04532
C	2.11944	0.55585	-0.76324
C	3.1622	1.47071	-0.79094
C	3.05398	2.68571	-0.09986
C	1.88437	2.96794	0.61586
C	0.84613	2.03602	0.63653
C	1.86776	-4.83288	0.18595
O	4.13686	3.52597	-0.19335
C	4.04369	4.77792	0.48217
H	-5.86898	0.48883	-0.36427
H	-5.14641	1.85915	-1.2618
H	-5.27084	1.92516	0.52398
H	-2.37388	1.90605	-1.04715
H	-2.52037	1.95653	0.72695

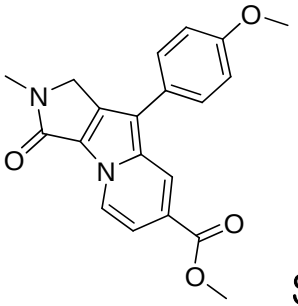
H	-2.71064	-3.71901	-0.03902
H	-0.8182	-5.3811	0.05544
H	1.98067	-2.08998	0.16613
H	2.20515	-0.36248	-1.34482
H	4.06985	1.27684	-1.36121
H	1.7744	3.90008	1.16729
H	-0.05181	2.2598	1.21406
H	2.03395	-5.31899	-0.7898
H	1.6521	-5.63358	0.91057
H	2.80801	-4.34838	0.48374
H	3.94551	4.64311	1.57213
H	3.19293	5.3735	0.11002
H	4.97766	5.30708	0.26545



SF14

C	0.09997	-0.03627	1.44354
C	0.70897	-1.24619	1.80917
C	1.13171	-1.49229	3.11769
C	0.94364	-0.51424	4.10338
C	0.32551	0.69618	3.76267
C	-0.08799	0.92545	2.4578
O	1.3143	-0.64672	5.42038
N	-3.41366	1.95898	-1.09779
C	-2.71371	1.60201	-2.25969
C	-1.51682	0.9661	-1.74044
C	-1.48149	0.92919	-0.36049
C	-2.72798	1.5955	0.14434
C	-0.32992	0.23898	0.07205
C	0.35315	-0.13166	-1.11968
N	-0.40802	0.32245	-2.2325
C	-0.00453	0.12185	-3.52353
C	1.182	-0.5178	-3.78009
C	1.99275	-0.96113	-2.69692
C	1.57616	-0.7666	-1.39022
O	-3.08051	1.81216	-3.42203
C	-4.6542	2.69138	-1.13125
H	-2.52393	2.49421	0.75441
H	-3.34943	0.92046	0.75952
H	-0.67812	0.50336	-4.2872
H	1.47587	-0.666	-4.81575
H	2.20856	-1.09254	-0.56681
H	-5.49719	2.09204	-0.74609
H	-4.85116	2.94539	-2.18087

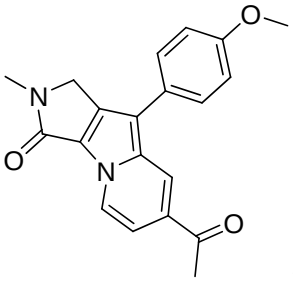
H	-4.58514	3.61959	-0.54093
O	3.20104	-1.58881	-2.86488
C	3.67646	-1.75695	-4.20093
H	3.82212	-0.7864	-4.70221
H	2.99399	-2.38335	-4.7972
H	4.64154	-2.26511	-4.10789
H	0.82793	-2.03082	1.06041
H	1.59226	-2.44936	3.35784
H	0.18837	1.4487	4.53986
H	-0.53905	1.88573	2.20251
C	1.92714	-1.87686	5.80059
H	1.25411	-2.7324	5.62695
H	2.13191	-1.78769	6.87301
H	2.87339	-2.04056	5.2593



SF15

C	-5.36257	1.74583	-0.69305
N	-4.12507	1.04256	-0.46448
C	-4.06477	-0.34537	-0.29332
C	-2.63739	-0.59396	-0.12859
C	-1.88045	0.5643	-0.20832
C	-2.82088	1.71182	-0.43378
N	-1.81212	-1.66728	0.02971
C	-0.47607	-1.17457	0.05082
C	-0.51407	0.24237	-0.11277
C	-2.10901	-3.00513	0.18039
C	-1.09404	-3.89748	0.36791
C	0.26122	-3.45425	0.41667
C	0.55012	-2.10582	0.26151
O	-5.02322	-1.12294	-0.29516
C	0.62853	1.15365	-0.17405
C	1.84351	0.80099	-0.79533
C	2.90718	1.69053	-0.85761
C	2.78962	2.97432	-0.30403
C	1.59037	3.35115	0.31032
C	0.5327	2.44452	0.36988
C	1.30972	-4.47083	0.64168
O	1.09362	-5.6598	0.83491
O	2.5694	-3.93762	0.61077
C	3.61997	-4.90059	0.83644
O	3.89656	3.77686	-0.41903

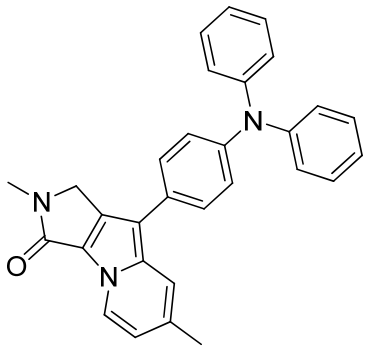
C	3.80366	5.09278	0.12487
H	-6.16866	1.00283	-0.6577
H	-5.37087	2.23811	-1.6805
H	-5.54106	2.5092	0.08275
H	-2.62456	2.24084	-1.38353
H	-2.79511	2.46393	0.37494
H	-3.16763	-3.25257	0.14467
H	-1.3076	-4.95706	0.49175
H	1.57746	-1.75431	0.31576
H	1.93934	-0.17266	-1.27606
H	3.84194	1.4184	-1.34882
H	1.47405	4.33844	0.75513
H	-0.38742	2.74217	0.87646
H	3.5447	-5.31915	1.84884
H	4.55407	-4.34406	0.71503
H	3.55551	-5.71759	0.10663
H	3.62467	5.06623	1.21284
H	3.00376	5.67353	-0.36319
H	4.77089	5.56767	-0.07137



SF16

C	-5.13666	1.6198	-0.44351
N	-3.87594	0.9362	-0.2994
C	-3.77508	-0.4584	-0.24751
C	-2.33985	-0.6789	-0.11101
C	-1.61566	0.50283	-0.10009
C	-2.59159	1.63729	-0.22027
N	-1.48395	-1.73728	-0.07566
C	-0.15804	-1.21181	-0.03675
C	-0.24034	0.21386	-0.0712
C	-1.74094	-3.0892	-0.06097
C	-0.69681	-3.96879	0.01006
C	0.65049	-3.49893	0.08445
C	0.89055	-2.12962	0.06313
O	-4.71098	-1.26019	-0.31263
C	0.87545	1.15959	-0.06919
C	2.08861	0.89791	-0.73936
C	3.13241	1.81116	-0.72583
C	2.9968	3.03031	-0.04626
C	1.79548	3.32152	0.61164
C	0.75742	2.39099	0.59516
C	1.81903	-4.41547	0.19592

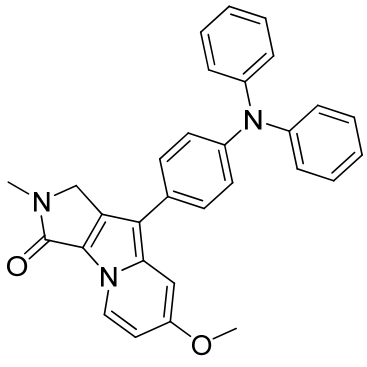
O	2.97337	-3.98405	0.16744
C	1.54938	-5.89958	0.3413
O	4.085	3.8623	-0.08669
C	3.94952	5.1394	0.53653
H	-5.92045	0.85312	-0.46603
H	-5.17603	2.20232	-1.37927
H	-5.32283	2.30188	0.40257
H	-2.41459	2.25221	-1.11994
H	-2.57974	2.3184	0.65014
H	-2.79295	-3.36186	-0.10543
H	-0.92108	-5.03353	0.01364
H	1.92062	-1.78207	0.13138
H	2.20243	-0.02505	-1.30733
H	4.0646	1.61086	-1.25259
H	1.66087	4.25885	1.14823
H	-0.15991	2.61688	1.14012
H	2.49898	-6.41845	0.50822
H	1.0774	-6.29849	-0.5706
H	0.86136	-6.10279	1.17637
H	3.77485	5.04195	1.62008
H	3.12914	5.71841	0.08296
H	4.89968	5.65639	0.36818



SF17

C	-6.92556	-0.25301	-0.11141
N	-5.62615	-0.87456	-0.09824
C	-5.45558	-2.26508	-0.04545
C	-4.01265	-2.41653	0.01969
C	-3.34171	-1.20918	0.00618
C	-4.37124	-0.11808	-0.05828
N	-3.10222	-3.44019	0.03759
C	-1.80871	-2.85819	0.03658
C	-1.95069	-1.44161	-0.00377
C	-3.29328	-4.80004	0.04885
C	-2.20599	-5.62994	0.08269
C	-0.87999	-5.10695	0.13346
C	-0.70832	-3.73478	0.11323
O	-6.35668	-3.11083	-0.05749
C	-0.85498	-0.47509	-0.05681
C	0.31777	-0.73442	-0.79307

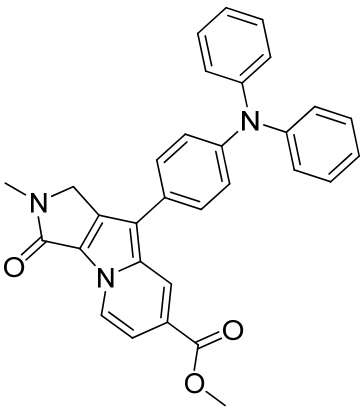
C	1.37464	0.16583	-0.81651
C	1.31098	1.36632	-0.08842
C	0.13145	1.6577	0.61843
C	-0.92656	0.75475	0.62438
N	2.42643	2.24139	-0.05999
C	2.24771	3.64879	-0.0724
C	3.73767	1.69535	0.00751
C	4.01182	0.60214	0.84679
C	5.297	0.06786	0.90462
C	6.33008	0.61619	0.14177
C	6.06119	1.70911	-0.68676
C	4.77556	2.24183	-0.7626
C	3.06734	4.47559	0.71672
C	2.89139	5.8572	0.70141
C	1.8883	6.43766	-0.07847
C	1.07136	5.6177	-0.86261
C	1.24845	4.23594	-0.86634
C	0.29202	-6.04351	0.22542
H	-7.66745	-1.06161	-0.11717
H	-7.06848	0.37032	-1.00908
H	-7.08488	0.37458	0.78152
H	-4.25903	0.5184	-0.95393
H	-4.34999	0.55017	0.82244
H	-4.33202	-5.1228	0.03349
H	-2.37163	-6.70719	0.08895
H	0.29112	-3.30435	0.16438
H	0.37966	-1.63997	-1.39763
H	2.26617	-0.05168	-1.40405
H	0.05896	2.58779	1.18249
H	-1.81597	0.98498	1.21311
H	3.20729	0.17841	1.44817
H	5.49212	-0.7801	1.56323
H	7.33514	0.19711	0.19103
H	6.85661	2.14457	-1.29354
H	4.5645	3.08948	-1.41459
H	3.84194	4.0231	1.33682
H	3.53485	6.48349	1.31979
H	1.74779	7.51898	-0.08199
H	0.29526	6.05947	-1.49019
H	0.6184	3.59887	-1.48601
H	0.27233	-6.78677	-0.58504
H	0.28157	-6.60428	1.17451
H	1.24486	-5.50033	0.16661



SF18

C	-0.20311	0.27501	-0.74961
C	0.5984	-0.84243	-0.442
C	0.66669	-1.35872	0.84949
C	-0.09265	-0.79595	1.88791
C	-0.92025	0.30116	1.58872
C	-0.96086	0.82434	0.30353
N	-0.03168	-1.31289	3.20739
N	-3.25974	2.43147	-3.69228
C	-2.22399	2.52575	-4.63303
C	-1.10065	1.91416	-3.9455
C	-1.41523	1.47951	-2.6756
C	-2.85928	1.80688	-2.42801
C	-0.29427	0.85179	-2.08843
C	0.73971	0.95004	-3.06524
N	0.20798	1.6006	-4.21456
C	0.9562	1.8399	-5.3327
C	2.27604	1.46959	-5.36725
C	2.86537	0.85306	-4.22795
C	2.10212	0.60272	-3.09776
O	-2.30942	3.01882	-5.76334
C	-4.57781	2.9637	-3.92383
H	-3.00527	2.51101	-1.58838
H	-3.46584	0.90913	-2.21583
H	0.43178	2.33405	-6.14734
H	2.8447	1.66938	-6.27057
H	2.56755	0.14864	-2.22618
H	-5.34612	2.17352	-3.88999
H	-4.57493	3.4132	-4.92499
H	-4.8374	3.73786	-3.18293
O	4.18493	0.48654	-4.16725
C	4.99252	0.73831	-5.31802
H	5.03424	1.81419	-5.55411
H	4.62751	0.18028	-6.19628
H	5.99587	0.38701	-5.05774
H	1.16752	-1.33064	-1.23505
H	1.29808	-2.22345	1.05458
H	-1.51654	0.75258	2.3822
H	-1.58265	1.6995	0.11187
C	-0.07968	-0.41968	4.31245
C	0.08742	-2.70909	3.43625

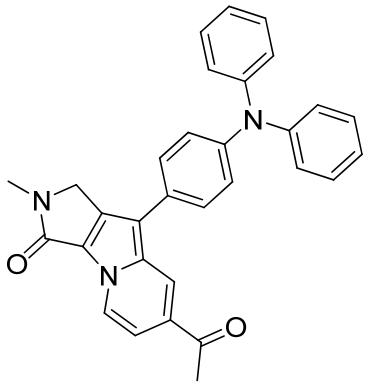
C	-0.84311	-0.73424	5.45033
C	-0.88094	0.14167	6.5333
C	-0.17343	1.3467	6.49913
C	0.58053	1.66541	5.36543
C	0.63777	0.78887	4.28343
C	-0.59646	-3.63273	2.6295
C	-0.46837	-5.00043	2.86635
C	0.32646	-5.4733	3.91204
C	1.00347	-4.55625	4.71819
C	0.8952	-3.18806	4.48138
H	-1.40287	-1.6702	5.47426
H	-1.48081	-0.11568	7.40783
H	-0.21105	2.03235	7.34617
H	1.14618	2.59809	5.32644
H	1.23572	1.03054	3.4039
H	-1.23379	-3.27396	1.82025
H	-1.01508	-5.7016	2.23299
H	0.42009	-6.54426	4.09452
H	1.63664	-4.90674	5.53526
H	1.43655	-2.47702	5.10664



SF19

C	-7.16568	-0.08034	-0.27706
N	-5.84834	-0.66209	-0.20324
C	-5.63886	-2.04207	-0.11264
C	-4.18867	-2.1493	-0.01937
C	-3.55708	-0.91598	-0.06204
C	-4.61884	0.13651	-0.18845
N	-3.25385	-3.13982	0.03893
C	-1.97775	-2.51301	0.03544
C	-2.16374	-1.10045	-0.05012
C	-3.40082	-4.50936	0.10404
C	-2.29054	-5.29782	0.19692
C	-0.98936	-4.71401	0.24345
C	-0.85213	-3.33478	0.16581
O	-6.5105	-2.91639	-0.11787
C	-1.08525	-0.11648	-0.12059
C	0.08235	-0.3743	-0.86523

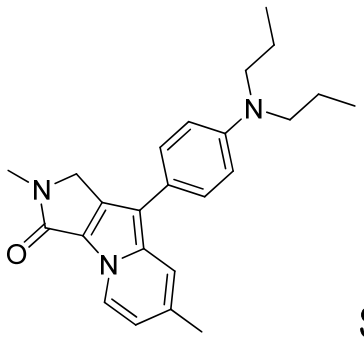
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C	1.08423	1.71887	-0.14832
C	-0.09482	2.01166	0.56021
C	-1.15555	1.11164	0.56287
N	2.21294	2.57352	-0.11107
C	2.07882	3.98357	-0.06261
C	3.51093	1.98389	-0.0805
C	3.77019	0.90258	0.77615
C	5.02631	0.30167	0.78745
C	6.04548	0.77934	-0.03893
C	5.79369	1.86491	-0.8815
C	4.53552	2.46372	-0.90973
C	3.00021	4.76143	0.66002
C	2.87444	6.14836	0.69437
C	1.82574	6.78951	0.02801
C	0.90514	6.01805	-0.68417
C	1.03005	4.63088	-0.7399
C	0.17474	-5.61366	0.38005
O	0.10816	-6.83231	0.46981
O	1.35905	-4.92754	0.39795
C	2.52406	-5.76698	0.5254
H	-7.88592	-0.90778	-0.26011
H	-7.30119	0.49376	-1.20782
H	-7.35991	0.58504	0.58073
H	-4.51987	0.72764	-1.11569
H	-4.6285	0.84787	0.65679
H	-4.42689	-4.86759	0.08279
H	-2.38754	-6.37961	0.25397
H	0.13222	-2.8754	0.2071
H	0.14205	-1.27993	-1.46988
H	2.02717	0.30671	-1.48144
H	-0.16194	2.93482	1.13581
H	-2.04211	1.33976	1.15688
H	2.97455	0.53888	1.42665
H	5.21028	-0.54096	1.45585
H	7.02928	0.30892	-0.02918
H	6.57933	2.23942	-1.53891
H	4.33488	3.30301	-1.57643
H	3.81353	4.27001	1.19313
H	3.59869	6.7342	1.26196
H	1.72938	7.87456	0.06617
H	0.08544	6.49983	-1.21858
H	0.32106	4.03643	-1.3154
H	2.49312	-6.32342	1.47154
H	3.37866	-5.08285	0.50574
H	2.57512	-6.48137	-0.30578



SF20

C	-6.92008	0.01148	-0.19729
N	-5.62095	-0.60996	-0.12054
C	-5.4511	-1.99705	-0.05428
C	-4.00588	-2.14638	0.05521
C	-3.33846	-0.93219	0.03458
C	-4.36965	0.15316	-0.06576
N	-3.10119	-3.16524	0.07459
C	-1.80309	-2.57734	0.076
C	-1.95098	-1.15647	0.02438
C	-3.28874	-4.52897	0.09215
C	-2.20067	-5.35579	0.13771
C	-0.87771	-4.81939	0.20047
C	-0.70893	-3.43928	0.17417
O	-6.34484	-2.8481	-0.09039
C	-0.86092	-0.18781	-0.0465
C	0.31564	-0.4618	-0.77087
C	1.36965	0.44001	-0.80717
C	1.29744	1.65855	-0.10972
C	0.1112	1.96424	0.58157
C	-0.94236	1.05754	0.60575
N	2.41021	2.53233	-0.0919
C	2.23334	3.9408	-0.10616
C	3.72529	1.99091	-0.02535
C	4.00763	0.90415	0.81845
C	5.29605	0.3765	0.87203
C	6.32161	0.92727	0.10164
C	6.04437	2.01463	-0.73087
C	4.75545	2.54032	-0.80264
C	3.04656	4.7655	0.691
C	2.87336	6.14727	0.67373
C	1.8827	6.73025	-0.12047
C	1.0726	5.912	-0.91348
C	1.24601	4.52969	-0.91368
C	0.33916	-5.66812	0.30344
C	0.16542	-7.17256	0.28355
O	1.4603	-5.16423	0.40002
H	-7.66421	-0.79452	-0.20294
H	-7.02724	0.60741	-1.11781
H	-7.10289	0.66698	0.67057
H	-4.24064	0.77734	-0.96744

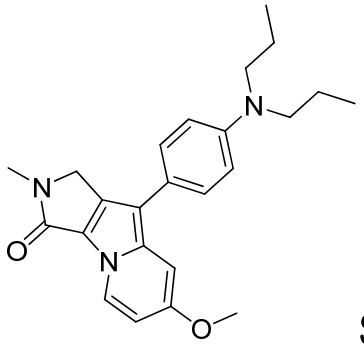
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H	0.30235	-3.0408	0.23461
H	0.38975	-1.38305	-1.34882
H	2.26709	0.206	-1.37888
H	0.035	2.90436	1.12799
H	-1.83362	1.2965	1.18836
H	3.20963	0.47806	1.42657
H	5.49752	-0.47058	1.52955
H	7.32843	0.51193	0.14657
H	6.83478	2.45088	-1.34326
H	4.53551	3.38129	-1.46062
H	3.81092	4.31106	1.32276
H	3.5099	6.77265	1.30002
H	1.74655	7.81216	-0.12828
H	0.30564	6.35554	-1.55132
H	0.62237	3.89373	-1.54114
H	1.15318	-7.64423	0.3029
H	-0.37916	-7.49631	-0.61695
H	-0.41957	-7.50855	1.15431



SF21

C	0.06192	0.45493	-0.73039
C	0.81445	-0.72408	-0.5967
C	0.97004	-1.37029	0.62549
C	0.34063	-0.8923	1.79709
C	-0.41915	0.29337	1.66299
C	-0.54778	0.94108	0.43967
N	0.43255	-1.54578	3.0287
N	-3.21315	2.67855	-3.37667
C	-2.25191	2.79894	-4.39068
C	-1.06265	2.22238	-3.78757
C	-1.28183	1.76371	-2.50047
C	-2.71081	2.05416	-2.15
C	-0.12483	1.12382	-2.01729
C	0.82952	1.24098	-3.06737
N	0.2175	1.91395	-4.1606
C	0.88799	2.16105	-5.33188
C	2.19398	1.76767	-5.45563

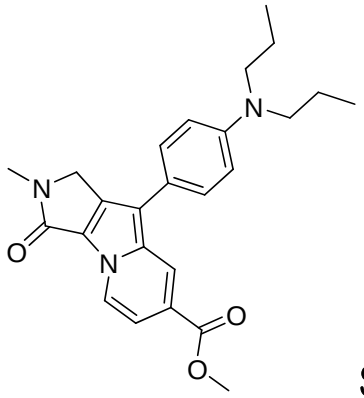
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C	-4.56164	3.16263	-3.52083
H	-2.81832	2.74671	-1.2941
H	-3.28128	1.14129	-1.90137
H	0.31125	2.67096	-6.10069
H	2.71204	1.96452	-6.39363
H	2.67416	0.40532	-2.36317
H	-5.29799	2.34373	-3.45494
H	-4.63229	3.62608	-4.51311
H	-4.80425	3.91548	-2.75315
C	4.31489	0.70446	-4.53708
H	4.79215	1.21462	-5.38405
H	4.40143	-0.37971	-4.71567
H	4.89467	0.93315	-3.63206
C	0.18888	-0.79007	4.2568
C	-1.23905	-0.90043	4.81189
C	-1.42704	-0.07647	6.0843
C	1.1917	-2.78385	3.16415
C	0.60495	-3.77316	4.17848
C	1.42266	-5.06506	4.23877
H	1.27683	-1.16783	-1.47942
H	1.59554	-2.26045	0.65439
H	-0.93538	0.71296	2.52453
H	-1.13546	1.85989	0.39062
H	0.44052	0.2705	4.08298
H	0.90041	-1.14144	5.02183
H	-1.46271	-1.96006	5.00911
H	-1.95274	-0.57922	4.03792
H	-0.74132	-0.40801	6.87926
H	-2.45223	-0.16525	6.46981
H	-1.23029	0.99163	5.90409
H	2.25212	-2.57883	3.42559
H	1.1986	-3.2866	2.18939
H	-0.43706	-3.99269	3.89575
H	0.57297	-3.31886	5.18139
H	1.43955	-5.57128	3.26105
H	1.00297	-5.7668	4.97204
H	2.46595	-4.86322	4.52744



SF22

N	-2.86265	2.97467	-3.23276
C	-1.92111	2.81634	-4.261
C	-0.85427	2.07475	-3.61789
C	-1.11447	1.79094	-2.2896
C	-2.45283	2.38347	-1.9556
C	-0.07957	0.99703	-1.75515
C	0.84927	0.83077	-2.82213
N	0.33703	1.49349	-3.97362
C	0.99982	1.49612	-5.16981
C	2.20694	0.85551	-5.28735
C	2.77953	0.21355	-4.15279
C	2.10634	0.21167	-2.9431
O	-2.03027	3.23874	-5.41855
C	-4.07794	3.72838	-3.398
H	-2.40262	3.15975	-1.1707
H	-3.17772	1.62153	-1.61721
H	0.50208	2.02781	-5.97736
H	2.7062	0.87214	-6.25277
H	2.56188	-0.25747	-2.07413
H	-4.9718	3.09771	-3.25936
H	-4.07576	4.12643	-4.41996
H	-4.12882	4.56866	-2.68491
O	3.99984	-0.41691	-4.17339
C	4.7263	-0.40054	-5.40148
H	4.96979	0.6288	-5.71138
H	4.17007	-0.90574	-6.20738
H	5.65408	-0.94693	-5.20572
C	0.04183	0.44207	-0.40857
C	0.6238	-0.81557	-0.16282
C	0.74855	-1.33574	1.12073
C	0.29193	-0.62153	2.25392
C	-0.33325	0.62378	2.0044
C	-0.43989	1.13427	0.71545
N	0.45732	-1.11153	3.54477
C	-0.07677	-0.38771	4.69029
C	-1.58141	-0.56915	4.94307
C	-2.06897	0.26634	6.12561
C	1.04492	-2.42454	3.77544
C	0.10415	-3.61936	3.56199
C	0.81664	-4.95406	3.77611
H	0.95645	-1.42605	-1.00389

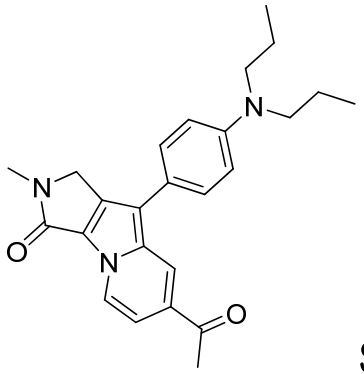
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H	-0.73026	1.21584	2.82764
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H	0.15014	0.68617	4.57662
H	0.48457	-0.71702	5.57938
H	-1.79012	-1.63596	5.11977
H	-2.13319	-0.29495	4.03057
H	-3.14494	0.12929	6.2986
H	-1.89312	1.33936	5.95325
H	-1.54432	-0.00921	7.05385
H	1.41436	-2.43891	4.81207
H	1.93762	-2.53851	3.137
H	-0.3185	-3.57121	2.54671
H	-0.74904	-3.53225	4.25323
H	1.6576	-5.07551	3.07549
H	0.13228	-5.80027	3.6214
H	1.22045	-5.03496	4.7972



SF23

C	-0.29083	0.56862	-0.36102
C	0.99246	0.30521	0.15113
C	1.18116	-0.21821	1.42697
C	0.08692	-0.53458	2.26465
C	-1.20323	-0.25109	1.75686
C	-1.37656	0.28426	0.48727
N	0.24575	-1.11395	3.52339
N	-3.1364	3.57329	-2.70343
C	-2.39192	3.31798	-3.86194
C	-1.39091	2.36318	-3.40409
C	-1.53095	2.03938	-2.06496
C	-2.69326	2.82027	-1.52593
C	-0.5188	1.14082	-1.68437
C	0.23617	0.90843	-2.87493
N	-0.32667	1.69132	-3.92504
C	0.18963	1.6976	-5.20186
C	1.2641	0.90754	-5.49621
C	1.83405	0.06569	-4.49252
C	1.31539	0.07976	-3.20488

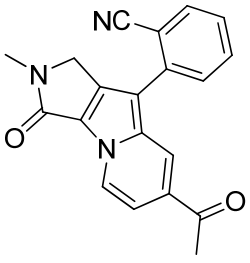
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C	-4.30051	4.4235	-2.70163
H	-2.39848	3.49834	-0.70494
H	-3.51219	2.18238	-1.14699
H	-0.32961	2.33979	-5.91004
H	1.66733	0.9063	-6.50464
H	1.74302	-0.58052	-2.45218
H	-5.20403	3.86997	-2.39563
H	-4.43178	4.79137	-3.72758
H	-4.1706	5.28431	-2.02568
C	2.96769	-0.84035	-4.7656
O	3.40958	-0.72965	-6.05811
O	3.4713	-1.60667	-3.95455
C	4.51342	-1.60034	-6.3787
H	4.74962	-1.39709	-7.42712
H	4.22581	-2.65091	-6.24104
H	5.37527	-1.38297	-5.73526
C	-0.8011	-0.91409	4.5297
C	-1.78645	-2.08089	4.67285
C	-2.87865	-1.78346	5.69905
C	1.58128	-1.44024	4.01755
C	1.60595	-2.61428	5.00013
C	3.02745	-2.94387	5.45835
H	1.87172	0.56702	-0.43862
H	2.20282	-0.33568	1.78345
H	-2.08783	-0.48446	2.34724
H	-2.39317	0.44751	0.12448
H	-1.35118	0.0109	4.29354
H	-0.31259	-0.73311	5.50112
H	-1.23043	-2.98677	4.95931
H	-2.23002	-2.30026	3.68856
H	-2.44942	-1.59463	6.69559
H	-3.58011	-2.62365	5.79437
H	-3.46246	-0.8935	5.41722
H	2.06929	-0.55636	4.47776
H	2.19906	-1.72928	3.15684
H	1.1539	-3.48639	4.50636
H	0.98637	-2.3946	5.88252
H	3.664	-3.2378	4.60943
H	3.02787	-3.77337	6.17765
H	3.49986	-2.07866	5.94417



SF24

C	-0.22874	0.60928	-0.24235
C	1.04176	0.30161	0.27808
C	1.20743	-0.21068	1.55924
C	0.10329	-0.43018	2.41648
C	-1.17656	-0.13328	1.88824
C	-1.32643	0.37252	0.60412
N	0.26646	-0.88541	3.71741
N	-2.99341	3.59962	-2.69633
C	-2.2217	3.3243	-3.83138
C	-1.25729	2.34771	-3.34408
C	-1.42706	2.05192	-2.00111
C	-2.59207	2.85262	-1.50031
C	-0.42615	1.15884	-1.58007
C	0.35472	0.89822	-2.75093
N	-0.18324	1.66711	-3.82895
C	0.36195	1.64725	-5.09291
C	1.4408	0.84681	-5.34337
C	1.99975	0.02844	-4.31526
C	1.44173	0.06968	-3.04147
O	-2.36693	3.82243	-4.9512
C	-4.11937	4.49861	-2.72157
H	-2.31637	3.5355	-0.67687
H	-3.428	2.22388	-1.14212
H	-0.13267	2.28565	-5.82248
H	1.85564	0.84657	-6.34884
H	1.86524	-0.57341	-2.2715
H	-5.06861	3.96849	-2.53503
H	-4.1521	4.94663	-3.72253
H	-4.00902	5.29841	-1.97146
C	3.16866	-0.86413	-4.54255
C	3.74767	-0.93881	-5.94195
O	3.65963	-1.52146	-3.62117
H	2.98532	-1.25693	-6.66896
H	4.57654	-1.65433	-5.94481
H	4.11534	0.04589	-6.26828
C	-0.88725	-1.08206	4.58549
C	-1.63372	-2.4118	4.4053
C	-2.89362	-2.48115	5.26825
C	1.57119	-1.32209	4.20018
C	2.02909	-2.70519	3.7135

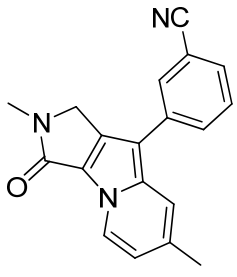
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H	2.21842	-0.42806	1.89921
H	-2.07237	-0.31911	2.47642
H	-2.33615	0.55745	0.23292
H	-1.58784	-0.24246	4.44025
H	-0.53605	-0.99624	5.62598
H	-0.95586	-3.24358	4.65511
H	-1.89272	-2.53736	3.34181
H	-3.40974	-3.44309	5.14564
H	-3.60436	-1.68451	4.99861
H	-2.65604	-2.36319	6.3371
H	1.52765	-1.32113	5.30035
H	2.3299	-0.567	3.93236
H	2.02059	-2.72183	2.61233
H	1.29758	-3.46077	4.03959
H	3.74516	-4.04352	3.87747
H	3.43933	-3.0821	5.33891
H	4.16867	-2.32133	3.91007



SF25

C	0.08001	-0.38952	2.04099
C	0.62475	-1.67305	2.24218
C	0.95025	-2.1395	3.51183
C	0.72886	-1.34109	4.63716
C	0.1874	-0.07033	4.47669
C	-0.12937	0.41326	3.19483
N	-3.32833	1.67226	-0.66094
C	-2.51815	1.4204	-1.76662
C	-1.32306	0.83269	-1.16847
C	-1.40266	0.73357	0.21211
C	-2.72384	1.31047	0.62611
C	-0.26501	0.05233	0.6899
C	0.5271	-0.2256	-0.46927
N	-0.1655	0.26387	-1.60882
C	0.33197	0.1329	-2.88478
C	1.55006	-0.46216	-3.06909
C	2.31951	-0.9131	-1.95478
C	1.79324	-0.78282	-0.67352
O	-2.78705	1.64769	-2.94965
C	-4.6041	2.33846	-0.76246
H	-2.60926	2.19731	1.2718

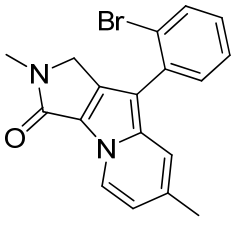
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H	-0.30494	0.52841	-3.67284
H	1.92232	-0.56304	-4.08663
H	2.39443	-1.11735	0.17193
H	-5.40269	1.73736	-0.29887
H	-4.82062	2.46796	-1.82988
H	-4.58216	3.32843	-0.27715
C	3.6806	-1.50285	-2.09894
C	4.26522	-1.62295	-3.48982
O	4.31534	-1.87582	-1.11118
H	4.3096	-0.63981	-3.98384
H	3.64639	-2.27703	-4.12187
H	5.27521	-2.03868	-3.41459
H	0.75874	-2.32509	1.37948
H	1.36236	-3.14311	3.62424
H	0.97676	-1.70489	5.63383
C	-0.63773	1.74058	3.0914
N	-1.05217	2.83447	3.0441
H	0.01135	0.57247	5.33826



SF26

C	0.15049	-0.33687	1.96514
C	1.4609	-0.62801	2.39647
C	1.73509	-0.92616	3.73168
C	0.72127	-0.92435	4.68482
C	-0.58802	-0.61245	4.28125
C	-0.86766	-0.33922	2.93413
N	-3.02488	2.08705	-0.60813
C	-2.29697	1.75373	-1.75391
C	-1.21354	0.93225	-1.22522
C	-1.28685	0.75792	0.14348
C	-2.50582	1.48993	0.62658
C	-0.17619	0.00842	0.58443
C	0.56678	-0.29508	-0.60075
N	-0.09814	0.31385	-1.70657
C	0.37271	0.23273	-2.99518
C	1.51993	-0.46888	-3.24584
C	2.20349	-1.1397	-2.19057
C	1.7084	-1.04852	-0.89469
O	-2.54639	2.09551	-2.91276
C	-4.26905	2.81711	-0.66209
H	-2.26974	2.26263	1.37875

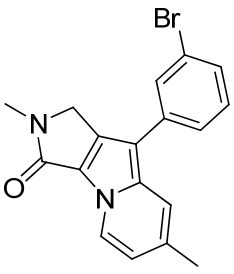
H	-3.26206	0.81729	1.07287
H	-0.22706	0.75079	-3.74062
H	1.8827	-0.51345	-4.26974
H	2.23185	-1.59407	-0.11228
H	-5.10997	2.20726	-0.29097
H	-4.44891	3.07514	-1.713
H	-4.21493	3.74233	-0.06711
C	3.44148	-1.94536	-2.41018
C	4.02255	-1.99039	-3.80659
O	3.97497	-2.54834	-1.47873
H	4.25252	-0.97694	-4.16971
H	3.30567	-2.43297	-4.51478
H	4.93866	-2.5909	-3.79335
C	-1.64358	-0.55034	5.24167
N	-2.51523	-0.47791	6.01832
H	2.28644	-0.58072	1.68915
H	2.75899	-1.14965	4.03106
H	0.92785	-1.14333	5.73086
H	-1.89773	-0.13035	2.6521



SF27

C	0.05533	-0.33182	2.11045
C	0.35847	-1.68673	2.36211
C	0.69451	-2.14404	3.63323
C	0.72866	-1.25367	4.70758
C	0.43762	0.09365	4.49644
C	0.11375	0.53732	3.21603
N	-3.36136	1.74141	-0.54785
C	-2.57119	1.48876	-1.67054
C	-1.37475	0.87349	-1.09986
C	-1.44584	0.75232	0.27918
C	-2.76422	1.31091	0.72124
C	-0.29803	0.09204	0.74763
C	0.48535	-0.17867	-0.412
N	-0.21368	0.31651	-1.54923
C	0.29738	0.21224	-2.8235
C	1.52232	-0.3707	-3.00755
C	2.27333	-0.8675	-1.89774
C	1.73872	-0.75999	-0.61954
O	-2.85969	1.73995	-2.84391
C	-4.66632	2.35105	-0.63135
H	-2.64682	2.15982	1.41444
H	-3.39393	0.55636	1.22117
H	-0.32873	0.62105	-3.61332

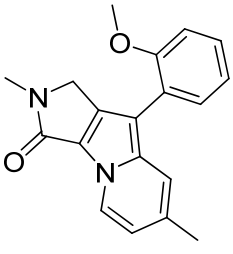
H	1.90795	-0.44763	-4.0225
H	2.31826	-1.13289	0.22444
H	-5.45479	1.66293	-0.28579
H	-4.84516	2.60092	-1.68397
H	-4.71411	3.27234	-0.02993
C	3.62147	-1.49235	-2.04468
C	4.30066	-1.43963	-3.39617
O	4.17236	-2.03117	-1.08355
H	4.2922	-0.42301	-3.81658
H	3.78277	-2.09554	-4.11363
H	5.33336	-1.78668	-3.28401
H	0.30808	-2.38709	1.52728
H	0.92752	-3.19824	3.78498
H	0.98584	-1.59691	5.71054
Br	-0.18923	2.43306	3.00272
H	0.47195	0.80814	5.31772



SF28

C	0.09808	-0.3429	2.10025
C	0.74981	-1.56237	2.37007
C	1.0517	-1.93496	3.67853
C	0.69934	-1.12213	4.75866
C	0.03592	0.0734	4.48864
C	-0.26453	0.47187	3.19072
N	-3.28177	1.81142	-0.48981
C	-2.52846	1.5276	-1.63129
C	-1.33243	0.8894	-1.08649
C	-1.36882	0.77597	0.2927
C	-2.6548	1.38929	0.7674
C	-0.23819	0.06412	0.73447
C	0.51549	-0.2175	-0.44741
N	-0.20313	0.29431	-1.56592
C	0.25693	0.16622	-2.85687
C	1.46246	-0.44001	-3.08031
C	2.25143	-0.92312	-1.99087
C	1.76058	-0.80184	-0.69634
O	-2.84504	1.76856	-2.79896
C	-4.55739	2.48392	-0.54168
H	-2.49758	2.25715	1.43005
H	-3.29042	0.66842	1.30826
H	-0.38829	0.58983	-3.62332
H	1.80592	-0.53928	-4.10778

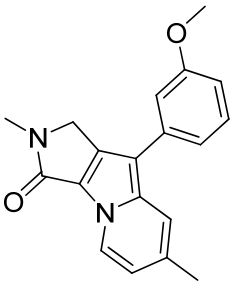
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H	-5.34728	1.87196	-0.07963
H	-4.80238	2.6458	-1.59802
H	-4.52197	3.45833	-0.02947
C	3.59087	-1.55727	-2.1785
C	4.14575	-1.66322	-3.58322
O	4.22576	-1.98907	-1.21513
H	4.20609	-0.67413	-4.06115
H	3.49235	-2.28452	-4.21542
H	5.14136	-2.11575	-3.5422
Br	-0.47185	1.21862	5.95231
H	0.98999	-2.23902	1.55037
H	1.55928	-2.8822	3.86363
H	0.92716	-1.4097	5.7839
H	-0.74779	1.43286	3.02266



SF29

C	-4.89273	1.38846	-0.79654
N	-3.58783	0.80846	-0.60582
C	-3.39696	-0.55173	-0.34813
C	-1.94946	-0.66071	-0.2187
C	-1.30263	0.55321	-0.38854
C	-2.34789	1.59272	-0.65137
N	-1.03183	-1.64313	-0.00714
C	0.25635	-1.03449	-0.04613
C	0.08737	0.36052	-0.29936
C	-1.20464	-2.98827	0.22635
C	-0.10971	-3.77487	0.44749
C	1.20359	-3.21287	0.4606
C	1.35886	-1.85356	0.21117
O	-4.27629	-1.41437	-0.26098
C	1.18694	1.3146	-0.46777
C	2.32042	0.963	-1.22031
C	3.39508	1.83359	-1.39138
C	3.34426	3.10119	-0.81743
C	2.22948	3.48899	-0.06765
C	1.15889	2.60863	0.11117
C	2.42398	-4.01948	0.73262
O	3.54473	-3.50575	0.71425
C	2.25631	-5.49782	1.02632
O	0.04213	2.91874	0.85038
C	0.0452	4.16287	1.54955
H	-5.62519	0.57565	-0.70884
H	-4.98788	1.84981	-1.79389

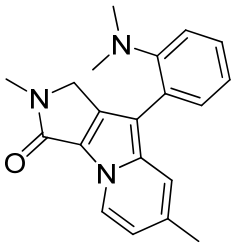
H	-5.11015	2.15295	-0.03188
H	-2.22533	2.07467	-1.63766
H	-2.34802	2.38693	0.11233
H	-2.2372	-3.32912	0.21338
H	-0.26753	-4.8375	0.61783
H	2.36275	-1.43057	0.23011
H	2.33683	-0.01759	-1.69833
H	4.25801	1.52624	-1.98252
H	4.16924	3.80294	-0.9491
H	2.20518	4.4832	0.37527
H	3.2357	-5.9245	1.26674
H	1.83304	-6.02218	0.15613
H	1.56767	-5.66239	1.87003
H	-0.88853	4.18534	2.12303
H	0.06625	5.01844	0.85492
H	0.90153	4.22977	2.2398



SF30

C	-4.79799	1.60949	0.5638
N	-3.53119	0.93073	0.45121
C	-3.43036	-0.45148	0.25701
C	-1.99308	-0.66017	0.12561
C	-1.27039	0.51846	0.22307
C	-2.24713	1.63718	0.43046
N	-1.13512	-1.71261	0.01328
C	0.19018	-1.18675	0.04122
C	0.10577	0.23142	0.19479
C	-1.38956	-3.05894	-0.11085
C	-0.34186	-3.92866	-0.23509
C	1.00448	-3.45533	-0.24927
C	1.24286	-2.09215	-0.11546
O	-4.3683	-1.25277	0.21791
C	1.21988	1.17384	0.30495
C	2.41363	0.84033	0.9623
C	3.44657	1.77648	1.05676
C	3.30554	3.0516	0.51953
C	2.11303	3.39846	-0.13018
C	1.07821	2.46655	-0.2414
C	2.17834	-4.36144	-0.40443
O	3.32296	-3.9115	-0.47777
C	1.92777	-5.85367	-0.47077
O	2.0622	4.6778	-0.62933
C	0.87347	5.06039	-1.3168

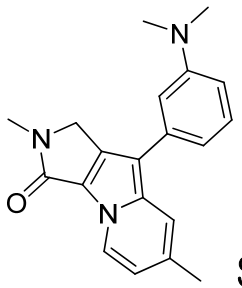
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H	-4.95596	2.31298	-0.27177
H	-4.87041	2.16658	1.51175
H	-2.23687	2.38765	-0.38065
H	-2.07374	2.17637	1.37887
H	-2.44104	-3.33747	-0.11284
H	-0.56331	-4.98887	-0.33832
H	2.27165	-1.7371	-0.146
H	2.51992	-0.1352	1.43455
H	4.37057	1.51047	1.5724
H	4.09861	3.79497	0.5892
H	0.16758	2.70862	-0.7856
H	2.89204	-6.37205	-0.50386
H	1.34926	-6.11024	-1.3718
H	1.34854	-6.20361	0.39771
H	-0.00739	5.01741	-0.65299
H	0.69686	4.42543	-2.20051
H	1.03427	6.09494	-1.63896



SF31

C	0.17364	-0.83402	1.53049
C	0.7589	-2.09934	1.71142
C	0.98595	-2.6352	2.97865
C	0.62685	-1.89237	4.10285
C	0.06805	-0.62265	3.95204
C	-0.15585	-0.06282	2.68139
H	0.78533	-2.2939	5.10509
N	-3.36831	0.87686	-1.19719
C	-2.50631	0.7921	-2.29459
C	-1.26785	0.29753	-1.70275
C	-1.3725	0.10358	-0.33402
C	-2.76023	0.48027	0.07863
C	-0.15801	-0.39986	0.16623
C	0.70389	-0.4866	-0.96851
N	-0.01709	-0.0496	-2.11897
C	0.54729	-0.03364	-3.37379
C	1.84818	-0.42535	-3.52861
C	2.62802	-0.83808	-2.4041
C	2.03796	-0.85882	-1.14583
O	-2.77689	1.08023	-3.46415
C	-4.72222	1.35927	-1.30682
H	-2.76224	1.3081	0.80813
H	-3.3102	-0.36062	0.5352
H	-0.10871	0.30316	-4.17352

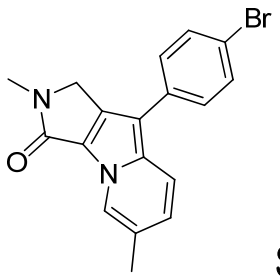
H	2.27322	-0.40859	-4.52967
H	2.6362	-1.17027	-0.289
H	-5.44993	0.58726	-1.0084
H	-4.89011	1.62194	-2.35906
H	-4.88275	2.25181	-0.68058
C	4.05521	-1.24847	-2.51695
C	4.69172	-1.24698	-3.8911
O	4.70141	-1.58352	-1.52269
H	0.97728	-2.69623	0.82596
H	1.41959	-3.62995	3.08201
H	-0.17343	-0.04642	4.84358
N	-0.73153	1.22652	2.53505
H	4.69468	-0.234	-4.32249
H	4.13184	-1.8913	-4.58579
H	5.72187	-1.6081	-3.80664
C	-1.37186	1.79564	3.71172
C	0.09005	2.22448	1.84416
H	-2.07083	1.07099	4.14978
H	-1.94078	2.6851	3.40381
H	-0.65383	2.11613	4.49486
H	-0.54981	3.05423	1.50742
H	0.57097	1.78414	0.96611
H	0.87315	2.63733	2.51061



SF32

C	0.50764	-0.13639	1.10263
C	1.85374	-0.19471	1.50798
C	2.15285	-0.47003	2.84207
C	1.15115	-0.68079	3.78644
C	-0.21074	-0.62848	3.40583
C	-0.50388	-0.34895	2.05378
H	1.42857	-0.88229	4.81918
N	-2.68557	2.30151	-1.44291
C	-1.99187	1.93161	-2.60049
C	-0.92959	1.07527	-2.08818
C	-0.97373	0.93534	-0.70974
C	-2.14957	1.7206	-0.2083
C	0.13555	0.1893	-0.27462
C	0.85086	-0.14709	-1.46391
N	0.16847	0.43161	-2.57572
C	0.62394	0.30293	-3.86775
C	1.75648	-0.42333	-4.10955
C	2.45141	-1.06976	-3.0423

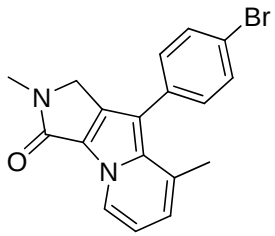
C	1.98327	-0.91843	-1.74202
O	-2.25478	2.28083	-3.75484
C	-3.8709	3.12173	-1.4739
H	-1.85803	2.50439	0.51308
H	-2.91398	1.09027	0.28385
H	0.02636	0.80842	-4.62332
H	2.10486	-0.50441	-5.13679
H	2.51187	-1.42291	-0.9346
H	-4.74338	2.58317	-1.06941
H	-4.06103	3.37753	-2.52399
H	-3.73032	4.05137	-0.89927
C	3.65999	-1.9126	-3.25958
C	4.18311	-2.06032	-4.67405
O	4.22035	-2.47665	-2.31828
H	2.65218	0.02575	0.80077
H	3.19507	-0.50193	3.16305
N	-1.22554	-0.85599	4.32523
H	-1.53821	-0.33821	1.71618
H	4.43659	-1.08009	-5.10806
H	3.42291	-2.51535	-5.32969
H	5.07528	-2.69582	-4.65918
C	-2.60393	-0.60602	3.94598
C	-0.89958	-1.01677	5.73036
H	-3.24912	-0.7738	4.81488
H	-2.93327	-1.29231	3.14753
H	-2.76115	0.43062	3.5927
H	-0.41645	-0.12118	6.16323
H	-0.22734	-1.87606	5.8862
H	-1.82055	-1.21162	6.28953



SF33

N	-3.07539	1.18111	-0.6501
C	-2.22863	1.0487	-1.7559
C	-0.99097	0.55983	-1.16635
C	-1.07277	0.40375	0.20348
C	-2.4531	0.81405	0.62645
C	0.13841	-0.12965	0.69007
C	0.97472	-0.266	-0.45831
N	0.24631	0.16138	-1.59708
C	0.77505	0.15892	-2.86689
C	2.06782	-0.25251	-3.0736
C	2.84205	-0.65345	-1.94506
C	2.3115	-0.65629	-0.67335

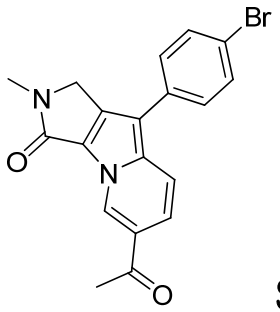
O	-2.5181	1.29899	-2.93012
C	-4.41953	1.69326	-0.75315
H	-2.45607	1.6727	1.31968
H	-3.00512	-0.00629	1.11827
H	0.10219	0.50255	-3.65069
C	2.65491	-0.28045	-4.45749
H	2.91755	-0.94734	0.18292
H	-5.16484	0.93852	-0.45156
H	-4.58618	1.96052	-1.80361
H	-4.55652	2.59002	-0.12656
H	3.88055	-0.94996	-2.09807
C	0.46892	-0.49169	2.06921
C	1.23745	-1.63006	2.38097
C	1.54085	-1.96606	3.70034
C	1.06922	-1.16086	4.73463
C	0.29603	-0.03189	4.46616
C	0.00433	0.29324	3.1431
Br	1.48092	-1.61859	6.55747
H	1.57493	-2.28628	1.57845
H	2.13082	-2.85465	3.92511
H	-0.06043	0.59087	5.28526
H	-0.57742	1.19373	2.93631
H	1.98486	0.17956	-5.19368
H	2.8508	-1.31457	-4.77824
H	3.61487	0.25487	-4.48808



SF34

N	-2.8357	1.76657	-1.00569
C	-2.10633	1.44367	-2.15477
C	-1.00476	0.64153	-1.63143
C	-1.04931	0.50841	-0.26097
C	-2.25946	1.24125	0.2374
C	0.10321	-0.17015	0.18465
C	0.84174	-0.49089	-0.99259
N	0.13509	0.05292	-2.10708
C	0.57576	-0.04797	-3.40434
C	1.73203	-0.73365	-3.65327
C	2.42928	-1.35734	-2.58874
C	2.00482	-1.26144	-1.274
O	-2.37415	1.7855	-3.31063
C	-4.04715	2.54749	-1.04089
H	-1.99874	2.05947	0.9308
H	-2.98354	0.5874	0.75171
H	-0.05393	0.4302	-4.1505

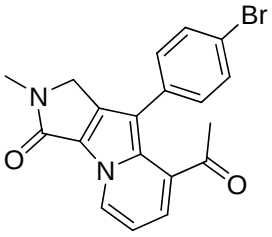
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C	2.73793	-1.99236	-0.18252
H	-4.90478	1.97947	-0.64466
H	-4.24135	2.80133	-2.09023
H	-3.94278	3.47964	-0.46147
H	3.31687	-1.95302	-2.81075
C	0.4621	-0.37965	1.59676
C	1.6868	0.07144	2.12356
C	1.98924	-0.06965	3.47727
C	1.0516	-0.65195	4.32878
C	-0.17755	-1.09806	3.84598
C	-0.46166	-0.95605	2.48817
Br	1.46392	-0.8447	6.19708
H	2.40223	0.56977	1.46895
H	2.93865	0.28566	3.87611
H	-0.90224	-1.55267	4.52019
H	-1.41747	-1.31583	2.10222
H	3.35743	-1.31595	0.42577
H	3.40081	-2.75025	-0.6195
H	2.04304	-2.48891	0.50694



SF35

N	-3.30925	1.33083	-0.38371
C	-2.49071	1.14537	-1.5019
C	-1.25604	0.62394	-0.92093
C	-1.32188	0.49974	0.44942
C	-2.68357	0.9547	0.88746
C	-0.11652	-0.0568	0.93867
C	0.70202	-0.24127	-0.20603
N	-0.03241	0.18163	-1.35755
C	0.47966	0.12893	-2.62047
C	1.76307	-0.33296	-2.82303
C	2.54367	-0.73133	-1.69689
C	2.02281	-0.68305	-0.42301
O	-2.79045	1.38014	-2.67384
C	-4.64161	1.87608	-0.47397
H	-2.65274	1.8195	1.57119
H	-3.24994	0.15183	1.38977
H	-0.16256	0.46799	-3.43097
C	2.26504	-0.36534	-4.23318
H	2.62608	-0.96773	0.43737
H	-5.40205	1.14736	-0.14733

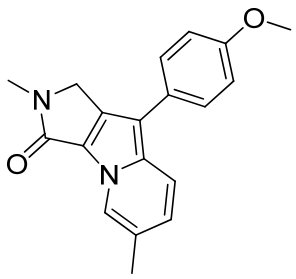
H	-4.8197	2.12994	-1.52577
H	-4.74204	2.78744	0.13763
H	3.56808	-1.06999	-1.84086
C	0.21729	-0.38869	2.3254
C	0.97405	-1.52839	2.65898
C	1.27583	-1.8405	3.9844
C	0.81084	-1.01045	5.00259
C	0.04737	0.11998	4.71151
C	-0.24167	0.42162	3.38248
Br	1.21758	-1.43601	6.8315
H	1.2988	-2.21012	1.87205
H	1.85627	-2.73017	4.22756
H	-0.30472	0.76005	5.51905
H	-0.81701	1.32211	3.15886
C	3.68922	-0.8183	-4.47061
O	1.53934	-0.03351	-5.16817
H	3.91518	-0.72507	-5.53765
H	3.8223	-1.86574	-4.16171
H	4.40036	-0.21379	-3.88834



SF36

N	-3.02573	2.08731	-0.9645
C	-2.31889	1.72981	-2.11639
C	-1.28145	0.84282	-1.60358
C	-1.3267	0.7052	-0.23362
C	-2.47737	1.52198	0.27375
C	-0.21726	-0.04874	0.2038
C	0.49056	-0.4089	-0.97339
N	-0.17882	0.19415	-2.08496
C	0.27973	0.11752	-3.37419
C	1.43112	-0.57609	-3.63208
C	2.10506	-1.23968	-2.57895
C	1.63538	-1.20205	-1.27313
O	-2.55566	2.10465	-3.26907
C	-4.15318	2.98721	-0.99031
H	-2.15085	2.31677	0.96689
H	-3.23849	0.91904	0.79668
H	-0.33188	0.62281	-4.11807
H	1.79758	-0.64058	-4.65547
C	2.20598	-2.16069	-0.26307
H	-5.06155	2.5068	-0.59333
H	-4.32367	3.26446	-2.03756
H	-3.95359	3.90076	-0.40504
H	2.97055	-1.85621	-2.82034

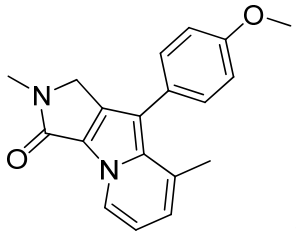
C	0.15708	-0.28813	1.60552
C	1.43904	0.0384	2.07974
C	1.78081	-0.13349	3.41927
C	0.82912	-0.63731	4.30354
C	-0.45332	-0.964	3.87025
C	-0.77897	-0.78576	2.52585
Br	1.29322	-0.87307	6.15622
H	2.17532	0.45815	1.39121
H	2.77677	0.1258	3.77724
H	-1.18615	-1.36114	4.57261
H	-1.77541	-1.06588	2.17945
C	3.70673	-2.33934	-0.1988
O	1.46219	-2.76904	0.49835
H	4.22349	-2.18083	-1.15232
H	3.93952	-3.32903	0.21057
H	4.08969	-1.58369	0.50721



SF37

N	-3.32061	1.44716	-1.22008
C	-2.47865	1.34813	-2.33632
C	-1.23099	0.86348	-1.76736
C	-1.3056	0.67321	-0.39999
C	-2.68605	1.05961	0.04188
C	-0.09283	0.12962	0.071
C	0.73677	0.02332	-1.08212
N	0.0022	0.47121	-2.21162
C	0.52471	0.48056	-3.48437
C	1.81647	0.06928	-3.70081
C	2.59983	-0.33616	-2.57979
C	2.07416	-0.35657	-1.30639
O	-2.78175	1.62413	-3.50181
C	-4.66327	1.96311	-1.30284
H	-2.69317	1.90574	0.75333
H	-3.22562	0.22517	0.52504
H	-0.15468	0.83005	-4.25938
C	2.39502	0.05423	-5.08915
H	2.67899	-0.6569	-0.45194
H	-5.41162	1.19928	-1.03358
H	-4.82777	2.26892	-2.34431
H	-4.80057	2.83643	-0.64304
H	3.64025	-0.62368	-2.74184
C	0.25008	-0.25704	1.43943
C	1.03963	-1.38314	1.72621

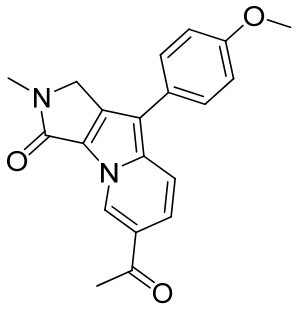
C	1.37491	-1.73739	3.0358
C	0.90497	-0.9654	4.10389
C	0.0916	0.1473	3.84376
C	-0.22398	0.49213	2.53629
O	1.17014	-1.21686	5.4286
H	1.37586	-2.02084	0.90765
H	1.98277	-2.62354	3.20822
H	-0.27235	0.73618	4.68659
H	-0.83399	1.37728	2.35324
C	2.00956	-2.33318	5.71812
H	1.73128	0.55102	-5.80959
H	2.55996	-0.97796	-5.43885
H	3.37044	0.56444	-5.1151
H	1.55966	-3.27796	5.36837
H	2.1067	-2.36138	6.80865
H	3.00752	-2.21301	5.26422



SF38

N	-2.98917	2.08471	-1.44746
C	-2.27402	1.82837	-2.6252
C	-1.21351	0.93649	-2.17843
C	-1.26008	0.69165	-0.82159
C	-2.43474	1.43433	-0.25614
C	-0.14689	-0.08227	-0.44002
C	0.57421	-0.33398	-1.64181
N	-0.10406	0.33404	-2.70576
C	0.33716	0.32461	-4.00631
C	1.46844	-0.37981	-4.31418
C	2.14341	-1.10982	-3.3031
C	1.71302	-1.11169	-1.98671
O	-2.52771	2.28602	-3.74427
C	-4.14593	2.94158	-1.40857
H	-2.13373	2.18021	0.50011
H	-3.18557	0.77123	0.21154
H	-0.27334	0.89386	-4.70403
H	1.82446	-0.38938	-5.34209
C	2.4144	-1.95398	-0.95814
H	-5.03172	2.40512	-1.02935
H	-4.34138	3.27276	-2.43658
H	-3.97449	3.82745	-0.77401
H	3.0155	-1.70884	-3.57019
C	0.18266	-0.45422	0.94536
C	1.3924	-0.08171	1.54703
C	1.67026	-0.37243	2.8862
C	0.71463	-1.03913	3.66127

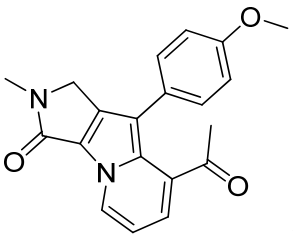
C	-0.50685	-1.4107	3.08176
C	-0.76198	-1.12245	1.7469
O	0.87502	-1.37292	4.98362
H	2.12364	0.47644	0.96004
H	2.62461	-0.06481	3.31203
H	-1.2376	-1.9367	3.69737
H	-1.71047	-1.43234	1.30326
C	2.10999	-1.01358	5.59642
H	3.06745	-2.68589	-1.45321
H	1.69568	-2.49582	-0.32647
H	3.03464	-1.34896	-0.2797
H	2.26394	0.07875	5.58572
H	2.96324	-1.50598	5.10185
H	2.04448	-1.36018	6.63287



SF39

C	-4.7097	1.62551	-0.37506
N	-3.44252	0.95915	-0.20764
C	-3.32338	-0.43421	-0.14533
C	-1.88762	-0.63443	-0.01186
C	-1.17617	0.5468	-0.0295
C	-2.16178	1.6705	-0.16088
N	-1.01254	-1.68821	0.03113
C	0.30643	-1.14598	0.04825
C	0.2096	0.2669	-0.01107
C	-1.26402	-3.03067	0.06725
C	-0.21412	-3.92093	0.12783
C	1.12261	-3.41926	0.18123
C	1.37042	-2.06776	0.15117
O	-4.2491	-1.25032	-0.1967
C	1.31967	1.22036	-0.058
C	2.49397	0.95737	-0.79286
C	3.53791	1.86967	-0.83776
C	3.43849	3.09136	-0.15589
C	2.27513	3.38393	0.56684
C	1.2378	2.45187	0.61056
C	-0.43851	-5.39414	0.15231
O	0.52062	-6.16547	0.17236
C	-1.85986	-5.91746	0.14382
O	4.51883	3.92886	-0.27061
C	4.44854	5.17471	0.42029
H	-5.48621	0.85113	-0.36638

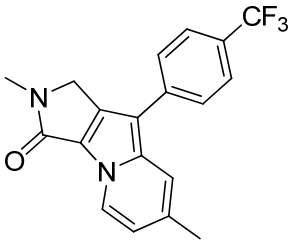
H	-4.75819	2.17029	-1.33339
H	-4.90133	2.33757	0.44527
H	-2.00025	2.2624	-1.07912
H	-2.14123	2.37321	0.69134
H	-2.31796	-3.30001	0.04047
H	1.92765	-4.14841	0.25514
H	2.38614	-1.68011	0.21381
H	2.57237	0.03273	-1.36544
H	4.44126	1.66747	-1.41185
H	2.1697	4.32361	1.10596
H	0.34955	2.67811	1.20224
H	-1.8339	-7.00403	0.2763
H	-2.35267	-5.68273	-0.81233
H	-2.46367	-5.46199	0.9425
H	4.33297	5.02554	1.50584
H	3.6165	5.79476	0.04607
H	5.39858	5.6823	0.22369



SF40

C	-5.39632	1.02739	-0.4608
N	-4.10948	0.38671	-0.35396
C	-3.95515	-1.00472	-0.36951
C	-2.52543	-1.17951	-0.15065
C	-1.85612	0.01894	-0.01712
C	-2.86369	1.1245	-0.12357
N	-1.61853	-2.20423	-0.14649
C	-0.32058	-1.62984	0.02593
C	-0.46863	-0.21733	0.06198
C	-1.83012	-3.54973	-0.3027
C	-0.75574	-4.39923	-0.30612
C	0.54653	-3.88884	-0.09247
C	0.76978	-2.53588	0.11952
O	-4.85215	-1.83588	-0.53958
C	0.59892	0.79149	0.05423
C	1.69299	0.68083	-0.81687
C	2.71928	1.6266	-0.83189
C	2.65364	2.73211	0.0273
C	1.55736	2.87039	0.89158
C	0.54892	1.91698	0.90041
C	2.15868	-2.15024	0.54886
O	3.13511	-2.65611	0.00305
C	2.31799	-1.25697	1.76087
O	3.59593	3.72573	0.09564
C	4.71895	3.61502	-0.77897

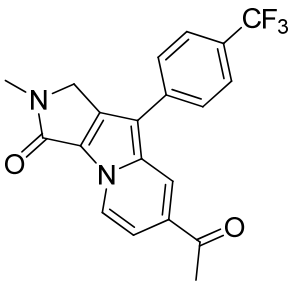
H	-6.13204	0.2421	-0.6765
H	-5.40559	1.76495	-1.2784
H	-5.68016	1.5365	0.47647
H	-2.64992	1.81559	-0.95864
H	-2.93576	1.73142	0.79672
H	-2.87201	-3.84255	-0.41645
H	-0.92337	-5.46657	-0.4357
H	1.40182	-4.5618	-0.03633
H	1.74138	-0.16275	-1.50729
H	3.55141	1.49833	-1.52258
H	1.52383	3.73644	1.55361
H	-0.28472	2.02494	1.5971
H	2.9546	-0.3987	1.50842
H	2.83912	-1.84624	2.53061
H	1.36421	-0.89645	2.16062
H	4.40486	3.62007	-1.83577
H	5.30006	2.70201	-0.5736
H	5.34016	4.49456	-0.58095



SF41

C	-5.01112	1.28724	0.80393
N	-3.73878	0.65062	0.56961
C	-3.60817	-0.72796	0.36127
C	-2.18326	-0.8885	0.1117
C	-1.49222	0.30402	0.15749
C	-2.48254	1.39398	0.44937
N	-1.30048	-1.91524	-0.10036
C	0.00046	-1.35402	-0.18939
C	-0.11179	0.0572	-0.00855
C	-1.53299	-3.26059	-0.22827
C	-0.48008	-4.1008	-0.47397
C	0.84299	-3.59707	-0.62465
C	1.05897	-2.23612	-0.47932
O	-4.51711	-1.56315	0.4007
C	0.97283	1.03108	0.02821
C	2.25328	0.7123	0.52323
C	3.27395	1.65612	0.55328
C	3.03822	2.95908	0.10244
C	1.76923	3.30256	-0.37445
C	0.75606	2.35284	-0.41073
C	4.14562	3.96982	0.09584
C	1.96683	-4.5339	-0.97531
H	-5.75842	0.48999	0.90474
H	-5.30188	1.94329	-0.03472

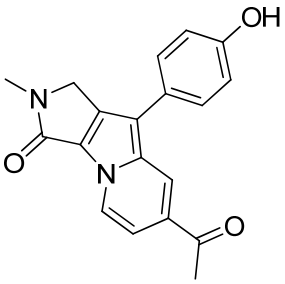
H	-4.99364	1.88437	1.7302
H	-2.55487	2.14177	-0.36107
H	-2.24991	1.9408	1.38016
H	-2.57209	-3.56426	-0.12257
H	-0.67376	-5.16876	-0.56922
H	2.05959	-1.82347	-0.60729
H	2.4368	-0.28139	0.93306
H	4.25293	1.38814	0.94882
H	1.57675	4.31801	-0.72148
H	-0.21992	2.63139	-0.80834
H	2.08105	-4.62202	-2.06815
H	1.77896	-5.54456	-0.58592
H	2.92643	-4.18446	-0.57088
F	4.87372	3.93269	-1.06712
F	5.0379	3.77027	1.11151
F	3.68046	5.2487	0.21621



SF42

C	-5.12533	1.64913	0.68602
N	-3.84639	1.01128	0.48795
C	-3.70669	-0.37292	0.3488
C	-2.27476	-0.53771	0.12291
C	-1.59137	0.66599	0.1247
C	-2.5931	1.75837	0.35629
N	-1.39039	-1.56655	-0.01538
C	-0.08832	-0.99906	-0.10965
C	-0.21135	0.42052	0.00414
C	-1.60833	-2.92309	-0.08379
C	-0.54568	-3.7627	-0.2751
C	0.77457	-3.24361	-0.42752
C	0.97744	-1.87094	-0.34549
O	-4.60607	-1.21373	0.42262
C	0.88238	1.38743	0.0253
C	2.11666	1.08922	0.63251
C	3.15006	2.01938	0.65819
C	2.96874	3.28253	0.08486
C	1.74462	3.60296	-0.51203
C	0.71666	2.6684	-0.5381
C	4.08649	4.28438	0.06834
C	1.95995	-4.11409	-0.67695
C	1.7501	-5.61284	-0.705
O	3.07642	-3.62667	-0.85532
H	-5.88625	0.86018	0.67146

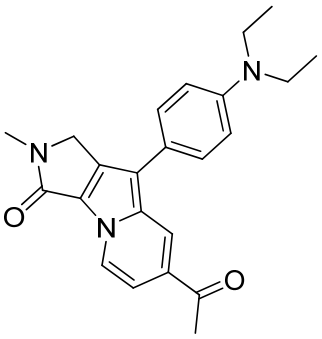
H	-5.33799	2.37425	-0.1167
H	-5.16889	2.17203	1.65544
H	-2.65702	2.47486	-0.48272
H	-2.37878	2.34402	1.2674
H	-2.64662	-3.23224	0.01207
H	-0.73649	-4.83266	-0.3213
H	1.98844	-1.48617	-0.47705
H	2.25516	0.12944	1.12956
H	4.09505	1.77195	1.14031
H	1.59849	4.58876	-0.95397
H	-0.22571	2.91948	-1.02641
H	2.71169	-6.10576	-0.87713
H	1.04694	-5.89715	-1.50385
H	1.31736	-5.96674	0.24356
F	4.77427	4.2652	-1.11751
F	5.00273	4.06097	1.05292
F	3.63128	5.56389	0.22563



SF43

C	-0.08217	-0.47097	1.91176
C	1.2013	-0.75506	2.41993
C	1.37764	-1.28517	3.69319
C	0.26772	-1.53903	4.50687
C	-1.01422	-1.23925	4.03603
C	-1.17962	-0.71657	2.75535
O	0.49998	-2.08246	5.74566
N	-2.84723	2.51423	-0.57079
C	-2.07025	2.22935	-1.69979
C	-1.10928	1.25596	-1.19984
C	-1.28574	0.96895	0.14394
C	-2.45264	1.7752	0.63238
C	-0.28556	0.07899	0.57285
C	0.49895	-0.19071	-0.59203
N	-0.03205	0.57163	-1.67495
C	0.51291	0.5364	-2.93843
C	1.58767	-0.27297	-3.18032
C	2.13975	-1.08433	-2.14428
C	1.58099	-1.02959	-0.87237
O	-2.20737	2.71802	-2.82433
C	-3.97573	3.41069	-0.61016
H	-2.18025	2.46419	1.45182
H	-3.29132	1.15069	0.99216
H	0.02302	1.17192	-3.67354

H	2.00543	-0.28334	-4.18461
H	1.99897	-1.67094	-0.09788
H	-4.9247	2.87939	-0.42677
H	-4.00195	3.85185	-1.61435
H	-3.87174	4.21579	0.13486
C	3.30021	-1.99491	-2.36087
C	3.89478	-2.0765	-3.75102
O	3.76434	-2.66183	-1.43396
H	3.13698	-2.38233	-4.48766
H	4.71272	-2.80418	-3.74571
H	4.28182	-1.09693	-4.07216
H	2.08161	-0.52644	1.82027
H	2.37458	-1.49783	4.07979
H	-1.88754	-1.43034	4.66421
H	-2.18967	-0.52204	2.391
H	-0.35236	-2.17952	6.20373



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N	-4.07871	2.01936	-1.96988
C	-3.63655	1.41332	-3.15093
C	-2.43724	0.70192	-2.72768
C	-2.15657	0.88216	-1.38177
C	-3.23741	1.74563	-0.80061
C	-0.93135	0.27166	-1.06677
C	-0.49012	-0.32756	-2.28788
N	-1.4423	-0.02409	-3.30686
C	-1.2914	-0.45494	-4.60567
C	-0.21264	-1.22679	-4.93587
C	0.75316	-1.59463	-3.94778
C	0.59286	-1.13435	-2.64464
O	-4.17076	1.50176	-4.26049
C	-5.27644	2.81798	-1.90593
C	-0.23467	0.27003	0.21646
H	-2.84461	2.67945	-0.35925
H	-3.82799	1.23702	-0.01618
H	-2.07459	-0.13894	-5.291
H	-0.11521	-1.55619	-5.96832
H	1.32501	-1.43421	-1.89689
H	-5.99932	2.39886	-1.18725
H	-5.7222	2.81635	-2.90859
H	-5.05299	3.85822	-1.61491

C	1.16872	0.32066	0.31592
C	1.82073	0.34394	1.54047
C	1.10187	0.34087	2.76055
C	-0.30909	0.27491	2.66057
C	-0.9476	0.24803	1.42691
N	1.74596	0.42466	3.99292
C	0.92385	0.30961	5.20301
C	3.17093	0.10387	4.07475
H	1.7704	0.37601	-0.59239
H	2.90859	0.38318	1.5392
H	-0.92336	0.22037	3.55732
H	-2.03637	0.172	1.40401
C	1.92651	-2.45521	-4.24928
C	2.05986	-3.01581	-5.65177
H	2.1805	-2.2046	-6.38766
H	1.16186	-3.58282	-5.94083
H	2.93786	-3.66976	-5.68996
O	2.77416	-2.70862	-3.38887
C	1.65845	0.58828	6.51002
C	3.48547	-1.38909	3.93713
H	0.4445	-0.68876	5.25697
H	0.10738	1.04245	5.11278
H	3.5442	0.47963	5.03456
H	3.70269	0.68748	3.30966
H	2.1535	1.57084	6.49434
H	2.40706	-0.17957	6.74913
H	0.92451	0.59484	7.32728
H	3.1332	-1.77772	2.97169
H	2.99645	-1.96565	4.7367
H	4.56925	-1.56602	4.00358