Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Evaluating the degree of hydrogen bonding control in the diastereoselective Diels-Alder cycloadditions of 9-(2-aminoethyl)-anthracene derivatives Supplementary information Calculations

R. A. Bawa,[1] F.-M. Gautier,[1] H. Adams,[1] Anthony J. H. M. Meijer,[1,*] and Simon Jones[1,†]

[1] *Department of Chemistry, University of Sheffield, Brook Hill, Sheffield, S3 7HF, United Kingdom*

(Dated: June 18, 2015)

* a.meijer@sheffield.ac.uk
† simon.jones@sheffield.ac.uk

CONTENTS

S1. BnNH - *anti* approach α - 1st isomer - product 8
S1.1. General Information 8
S1.2. Cartesian Co-ordinates (XYZ format) 8

S2. BnNH - *anti* approach α - 1st isomer - TS 10
S2.1. General Information 10
S2.2. Cartesian Co-ordinates (XYZ format) 10

S3. BnNH - *anti* approach α - 2nd isomer - product 12
S3.1. General Information 12
S3.2. Cartesian Co-ordinates (XYZ format) 12

S4. BnNH - *anti* approach α - 2nd isomer - TS 14
S4.1. General Information 14
S4.2. Cartesian Co-ordinates (XYZ format) 14

S5. BnNH - *anti* approach α - 3rd isomer - product 16
S5.1. General Information 16
S5.2. Cartesian Co-ordinates (XYZ format) 16

S6. BnNH - *anti* approach α - 3rd isomer - TS 18
S6.1. General Information 18
S6.2. Cartesian Co-ordinates (XYZ format) 18

S7. BnNH - *anti* approach α - 4th isomer - product 20
S7.1. General Information 20
S7.2. Cartesian Co-ordinates (XYZ format) 20

S8. BnNH - *anti* approach α - 4th isomer - TS 22
S8.1. General Information 22
S8.2. Cartesian Co-ordinates (XYZ format) 22

S9. BnNH - *anti* approach α - 5th isomer - product 24
S9.1. General Information 24
S9.2. Cartesian Co-ordinates (XYZ format) 24

S10. BnNH - *anti* approach α - 5th isomer - TS 26
S10.1. General Information 26
S10.2. Cartesian Co-ordinates (XYZ format) 26

S11. BnNH - *anti* approach β - 1st isomer - product 28
S11.1. General Information 28
S11.2. Cartesian Co-ordinates (XYZ format) 28

S12. BnNH - *anti* approach β - 1st isomer - TS 30
S12.1. General Information 30
S12.2. Cartesian Co-ordinates (XYZ format) 30

S13. BnNH - *anti* approach β - 2nd isomer - product 32

S13.1. General Information 32
S13.2. Cartesian Co-ordinates (XYZ format) 32

S14. BnNH - *anti* approach β - 2^{nd} isomer - TS 34
S14.1. General Information 34
S14.2. Cartesian Co-ordinates (XYZ format) 34

S15. BnNH - *anti* approach γ - product 36
S15.1. General Information 36
S15.2. Cartesian Co-ordinates (XYZ format) 36

S16. BnNH - *anti* approach γ - TS 38
S16.1. General Information 38
S16.2. Cartesian Co-ordinates (XYZ format) 38

S17. BnNH - *syn* approach α - 1^{st} isomer - product 40
S17.1. General Information 40
S17.2. Cartesian Co-ordinates (XYZ format) 40

S18. BnNH - *syn* approach α - 1^{st} isomer - TS 42
S18.1. General Information 42
S18.2. Cartesian Co-ordinates (XYZ format) 42

S19. BnNH - *syn* approach α - 2^{nd} isomer - product 44
S19.1. General Information 44
S19.2. Cartesian Co-ordinates (XYZ format) 44

S20. BnNH - *syn* approach α - 2^{nd} isomer - TS 46
S20.1. General Information 46
S20.2. Cartesian Co-ordinates (XYZ format) 46

S21. BnNH - *syn* approach α - 3^{rd} isomer - product 48
S21.1. General Information 48
S21.2. Cartesian Co-ordinates (XYZ format) 48

S22. BnNH - *syn* approach α - 3^{rd} isomer - TS 50
S22.1. General Information 50
S22.2. Cartesian Co-ordinates (XYZ format) 50

S23. BnNH - *syn* approach α - 4^{th} isomer - product 52
S23.1. General Information 52
S23.2. Cartesian Co-ordinates (XYZ format) 52

S24. BnNH - *syn* approach α - 4^{th} isomer - TS 54
S24.1. General Information 54
S24.2. Cartesian Co-ordinates (XYZ format) 54

S25. BnNH - *syn* approach β - 1^{st} isomer - product 56
S25.1. General Information 56
S25.2. Cartesian Co-ordinates (XYZ format) 56

S26. BnNH - *syn* approach β - 1st isomer - TS 58
S26.1. General Information 58
S26.2. Cartesian Co-ordinates (XYZ format) 58

S27. BnNH - *syn* approach β - 2nd isomer - product 60
S27.1. General Information 60
S27.2. Cartesian Co-ordinates (XYZ format) 60

S28. BnNH - *syn* approach β - 2nd isomer - TS 62
S28.1. General Information 62
S28.2. Cartesian Co-ordinates (XYZ format) 62

S29. BnNH - *syn* approach γ - product 64
S29.1. General Information 64
S29.2. Cartesian Co-ordinates (XYZ format) 64

S30. BnNH - *syn* approach γ - TS 66
S30.1. General Information 66
S30.2. Cartesian Co-ordinates (XYZ format) 66

S31. MeC(O)NH - *anti* approach α - product 68
S31.1. General Information 68
S31.2. Cartesian Co-ordinates (XYZ format) 68

S32. MeC(O)NH - *anti* approach α - TS 70
S32.1. General Information 70
S32.2. Cartesian Co-ordinates (XYZ format) 70

S33. MeC(O)NH - *anti* approach β - product 72
S33.1. General Information 72
S33.2. Cartesian Co-ordinates (XYZ format) 72

S34. MeC(O)NH - *anti* approach β - TS 74
S34.1. General Information 74
S34.2. Cartesian Co-ordinates (XYZ format) 74

S35. MeC(O)NH - *anti* approach γ - product 76
S35.1. General Information 76
S35.2. Cartesian Co-ordinates (XYZ format) 76

S36. MeC(O)NH - *anti* approach γ - TS 78
S36.1. General Information 78
S36.2. Cartesian Co-ordinates (XYZ format) 78

S37. MeC(O)NH - *syn* approach α - product 80
S37.1. General Information 80
S37.2. Cartesian Co-ordinates (XYZ format) 80

S38. MeC(O)NH - *syn* approach α - TS 82
S38.1. General Information 82

S38.2. Cartesian Co-ordinates (XYZ format) 82

S39. MeC(O)NH - *syn* approach β - product 84
S39.1. General Information 84
S39.2. Cartesian Co-ordinates (XYZ format) 84

S40. MeC(O)NH - *syn* approach β - TS 86
S40.1. General Information 86
S40.2. Cartesian Co-ordinates (XYZ format) 86

S41. MeC(O)NH - *syn* approach γ - product 88
S41.1. General Information 88
S41.2. Cartesian Co-ordinates (XYZ format) 88

S42. MeC(O)NH - *syn* approach γ - TS 90
S42.1. General Information 90
S42.2. Cartesian Co-ordinates (XYZ format) 90

S43. $CF_3C(O)NH$ - *anti* approach α - product 92
S43.1. General Information 92
S43.2. Cartesian Co-ordinates (XYZ format) 92

S44. $CF_3C(O)NH$ - *anti* approach α - TS 94
S44.1. General Information 94
S44.2. Cartesian Co-ordinates (XYZ format) 94

S45. $CF_3C(O)NH$ - *anti* approach β - product 96
S45.1. General Information 96
S45.2. Cartesian Co-ordinates (XYZ format) 96

S46. $CF_3C(O)NH$ - *anti* approach β - TS 98
S46.1. General Information 98
S46.2. Cartesian Co-ordinates (XYZ format) 98

S47. $CF_3C(O)NH$ - *anti* approach γ - product 100
S47.1. General Information 100
S47.2. Cartesian Co-ordinates (XYZ format) 100

S48. $CF_3C(O)NH$ - *anti* approach γ - TS 102
S48.1. General Information 102
S48.2. Cartesian Co-ordinates (XYZ format) 102

S49. $CF_3C(O)NH$ - *syn* approach α - product 104
S49.1. General Information 104
S49.2. Cartesian Co-ordinates (XYZ format) 104

S50. $CF_3C(O)NH$ - *syn* approach α - TS 106
S50.1. General Information 106
S50.2. Cartesian Co-ordinates (XYZ format) 106

S51. $CF_3C(O)NH$ - *syn* approach β - product 108

S51.1. General Information 108
S51.2. Cartesian Co-ordinates (XYZ format) 108

S52. $CF_3C(O)NH$ - *syn* approach β - TS 110
S52.1. General Information 110
S52.2. Cartesian Co-ordinates (XYZ format) 110

S53. $CF_3C(O)NH$ - *syn* approach γ - product 112
S53.1. General Information 112
S53.2. Cartesian Co-ordinates (XYZ format) 112

S54. $CF_3C(O)NH$ - *syn* approach γ - TS 114
S54.1. General Information 114
S54.2. Cartesian Co-ordinates (XYZ format) 114

S55. tBuC(O)NH - *anti* approach α - product 116
S55.1. General Information 116
S55.2. Cartesian Co-ordinates (XYZ format) 116

S56. tBuC(O)NH - *anti* approach α - TS 118
S56.1. General Information 118
S56.2. Cartesian Co-ordinates (XYZ format) 118

S57. tBuC(O)NH - *anti* approach β - product 120
S57.1. General Information 120
S57.2. Cartesian Co-ordinates (XYZ format) 120

S58. tBuC(O)NH - *anti* approach β - TS 122
S58.1. General Information 122
S58.2. Cartesian Co-ordinates (XYZ format) 122

S59. tBuC(O)NH - *anti* approach γ - product 124
S59.1. General Information 124
S59.2. Cartesian Co-ordinates (XYZ format) 124

S60. tBuC(O)NH - *anti* approach γ - TS 126
S60.1. General Information 126
S60.2. Cartesian Co-ordinates (XYZ format) 126

S61. tBuC(O)NH - *syn* approach α - product 128
S61.1. General Information 128
S61.2. Cartesian Co-ordinates (XYZ format) 128

S62. tBuC(O)NH - *syn* approach α - TS 130
S62.1. General Information 130
S62.2. Cartesian Co-ordinates (XYZ format) 130

S63. tBuC(O)NH - *syn* approach β - product 132
S63.1. General Information 132
S63.2. Cartesian Co-ordinates (XYZ format) 132

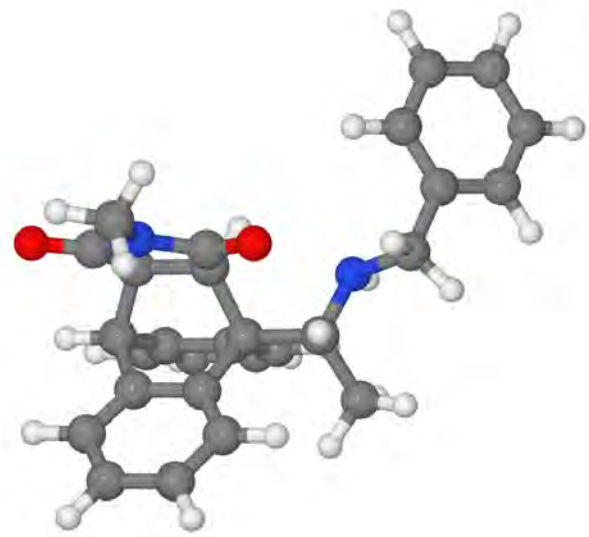
S64. tBuC(O)NH - *syn* approach β - TS 134
S64.1. General Information 134
S64.2. Cartesian Co-ordinates (XYZ format) 134

S65. tBuC(O)NH - *syn* approach γ - product 136
S65.1. General Information 136
S65.2. Cartesian Co-ordinates (XYZ format) 136

S66. tBuC(O)NH - *syn* approach γ - TS 138
S66.1. General Information 138
S66.2. Cartesian Co-ordinates (XYZ format) 138

S1. BnNH - *ANTI* APPROACH α - 1st ISOMER - PRODUCT

S1.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.0944	Debye
Energy	:	-1342.96259315	a.u.
Number of imaginary frequencies	:	0	

S1.2. Cartesian Co-ordinates (XYZ format)

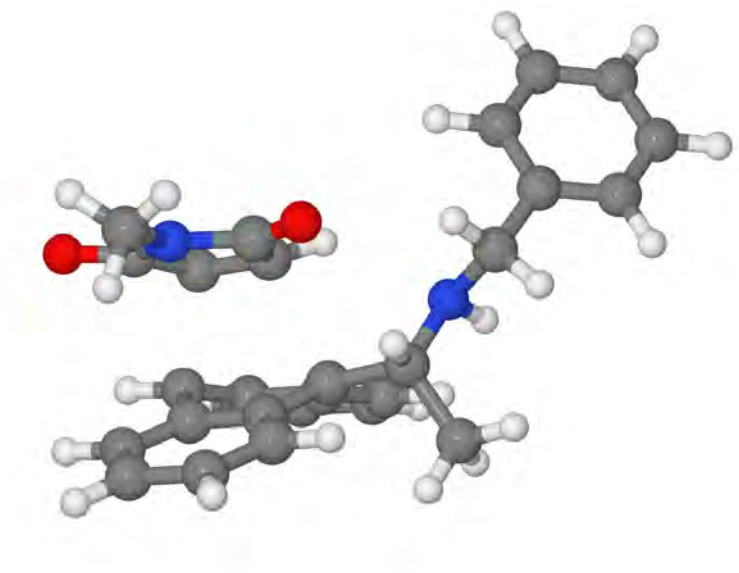
58

C	-1.55369508	-0.27037206	3.26800966
C	-0.66957510	0.41910702	2.43441772
C	-0.22578253	-0.16360310	1.24715710
C	-0.72249925	-1.42896128	0.88840240
C	-1.60763359	-2.11224437	1.71482182
C	-2.01581860	-1.53533757	2.91754580
C	0.69653368	0.46799946	0.18542831
C	-0.25746185	-1.91212344	-0.46605834
C	1.25001693	-1.84785628	-0.49424765
C	1.77090466	-0.58249849	-0.17092457
C	3.15134645	-0.39955312	-0.24752750
H	3.60453987	0.55634326	-0.03129574
C	3.98988914	-1.45877194	-0.60479128
C	3.46125364	-2.71057487	-0.90040815
C	2.08038640	-2.90274978	-0.85256112
H	-1.88156867	0.18990107	4.19327068
H	-0.34568888	1.40896106	2.72629023
H	-1.98373020	-3.08491373	1.41648638
H	-2.69986343	-2.06624341	3.56977367

H	5.06087160	-1.29667139	-0.65034658
H	4.11608982	-3.53015089	-1.17357099
H	1.65113747	-3.86887050	-1.09672976
C	1.20948005	1.88861752	0.57238221
H	-0.64580941	-2.89950013	-0.71463954
C	-0.21174376	0.54636997	-1.11916053
C	-0.72401279	-0.85419697	-1.52031779
C	-1.48305380	1.37631822	-0.95437884
H	-0.36690554	-1.16063225	-2.50569844
H	0.39131519	1.02092385	-1.89283299
O	-1.58586693	2.54390502	-0.64370334
C	-2.23827386	-0.73393649	-1.58399940
O	-3.02860880	-1.60582769	-1.86781836
N	-2.57893157	0.57176477	-1.25241554
C	-3.95041394	1.05740631	-1.19483626
H	-4.05580282	1.94609809	-1.81780362
H	-4.59741068	0.26184022	-1.55861914
H	-4.21779394	1.31249011	-0.16806355
C	2.14582300	1.93379486	1.80411065
H	2.12857103	2.93396401	2.24451804
H	1.85548437	1.22537756	2.58049154
H	3.18081737	1.71544611	1.53961074
H	0.30597112	2.44394135	0.82915765
C	1.65494323	4.05359268	-0.53957778
H	0.59264112	4.29413748	-0.43716714
H	2.17338991	4.48967648	0.32864577
N	1.75654221	2.58841681	-0.60085636
H	2.72427726	2.32875991	-0.76024896
C	2.20219779	4.68417645	-1.80136526
C	3.38598490	5.42506170	-1.78167856
C	1.53501940	4.51867151	-3.02126861
C	3.89422989	5.99386597	-2.95042396
H	3.91329837	5.56253195	-0.84266651
C	2.03701329	5.08506203	-4.18876410
H	0.61407566	3.94648457	-3.04482198
C	3.22049618	5.82478380	-4.15677214
H	4.81357765	6.56809807	-2.91621828
H	1.50492966	4.95426321	-5.12475443
H	3.61117101	6.26715517	-5.06639051

S2. BnNH - *ANTI* APPROACH α - 1st ISOMER - TS

S2.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.6307	Debye
Energy	:	-1342.90581934	a.u.
Number of imaginary frequencies	:	1	

S2.2. Cartesian Co-ordinates (XYZ format)

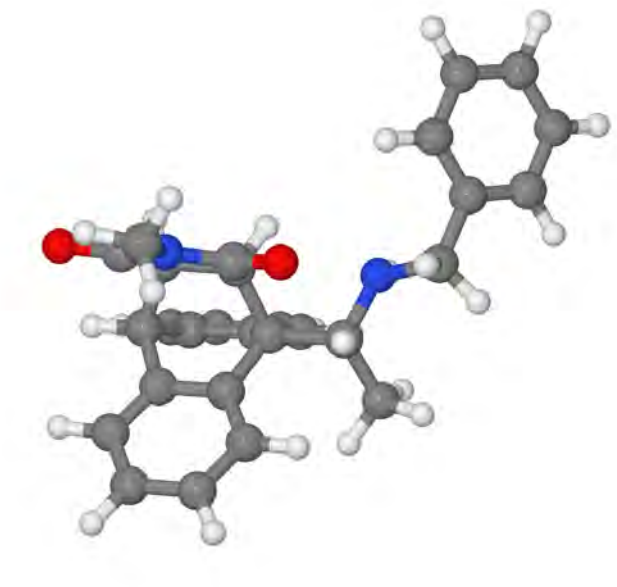
58

C	3.30053210	-1.41015220	2.57673478
C	2.10303259	-0.78133923	2.30344224
C	1.94367480	0.00480652	1.13441420
C	3.04034948	0.07981399	0.23048411
C	4.24309492	-0.60115618	0.51186967
C	4.38164186	-1.32007790	1.68010795
C	0.71063930	0.66908085	0.75758600
C	2.81980705	0.77363741	-1.00520957
C	1.93317854	1.90495420	-0.97950172
C	0.83690596	1.85173869	-0.07596555
C	-0.07891826	2.93086600	-0.09447578
H	-0.91414362	2.95278406	0.58871984
C	0.09501380	4.00207663	-0.94817364
C	1.17249608	4.03127670	-1.85012996
C	2.07274532	2.98610806	-1.87128770
H	3.40732336	-1.98117983	3.49207807
H	1.29077315	-0.88271993	3.00955296
H	5.05909824	-0.54199946	-0.19951402
H	5.31701279	-1.81852007	1.90691388

H	-0.60766298	4.82700872	-0.92092949
H	1.29670668	4.87388849	-2.52046704
H	2.90948772	2.99391437	-2.56161737
C	-0.53766358	0.41608402	1.61246991
H	3.63150311	0.78436077	-1.72564781
C	0.35144621	-0.73167819	-1.10699022
C	1.45935500	-0.55730355	-1.95261931
C	0.46123147	-2.06994319	-0.48478776
H	1.44440901	0.01503706	-2.86845732
H	-0.60682750	-0.24114637	-1.16552377
O	-0.29518047	-2.62772250	0.28941357
C	2.25360322	-1.82646978	-1.91953790
O	3.23656178	-2.12335181	-2.56567645
N	1.65132225	-2.63969326	-0.96211708
C	2.16779590	-3.92998767	-0.54442471
H	1.34222245	-4.50937939	-0.13392678
H	2.59665680	-4.43972874	-1.40692377
H	2.94005799	-3.81121111	0.22028539
C	-0.54462630	1.27149725	2.90162754
H	-1.39505792	0.98939037	3.52803636
H	0.36607134	1.13304198	3.48787618
H	-0.62702531	2.33623242	2.67389345
H	-0.47813582	-0.63223249	1.90846395
C	-2.83184695	-0.42889178	1.28231525
H	-2.44683743	-1.43403423	1.09242368
H	-3.04842758	-0.35681441	2.36006570
N	-1.79269183	0.52137685	0.84454316
H	-2.17302537	1.45963514	0.89976060
C	-4.11303997	-0.20672573	0.51052713
C	-5.21044827	0.42071256	1.10575783
C	-4.21328688	-0.60339236	-0.82841915
C	-6.38384008	0.64664304	0.38543314
H	-5.14899540	0.72975242	2.14477706
C	-5.38198805	-0.38135958	-1.55065393
H	-3.36943793	-1.09571159	-1.29933989
C	-6.47159815	0.24622658	-0.94520295
H	-7.22718763	1.13155603	0.86469609
H	-5.44627476	-0.70086551	-2.58501196
H	-7.38289165	0.41743672	-1.50726378

S3. BnNH - *ANTI* APPROACH α - 2nd ISOMER - PRODUCT

S3.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.1684	Debye
Energy	:	-1342.96259690	a.u.
Number of imaginary frequencies	:	0	

S3.2. Cartesian Co-ordinates (XYZ format)

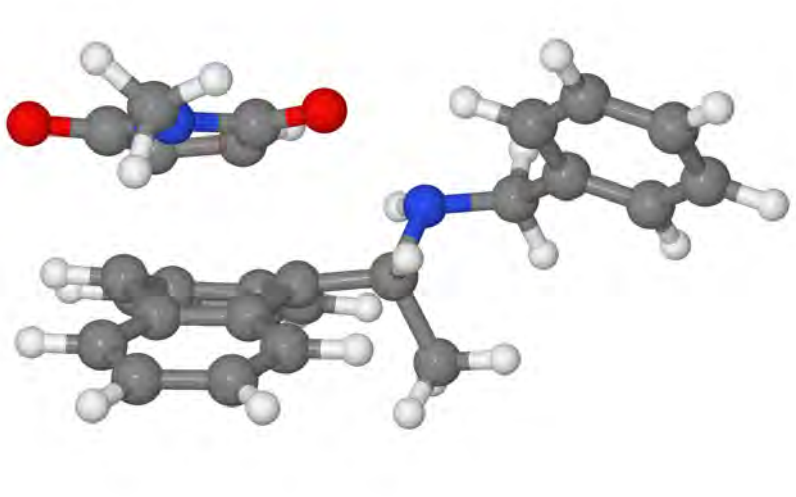
58

C	-1.28806925	-0.36101562	3.50793982
C	-0.60838729	0.38011560	2.53799319
C	-0.24098353	-0.21509244	1.33128905
C	-0.60602564	-1.55239594	1.09669125
C	-1.28877044	-2.28751183	2.05928874
C	-1.62117589	-1.69219697	3.27643561
C	0.45725346	0.45861095	0.13378015
C	-0.24221851	-2.05850244	-0.28077438
C	1.23045170	-1.80742049	-0.49628359
C	1.61371303	-0.46948549	-0.29659182
C	2.94313049	-0.12147748	-0.53379673
H	3.28888106	0.89385158	-0.40737087
C	3.86911488	-1.08778918	-0.93597627
C	3.47846413	-2.41048217	-1.11414444
C	2.14778590	-2.77017355	-0.89891398
H	-1.55814767	0.11050364	4.44611931
H	-0.38035846	1.41786385	2.74103999
H	-1.56717575	-3.31609178	1.85665822
H	-2.14677000	-2.26247430	4.03387785

H	4.89942026	-0.79765505	-1.10815597
H	4.20110893	-3.15708852	-1.42316341
H	1.82507372	-3.79561162	-1.04585290
C	0.82032603	1.95262623	0.38586789
H	-0.52240723	-3.10075641	-0.43148050
C	-0.60007149	0.33907688	-1.04945791
C	-0.96373641	-1.13730025	-1.31886733
C	-1.94303870	1.00891566	-0.76485604
H	-0.68461639	-1.45721531	-2.32491636
H	-0.16385873	0.83785522	-1.91445923
O	-2.16445470	2.16961813	-0.49375632
C	-2.47766304	-1.21455741	-1.20251608
O	-3.17167997	-2.19580245	-1.34753358
N	-2.94886947	0.05480859	-0.89127183
C	-4.35679483	0.36475211	-0.68706256
H	-4.65642643	1.18277109	-1.34298456
H	-4.92834902	-0.53207260	-0.91700983
H	-4.53125095	0.66102952	0.34853223
C	1.88177264	2.18719864	1.49157059
H	1.72723138	3.16352367	1.95774019
H	1.84210062	1.43456495	2.27970243
H	2.89546657	2.18156624	1.08855820
H	-0.11196772	2.40716314	0.72516376
C	0.94632781	4.09417677	-0.84366518
H	-0.08699735	4.28138161	-0.53527993
H	1.59832120	4.59538746	-0.11137242
N	1.12400365	2.63670683	-0.87979496
H	2.06497812	2.42260647	-1.19350231
C	1.18778706	4.70135498	-2.20864224
C	2.28992748	5.52523613	-2.44663668
C	0.31117824	4.43087673	-3.26653695
C	2.51445842	6.07304955	-3.71060824
H	2.97729373	5.74412727	-1.63525033
C	0.52981573	4.97634697	-4.52756977
H	-0.54736525	3.79276657	-3.08858681
C	1.63451064	5.79949379	-4.75390005
H	3.37460637	6.71216822	-3.87733078
H	-0.16209196	4.76395035	-5.33533192
H	1.80440009	6.22515917	-5.73659658

S4. BnNH - *ANTI* APPROACH α - 2nd ISOMER - TS

S4.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.1684	Debye
Energy	:	-1342.90086062	a.u.
Number of imaginary frequencies	:	1	

S4.2. Cartesian Co-ordinates (XYZ format)

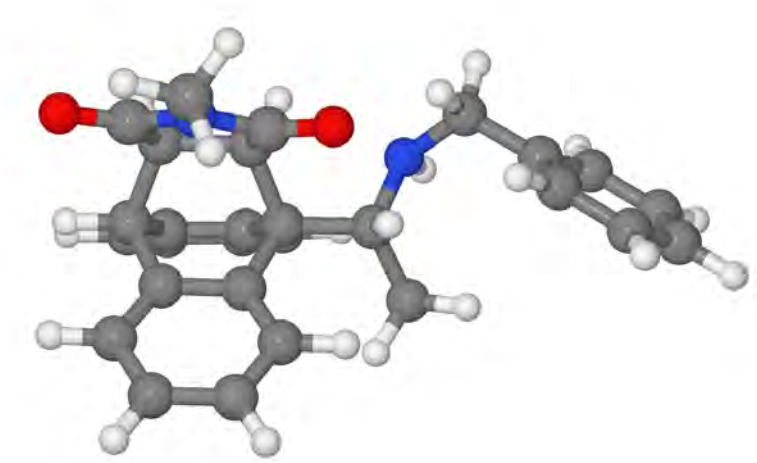
58

C	3.92760324	-0.69995856	2.50116301
C	2.64648938	-0.22326164	2.31436372
C	2.27338004	0.40224698	1.09786510
C	3.24658084	0.47168791	0.06160461
C	4.53931808	-0.05433942	0.26185623
C	4.88541126	-0.61401707	1.47360539
C	0.94731575	0.91875708	0.81920016
C	2.81480169	0.98891860	-1.20656681
C	1.83362424	2.04009271	-1.18484855
C	0.86514080	2.00571632	-0.14500338
C	-0.12281459	3.02367425	-0.14331906
H	-0.85549307	3.07466745	0.64856273
C	-0.14574401	4.00280237	-1.11702192
C	0.79912090	4.00139904	-2.15694404
C	1.77085996	3.02281785	-2.19141150
H	4.19669437	-1.14818656	3.45082378
H	1.93394041	-0.31790918	3.12165952
H	5.25849628	-0.00338256	-0.54787004
H	5.88870096	-0.99127501	1.63439953

H	-0.89732075	4.78261185	-1.07199764
H	0.76979309	4.77107620	-2.91936588
H	2.51290011	3.01190639	-2.98257518
C	-0.15093622	0.70049137	1.86284935
H	3.53892469	0.99562413	-2.01498675
C	0.56383121	-0.77260154	-0.86232138
C	1.52956438	-0.53199983	-1.85455370
C	0.94221711	-2.01580834	-0.15335943
H	1.31920981	-0.06077142	-2.80376172
H	-0.46103969	-0.44247043	-0.84774894
O	0.37826267	-2.59537935	0.75382358
C	2.48846722	-1.68524384	-1.83618200
O	3.41102529	-1.91278243	-2.59057832
N	2.13407516	-2.46938801	-0.74520928
C	2.87005639	-3.64141417	-0.30802748
H	2.21074271	-4.23433542	0.32379070
H	3.18147945	-4.22011423	-1.17786145
H	3.75557303	-3.35260272	0.26402423
C	-0.05315264	1.75794411	2.99653745
H	-0.70610237	1.48082364	3.82680511
H	0.96607506	1.81127369	3.38340044
H	-0.33114257	2.75839019	2.66151810
H	0.04728011	-0.27009219	2.32117629
C	-2.64376831	0.55037749	2.12245297
H	-2.73307872	1.46034789	2.73602843
H	-3.52128148	0.54308778	1.46538603
N	-1.47903061	0.56307399	1.23468876
H	-1.62460780	1.26525390	0.52311909
C	-2.72915196	-0.65176046	3.04689312
C	-2.24243474	-1.90661252	2.66900682
C	-3.35396481	-0.51913202	4.29176998
C	-2.38491464	-3.00260711	3.51888251
H	-1.72601724	-2.01972890	1.72427726
C	-3.50630808	-1.61645973	5.13693285
H	-3.72639322	0.45270294	4.60248613
C	-3.02115130	-2.86491513	4.75144291
H	-1.99205053	-3.96662307	3.21461320
H	-3.99607968	-1.49456298	6.09699249
H	-3.13112664	-3.72005725	5.40924358

S5. BnNH - *ANTI* APPROACH α - 3rd ISOMER - PRODUCT

S5.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.8415	Debye
Energy	:	-1342.96116108	a.u.
Number of imaginary frequencies	:	0	

S5.2. Cartesian Co-ordinates (XYZ format)

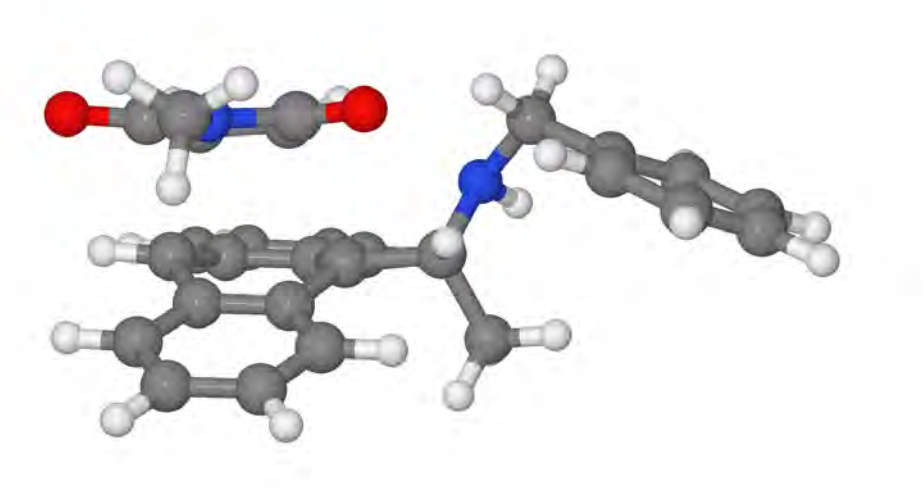
58

C	3.50585365	-0.84894729	2.76150179
C	2.20531511	-0.55517823	2.34420013
C	1.98353398	0.02966138	1.09694266
C	3.08577919	0.26604000	0.25655580
C	4.37974405	-0.03164171	0.66969949
C	4.59241247	-0.58024406	1.93447745
C	0.62389183	0.36410087	0.45163512
C	2.71670461	0.79740399	-1.10910320
C	1.85416114	2.02026772	-0.92073268
C	0.72175431	1.79623747	-0.11897109
C	-0.19141854	2.83954501	0.03317208
H	-1.09566462	2.71280980	0.60756403
C	0.04279314	4.08170700	-0.56181848
C	1.18302488	4.29593182	-1.32909751
C	2.08952188	3.25303721	-1.51768541
H	3.66407394	-1.29229891	3.73818684
H	1.38176322	-0.79569483	3.00273609
H	5.21564102	0.15509838	0.00406693
H	5.59938765	-0.80742192	2.26555371

H	-0.67568260	4.88160515	-0.42211163
H	1.36190403	5.26286602	-1.78546560
H	2.97323155	3.39622331	-2.13074851
C	-0.60331589	0.07586641	1.37624860
H	3.58832502	0.98340440	-1.73626280
C	0.58169258	-0.56302196	-0.84165061
C	1.77112401	-0.25556621	-1.77966046
C	0.71610153	-2.05849838	-0.55518502
H	1.45005679	0.13055570	-2.74901557
H	-0.38716027	-0.39654934	-1.31448030
O	0.01491543	-2.75822043	0.14576788
C	2.47102737	-1.58494711	-2.00678945
O	3.44427872	-1.79002988	-2.69628143
N	1.80085814	-2.55361342	-1.26889658
C	2.20178223	-3.95280504	-1.22232604
H	1.35722196	-4.58969164	-1.48699343
H	3.01370239	-4.08640957	-1.93424034
H	2.54122138	-4.21485996	-0.21892270
C	-0.66338968	0.94634140	2.65051603
H	-1.29471719	0.45601356	3.39421511
H	0.31912428	1.11500013	3.09203029
H	-1.09565437	1.92803180	2.45392513
H	-0.47318277	-0.95892787	1.69530201
C	-2.77984905	-1.02511179	0.76682222
H	-2.25445008	-1.91651273	0.42207545
H	-3.61535954	-0.85242081	0.08080412
N	-1.86422312	0.11898374	0.61046934
H	-2.36377978	0.97984588	0.79860091
C	-3.32391500	-1.27310121	2.16582775
C	-4.33415127	-0.46091947	2.69569969
C	-2.81487608	-2.30505705	2.96077347
C	-4.81437445	-0.66474283	3.98643398
H	-4.75423479	0.33538342	2.08769155
C	-3.29103875	-2.51250744	4.25573874
H	-2.04332066	-2.95312810	2.55770707
C	-4.29026127	-1.69135833	4.77294874
H	-5.60125971	-0.02914630	4.37790632
H	-2.88456368	-3.31818056	4.85745001
H	-4.66421270	-1.85300255	5.77776861

S6. BnNH - *ANTI* APPROACH α - 3rd ISOMER - TS

S6.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.4012	Debye
Energy	:	-1342.90494410	a.u.
Number of imaginary frequencies	:	1	

S6.2. Cartesian Co-ordinates (XYZ format)

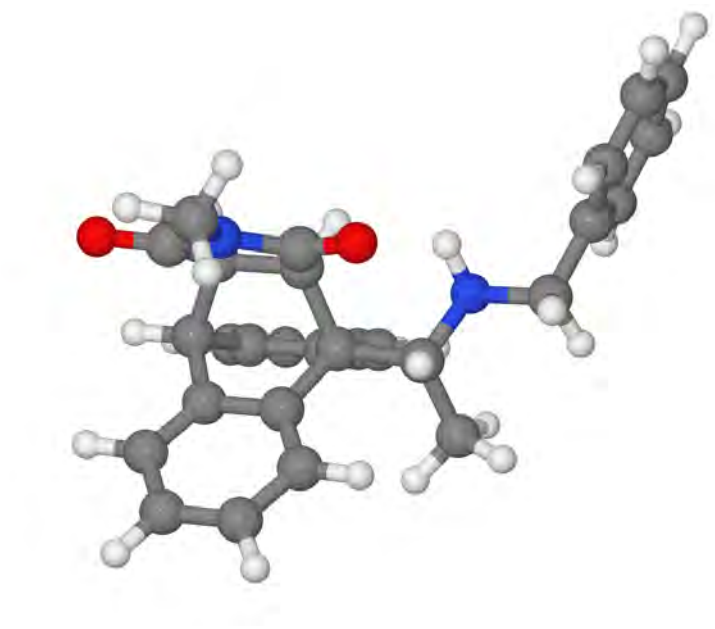
58

C	1.29076540	-1.85775280	2.97775459
C	0.53058171	-0.96344471	2.25203705
C	1.14066064	-0.04549400	1.35970819
C	2.55341220	-0.11260951	1.20275426
C	3.30705404	-1.05881774	1.92787302
C	2.68845034	-1.90785515	2.82090950
C	0.41152599	0.90252596	0.53838772
C	3.13971066	0.73771316	0.20726725
C	2.53103733	2.02227116	-0.00792748
C	1.12055862	2.10739851	0.14518586
C	0.50448608	3.34800220	-0.14821449
H	-0.56241632	3.46319818	-0.04717250
C	1.25104153	4.44018126	-0.54313314
C	2.64402056	4.33742476	-0.70215273
C	3.27200246	3.13523126	-0.45091656
H	0.80366659	-2.52942634	3.67556119
H	-0.54132557	-0.96139121	2.39155316
H	4.38023281	-1.10063827	1.77956653
H	3.27389503	-2.61424327	3.39806890

H	0.75574362	5.38526440	-0.73479104
H	3.21978998	5.19984245	-1.01784527
H	4.34547758	3.03772211	-0.57306713
C	-1.12412190	0.84876746	0.56389207
H	4.20930195	0.65254414	0.04327546
C	0.98643398	-0.20565224	-1.47582328
C	2.38888693	-0.16152766	-1.55898833
C	0.59573859	-1.60088015	-1.17483747
H	2.94023561	0.50214326	-2.20867920
H	0.28828782	0.47316974	-1.93878865
O	-0.51496768	-2.08408380	-1.04207861
C	2.89426112	-1.55917609	-1.37787664
O	4.03217411	-1.97112536	-1.46070361
N	1.78250563	-2.33855462	-1.06455398
C	1.84299815	-3.74515533	-0.71195835
H	0.89528745	-4.20838308	-0.98252058
H	2.66222262	-4.21066761	-1.25897253
H	2.01185489	-3.87127948	0.36086583
C	-1.68946993	1.55048454	1.82004261
H	-1.53867757	2.63152695	1.76929057
H	-2.76117182	1.35534084	1.89621055
H	-1.20747411	1.19865096	2.73412514
H	-1.38136876	-0.20880786	0.63352281
C	-2.70471382	0.44703031	-1.33862948
H	-2.16432762	-0.45204037	-1.63643670
H	-3.02867150	0.95513201	-2.25234509
N	-1.74326146	1.35224867	-0.67808825
H	-2.19605517	2.24223495	-0.50556737
C	-3.92530370	0.04681748	-0.52368903
C	-4.97860479	0.94683409	-0.31871355
C	-4.01416636	-1.22523117	0.05169719
C	-6.08487892	0.59185356	0.44845065
H	-4.93614960	1.93329787	-0.77203852
C	-5.12002563	-1.58454049	0.82311875
H	-3.21231008	-1.93720472	-0.11456893
C	-6.15680265	-0.67673135	1.02547050
H	-6.89443636	1.29949677	0.59091711
H	-5.17288876	-2.57551622	1.26078928
H	-7.01864147	-0.95582783	1.62130237

S7. BnNH - *ANTI* APPROACH α - 4th ISOMER - PRODUCT

S7.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	0.4896	Debye
Energy	:	-1342.96155621	a.u.
Number of imaginary frequencies	:	0	

S7.2. Cartesian Co-ordinates (XYZ format)

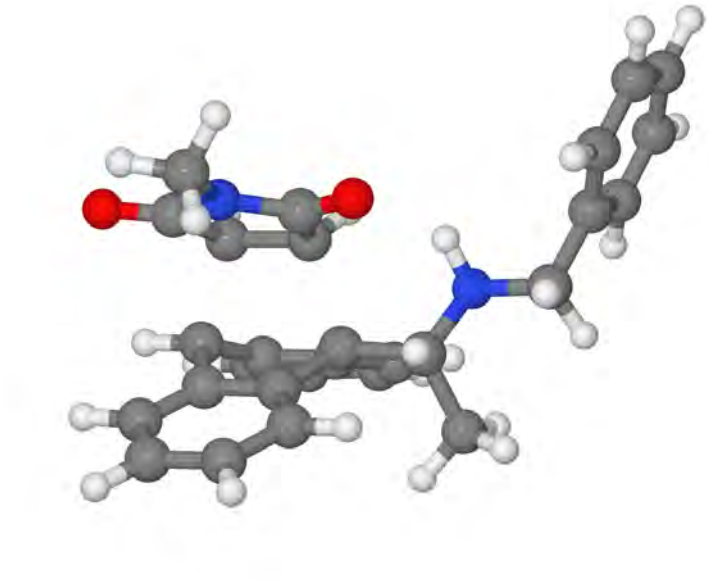
58

C	-1.56611419	-0.10623644	3.28473234
C	-0.66195446	0.51046938	2.41711593
C	-0.27261072	-0.12676711	1.23738039
C	-0.83680320	-1.37560916	0.93111545
C	-1.74330115	-1.98704398	1.79032362
C	-2.10201716	-1.35389507	2.97964573
C	0.68616116	0.41981998	0.15652317
C	-0.41330835	-1.92313874	-0.40934002
C	1.09730506	-1.94263625	-0.45613959
C	1.69250166	-0.69814622	-0.18847920
C	3.07235169	-0.56869793	-0.33844101
H	3.54060888	0.39743558	-0.23092233
C	3.84699106	-1.68037808	-0.67861015
C	3.25286746	-2.92024660	-0.89554203
C	1.86688173	-3.04800296	-0.80012989
H	-1.85004687	0.39669985	4.20226669
H	-0.27429625	1.48482430	2.68081474
H	-2.17191291	-2.94802690	1.52740717
H	-2.80227256	-1.82789075	3.65797663

H	4.92064953	-1.56898487	-0.78182101
H	3.86083531	-3.77928376	-1.15614796
H	1.38717103	-4.00041533	-1.00061727
C	1.28887749	1.79555726	0.56885272
H	-0.85873169	-2.89370441	-0.62603068
C	-0.19675699	0.50258625	-1.16875386
C	-0.84224212	-0.86770236	-1.48026919
C	-1.37390327	1.46770227	-1.09148586
H	-0.56054366	-1.23351562	-2.47010636
H	0.45107406	0.82058465	-1.98662186
O	-1.33334875	2.66890049	-0.92820692
C	-2.34254837	-0.61037672	-1.48795402
O	-3.22166896	-1.42179787	-1.66381979
N	-2.54890394	0.74921644	-1.26402843
C	-3.86691093	1.36764824	-1.22048044
H	-3.91233087	2.19413686	-1.93029046
H	-4.59751940	0.60478544	-1.48140955
H	-4.07120800	1.74906254	-0.21876933
C	2.25385380	1.70334971	1.77227783
H	2.22113633	2.62292337	2.36113143
H	1.99820638	0.87799066	2.43580747
H	3.28345037	1.55703568	1.44678235
H	0.43082544	2.40649891	0.88267797
C	2.38346291	3.83603930	-0.26779202
H	3.21723676	3.79662418	0.43799219
H	1.58132267	4.41959047	0.21321079
N	1.95221901	2.45826745	-0.56960040
H	1.26934052	2.54487967	-1.31608200
C	2.82467103	4.54143953	-1.53033531
C	2.00587678	5.49684429	-2.13811684
C	4.04860592	4.22660208	-2.13190556
C	2.40163565	6.13184214	-3.31554484
H	1.05125916	5.74516630	-1.68543959
C	4.44773865	4.85818863	-3.30630898
H	4.68988848	3.48158169	-1.67311215
C	3.62431216	5.81457186	-3.90164328
H	1.75543392	6.87349939	-3.77197981
H	5.40165758	4.60739708	-3.75721240
H	3.93574452	6.30852842	-4.81526804

S8. BnNH - *ANTI* APPROACH α - 4th ISOMER - TS

S8.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.2382	Debye
Energy	:	-1342.90596197	a.u.
Number of imaginary frequencies	:	1	

S8.2. Cartesian Co-ordinates (XYZ format)

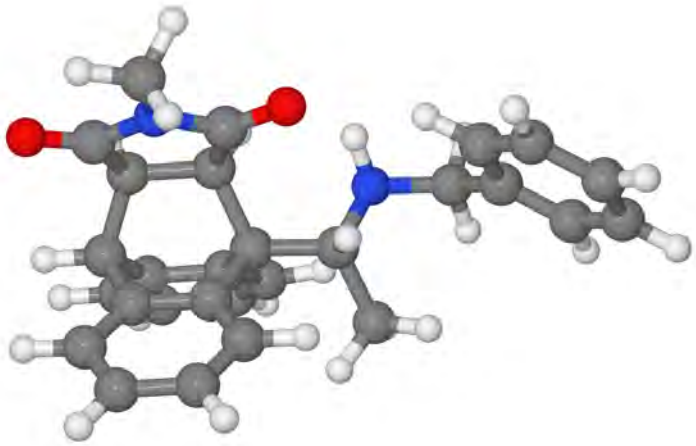
58

C	3.26186299	-1.54378223	2.48667383
C	2.06810975	-0.89947850	2.23780775
C	1.91682243	-0.04972352	1.11051595
C	3.02274680	0.07173398	0.22524256
C	4.22307205	-0.62216616	0.47951829
C	4.35134315	-1.40498579	1.60684311
C	0.69801408	0.66367185	0.78436601
C	2.81653976	0.83123553	-0.97784454
C	1.93632019	1.96979547	-0.89290524
C	0.82432270	1.87047958	-0.01247499
C	-0.11568226	2.93109250	-0.00686332
H	-1.00023043	2.84475183	0.60533327
C	0.07270923	4.04400587	-0.80180216
C	1.18051779	4.13488579	-1.66306758
C	2.08915830	3.09734631	-1.72105241
H	3.35970855	-2.16366720	3.37061930
H	1.25325334	-1.03640068	2.93389797
H	5.04442215	-0.52490413	-0.22096935
H	5.28471994	-1.91551948	1.81393957

H	-0.64836717	4.85288239	-0.76703292
H	1.31516922	5.01333570	-2.28380084
H	2.93914628	3.14629722	-2.39338589
C	-0.51743174	0.40527269	1.67580068
H	3.65577984	0.90145195	-1.66308630
C	0.36402056	-0.60233021	-1.32322121
C	1.57553947	-0.43512216	-2.01920080
C	0.32459399	-1.95823073	-0.75762528
H	1.65722048	0.12907669	-2.93796921
H	-0.54160607	-0.05470294	-1.52429175
O	-0.55430460	-2.50463891	-0.11496611
C	2.29858613	-1.75279999	-1.94307530
O	3.33633041	-2.07493329	-2.48099136
N	1.54565573	-2.56691766	-1.10328603
C	1.94545019	-3.89889550	-0.68753034
H	1.06870711	-4.39586639	-0.27543783
H	2.32255340	-4.45373821	-1.54715633
H	2.72741461	-3.84896827	0.07423494
C	-0.44452640	1.25246978	2.96631026
H	-1.23628306	0.95775312	3.65839744
H	0.51035261	1.11341131	3.47491908
H	-0.56082505	2.31403542	2.74471092
H	-0.46755213	-0.65239149	1.96854806
C	-2.95028925	0.03603135	1.67138231
H	-3.20657086	0.64773905	2.54003906
H	-2.71204042	-0.97442120	2.04203010
N	-1.79451835	0.63813502	0.97981024
H	-1.73650789	0.19218954	0.07120506
C	-4.13813114	-0.04263708	0.74020177
C	-4.28640270	-1.13971746	-0.11594240
C	-5.08255291	0.98629558	0.68521833
C	-5.35930967	-1.20880473	-1.00270784
H	-3.55396438	-1.94046676	-0.08610760
C	-6.15780449	0.91904294	-0.19849837
H	-4.97457743	1.84397721	1.34116256
C	-6.29879284	-0.17983426	-1.04461908
H	-5.46390629	-2.06743479	-1.65675199
H	-6.88568068	1.72249651	-0.22574081
H	-7.13654518	-0.23469271	-1.73081684

S9. BnNH - *ANTI* APPROACH α - 5th ISOMER - PRODUCT

S9.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	0.4903	Debye
Energy	:	-1342.96020426	a.u.
Number of imaginary frequencies	:	0	

S9.2. Cartesian Co-ordinates (XYZ format)

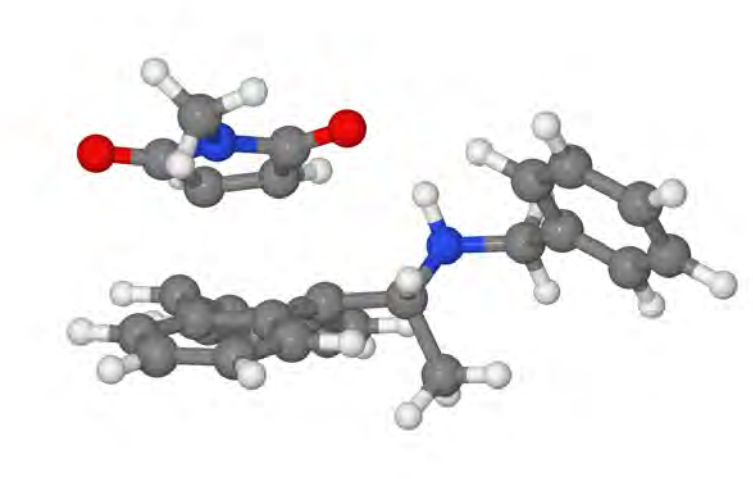
58

C	-1.80807328	-0.58474982	3.20657396
C	-0.92141616	0.15361181	2.41972446
C	-0.43441457	-0.37529159	1.22222996
C	-0.88572270	-1.64150631	0.81671226
C	-1.77429485	-2.37477994	1.59570765
C	-2.23014331	-1.84823191	2.80340791
C	0.52087313	0.31179827	0.22181958
C	-0.36855289	-2.06797576	-0.53406769
C	1.13911772	-1.96968627	-0.51906121
C	1.62452304	-0.70180738	-0.15574475
C	2.99298978	-0.45678556	-0.26491991
H	3.38479614	0.53299528	-0.09172241
C	3.86217141	-1.48105526	-0.64805514
C	3.37542081	-2.74890661	-0.95236111
C	2.00219870	-2.98879576	-0.90550601
H	-2.16818094	-0.16399297	4.13862419
H	-0.62512374	1.13638568	2.75964665
H	-2.11394668	-3.34717774	1.25596178
H	-2.91728210	-2.41683984	3.41961384

H	4.92518568	-1.27810931	-0.71626770
H	4.05616760	-3.54032302	-1.24510491
H	1.60374081	-3.96038079	-1.17877400
C	1.00182092	1.70201969	0.74502242
H	-0.72826147	-3.05327678	-0.82930934
C	-0.30586118	0.41142514	-1.13941860
C	-0.83494765	-0.98096979	-1.55687082
C	-1.55242693	1.28304482	-1.07770145
H	-0.49084085	-1.26266694	-2.55462980
H	0.36142910	0.82741076	-1.89511251
O	-1.60630035	2.47946095	-0.87682599
C	-2.34888053	-0.83455300	-1.61111355
O	-3.15897655	-1.69525039	-1.86491382
N	-2.66413856	0.49334437	-1.32579291
C	-4.02453375	1.01398313	-1.31360829
H	-4.10067940	1.86832273	-1.98688900
H	-4.68546486	0.21427348	-1.64124751
H	-4.29759789	1.33088899	-0.30588359
C	1.94645929	1.59617674	1.95819986
H	1.92063797	2.52193880	2.53657150
H	1.64812648	0.78341311	2.61921501
H	2.97965980	1.41340685	1.66799593
H	0.09547091	2.21039486	1.09528089
C	2.30758357	3.72455764	0.01492117
H	2.64284396	4.16773653	-0.92982709
H	3.22019815	3.47473335	0.56165189
N	1.61217582	2.48466659	-0.34816113
H	0.87698740	2.72029805	-1.00632238
C	1.54792798	4.78928518	0.80378079
C	2.23208284	5.57886887	1.73456454
C	0.18737553	5.03717661	0.59197855
C	1.58268833	6.59717083	2.42964005
H	3.28677154	5.39423800	1.91705084
C	-0.46648115	6.05127239	1.29091167
H	-0.37341595	4.42854357	-0.10828763
C	0.22764343	6.83701086	2.20915699
H	2.13260317	7.19813251	3.14582491
H	-1.52277064	6.22572660	1.11682355
H	-0.28316998	7.62495852	2.75131750

S10. BnNH - *ANTI* APPROACH α - 5th ISOMER - TS

S10.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.4356	Debye
Energy	:	-1342.90479846	a.u.
Number of imaginary frequencies	:	1	

S10.2. Cartesian Co-ordinates (XYZ format)

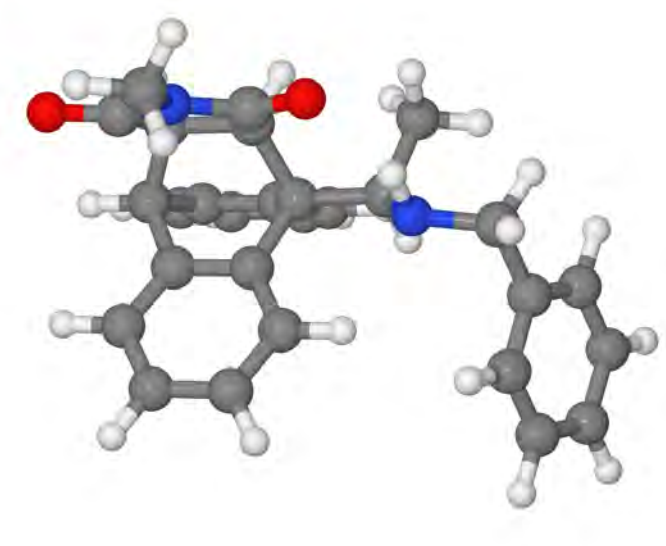
58

C	-2.40614986	-0.23243889	2.79054475
C	-1.25707710	0.31769395	2.26235175
C	-0.52406400	-0.35336649	1.24771345
C	-1.03809536	-1.59254682	0.77569592
C	-2.23429561	-2.11966801	1.30352914
C	-2.90308166	-1.45888531	2.31149817
C	0.68694526	0.16177420	0.64072418
C	-0.34554976	-2.21371937	-0.31935489
C	1.08483255	-2.04501772	-0.37516871
C	1.61261380	-0.80426764	0.07588923
C	2.99785590	-0.57015860	-0.10961777
H	3.41067553	0.38937274	0.15609151
C	3.81225252	-1.53990626	-0.65917736
C	3.28078198	-2.76996636	-1.08565331
C	1.92667007	-3.00704527	-0.96433377
H	-2.93054008	0.28738832	3.58425736
H	-0.90953237	1.26170778	2.65681577
H	-2.61389828	-3.05592275	0.91087240
H	-3.80785441	-1.88015854	2.73420978

H	4.87295723	-1.34536016	-0.77157509
H	3.93087459	-3.52286196	-1.51648402
H	1.49773371	-3.94201469	-1.30907583
C	1.14403629	1.56179607	1.07049191
H	-0.75152630	-3.15076208	-0.68803614
C	-0.32212624	0.33928409	-1.61027825
C	-0.83985716	-0.94417793	-1.86316574
C	-1.43525970	1.24091876	-1.29066420
H	-0.44217324	-1.60678041	-2.61927795
H	0.61735195	0.71986306	-1.97486591
O	-1.41497552	2.43710661	-1.05340230
C	-2.33599758	-0.83481085	-1.74771464
O	-3.17353606	-1.68303263	-1.96785665
N	-2.60344243	0.46012485	-1.31268179
C	-3.92864990	0.95338637	-0.98435187
H	-4.26607752	0.54908848	-0.02694664
H	-3.87171149	2.03869557	-0.92045003
H	-4.63483667	0.66033202	-1.76200771
C	1.99267566	1.47668684	2.35766149
H	2.13328004	2.46967483	2.78822947
H	1.48388278	0.86213976	3.10184526
H	2.97237945	1.03456247	2.17364502
H	0.23920211	2.12197208	1.32686400
C	2.50527477	3.52996445	0.31593016
H	2.90595007	3.91670346	-0.62776625
H	3.37637019	3.32699800	0.94478697
N	1.85265172	2.25888062	-0.01880443
H	1.17783034	2.42728901	-0.75734180
C	1.67381072	4.62733603	0.97629112
C	2.25265193	5.44437027	1.95319808
C	0.34902033	4.87383509	0.59854746
C	1.53559160	6.48894119	2.53407240
H	3.27801085	5.26196146	2.26177096
C	-0.37219334	5.91410446	1.18281484
H	-0.13183731	4.24608421	-0.14373577
C	0.21769509	6.72716570	2.14941883
H	2.00400186	7.11177397	3.28847241
H	-1.39912999	6.08815765	0.88036239
H	-0.34567091	7.53580570	2.60161662

S11. BnNH - *ANTI* APPROACH β - 1st ISOMER - PRODUCT

S11.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.7723	Debye
Energy	:	-1342.95964406	a.u.
Number of imaginary frequencies	:	0	

S11.2. Cartesian Co-ordinates (XYZ format)

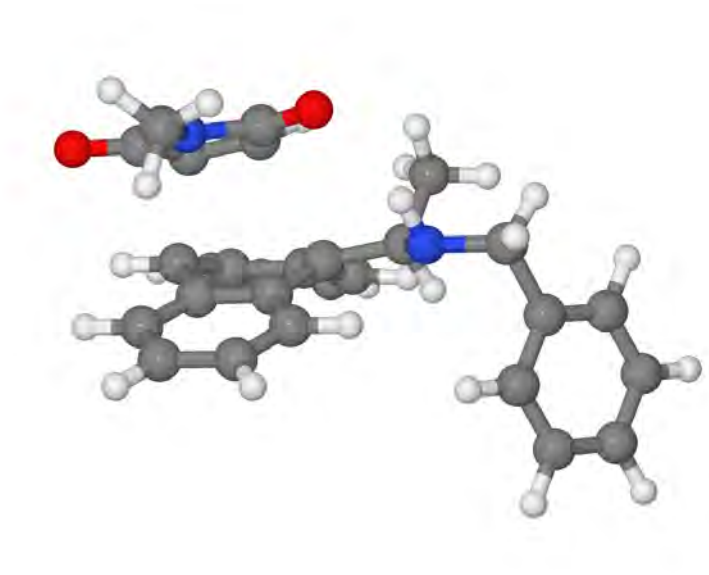
58

C	-0.94297552	-0.23663121	3.44165277
C	-0.39993432	0.52180141	2.40125346
C	-0.04339682	-0.09214810	1.20141768
C	-0.22902091	-1.48242283	1.07181311
C	-0.78458118	-2.23161292	2.10259056
C	-1.14433336	-1.60552490	3.29615831
C	0.58180940	0.56547570	-0.05028228
C	0.25723261	-2.06519914	-0.23755230
C	1.69585311	-1.63399673	-0.39862701
C	1.88574421	-0.24578461	-0.29606932
C	3.18661189	0.25277516	-0.36709526
H	3.38917208	1.31031561	-0.26706472
C	4.26604033	-0.61403245	-0.55968314
C	4.06096125	-1.98389566	-0.68366843
C	2.76606202	-2.49679232	-0.59895819
H	-1.21089995	0.25349534	4.37139606
H	-0.27594465	1.58799946	2.50176048
H	-0.92451239	-3.30010676	1.97762656
H	-1.57102239	-2.18596125	4.10655546

H	5.27041054	-0.20866604	-0.60811085
H	4.90200520	-2.65132785	-0.83324289
H	2.59184813	-3.56508446	-0.67415357
C	0.89481920	2.10186934	0.00776626
H	0.12997010	-3.14645600	-0.28584391
C	-0.37240741	0.16533205	-1.26549804
C	-0.51879495	-1.36850643	-1.38847840
C	-1.81708407	0.66182041	-1.17814767
H	-0.14573950	-1.74005342	-2.34557819
H	0.04911902	0.58638775	-2.17844176
O	-2.21556091	1.80853283	-1.12934160
C	-2.01097655	-1.64833224	-1.33198822
O	-2.55626225	-2.72627735	-1.38187182
N	-2.67041183	-0.42803240	-1.21775055
C	-4.11976433	-0.29733688	-1.14955294
H	-4.46985626	0.37073159	-1.93696642
H	-4.54500628	-1.29026711	-1.27933013
H	-4.41490507	0.11013646	-0.18158570
C	1.29228878	2.65529346	-1.38403070
H	1.83032131	3.59940362	-1.28066909
H	1.93719614	1.97827077	-1.94580054
H	0.39689308	2.85058212	-1.97989130
H	1.75846410	2.19122267	0.67318445
C	0.17074256	4.31318951	0.88574094
H	0.51243055	4.84957457	-0.01250210
H	-0.76162261	4.79682064	1.19360936
N	-0.16316147	2.90438318	0.63718379
H	-1.00436974	2.85633397	0.07097527
C	1.20489371	4.50497961	1.97996545
C	0.92287964	4.13581324	3.30096507
C	2.45152903	5.07082748	1.70106494
C	1.86189616	4.32143688	4.31096363
H	-0.04517096	3.70708466	3.53629494
C	3.39765310	5.25900793	2.70971441
H	2.68408823	5.37347698	0.68475842
C	3.10556388	4.88282156	4.01759481
H	1.62387490	4.03304291	5.32896852
H	4.35980654	5.69934559	2.47195792
H	3.83758855	5.02770948	4.80418015

S12. BnNH - *ANTI* APPROACH β - 1st ISOMER - TS

S12.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.0936	Debye
Energy	:	-1342.89758024	a.u.
Number of imaginary frequencies	:	1	

S12.2. Cartesian Co-ordinates (XYZ format)

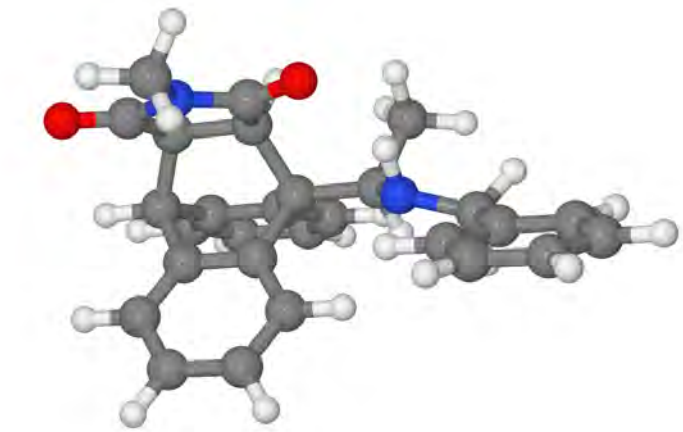
58

C	0.78629577	-2.08931994	2.64249253
C	0.12820418	-1.42161918	1.63169003
C	0.71053296	-0.29207289	0.99317241
C	2.01037669	0.10462110	1.43773401
C	2.68006158	-0.62227875	2.44418669
C	2.07377648	-1.69834638	3.05348921
C	0.09217773	0.49186406	-0.06334433
C	2.63939643	1.21194017	0.77824920
C	1.77052307	2.26708102	0.33275148
C	0.46506375	1.90108180	-0.09192298
C	-0.40307978	2.94294858	-0.50669527
H	-1.42426312	2.72388887	-0.78535813
C	0.01463560	4.25880718	-0.51940978
C	1.32795405	4.59737587	-0.15040609
C	2.19521523	3.60770202	0.26441130
H	0.29906455	-2.92765880	3.12830448
H	-0.84970301	-1.73841774	1.31032264
H	3.67310882	-0.30592459	2.74232912
H	2.58041334	-2.23430705	3.84806180

H	-0.68096679	5.03715897	-0.81159484
H	1.64945984	5.63216066	-0.17386730
H	3.20542192	3.85474896	0.57309282
C	-1.21586466	0.11971323	-0.79968572
H	3.63386965	1.48862755	1.11345410
C	1.94107056	-0.05971253	-1.69263017
C	3.11350083	0.38132465	-1.06602812
C	1.88345885	-1.52668786	-1.59855425
H	3.68088269	1.24380243	-1.38588381
H	1.38801539	0.47386551	-2.44404078
O	1.03898156	-2.30167580	-2.01822639
C	3.86878753	-0.84521890	-0.63734639
O	4.97219419	-0.91915685	-0.14087605
N	3.03715038	-1.92830813	-0.90621072
C	3.33931398	-3.29938698	-0.53721982
H	2.65711069	-3.94847989	-1.08346605
H	4.37143183	-3.53184962	-0.80115944
H	3.20339298	-3.44937277	0.53667861
C	-1.19930482	0.50861943	-2.30344868
H	-2.22184587	0.58935136	-2.67759681
H	-0.70617992	1.45842922	-2.50377870
H	-0.69412941	-0.27408645	-2.87229609
H	-1.99385524	0.71846801	-0.30803886
C	-2.98664713	-1.59754121	-1.08120215
H	-3.17234635	-1.35065985	-2.13708162
H	-3.08639169	-2.68546486	-1.00251460
N	-1.62712646	-1.27910101	-0.63082957
H	-0.96236473	-1.87910616	-1.11317265
C	-4.06635666	-0.94241059	-0.23865725
C	-4.04742575	-1.03622818	1.15833008
C	-5.12245178	-0.25742090	-0.84547645
C	-5.05862522	-0.46356747	1.92426097
H	-3.23171711	-1.55966866	1.64329922
C	-6.13993454	0.31539667	-0.08181073
H	-5.15093374	-0.17314820	-1.92742717
C	-6.11032915	0.21429959	1.30633032
H	-5.02850676	-0.54705542	3.00517273
H	-6.95104170	0.84239441	-0.57219785
H	-6.89768934	0.66027796	1.90360296

S13. BnNH - *ANTI* APPROACH β - 2nd ISOMER - PRODUCT

S13.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.2282	Debye
Energy	:	-1342.96108246	a.u.
Number of imaginary frequencies	:	0	

S13.2. Cartesian Co-ordinates (XYZ format)

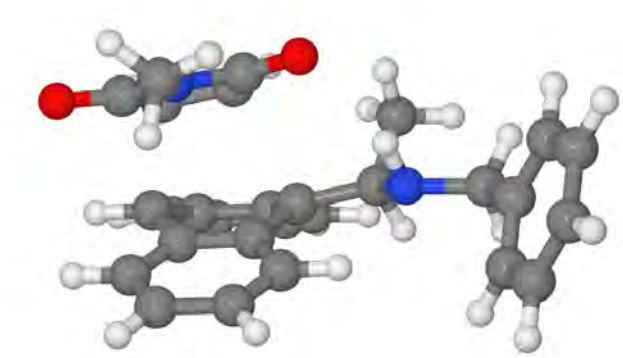
58

C	-1.03762281	-0.11340331	3.38779092
C	-0.49277413	0.63719827	2.34266019
C	-0.09813588	0.00857971	1.16166556
C	-0.23788232	-1.38865733	1.06135011
C	-0.79806334	-2.13094211	2.09484506
C	-1.20292377	-1.48964119	3.26545715
C	0.55159873	0.65440202	-0.08246683
C	0.31404021	-1.98535371	-0.21578771
C	1.74567878	-1.51332068	-0.32905939
C	1.89007199	-0.11761669	-0.24855134
C	3.17677164	0.41975784	-0.26675066
H	3.34192824	1.48509693	-0.17973916
C	4.28988600	-0.41700870	-0.38960552
C	4.13143682	-1.79443371	-0.49588221
C	2.84976196	-2.34579444	-0.46118650
H	-1.33644044	0.38901168	4.30123806
H	-0.39829341	1.70750010	2.43524718
H	-0.90385157	-3.20556402	1.99111223
H	-1.63380063	-2.06375289	4.07805920

H	5.28306818	0.01764433	-0.39873391
H	4.99814081	-2.43838930	-0.59220642
H	2.71224332	-3.42036915	-0.52122891
C	0.79344380	2.20094252	-0.03015301
H	0.22142681	-3.07078099	-0.24232733
C	-0.32114017	0.19938257	-1.33681810
C	-0.43900055	-1.33974993	-1.40942335
C	-1.77417850	0.67701811	-1.36324358
H	-0.03402831	-1.73531127	-2.34387994
H	0.15611899	0.59518063	-2.23371148
O	-2.18746591	1.81694615	-1.42627311
C	-1.92837858	-1.64158940	-1.38703632
O	-2.45420647	-2.73031473	-1.39688039
N	-2.60975146	-0.42851317	-1.36614597
C	-4.06243038	-0.31844360	-1.37495649
H	-4.38206911	0.30326673	-2.21169472
H	-4.46748543	-1.32341957	-1.47321403
H	-4.41090155	0.13304678	-0.44495454
C	1.26722229	2.77004433	-1.38951457
H	1.70031440	3.76290560	-1.25059927
H	2.01830149	2.15174723	-1.88280296
H	0.41461259	2.87609100	-2.06477261
H	1.59740174	2.33599663	0.70144582
C	-0.00961647	4.29632616	0.98099601
H	0.77511144	4.18823671	1.74292529
H	0.41552958	4.95497656	0.20581162
N	-0.34425265	2.96136189	0.49876711
H	-1.08320272	3.00345492	-0.19686942
C	-1.19313025	5.01662874	1.60394979
C	-2.32222509	4.33338308	2.06363249
C	-1.14897835	6.40824890	1.75011158
C	-3.37691116	5.02455902	2.66045690
H	-2.37263560	3.25848579	1.94442034
C	-2.19687176	7.09913158	2.35190868
H	-0.28449970	6.95587826	1.38642859
C	-3.31808376	6.40770626	2.81040335
H	-4.24727249	4.47798061	3.00734687
H	-2.14248276	8.17733097	2.45615363
H	-4.13876295	6.94381332	3.27383924

S14. BnNH - *ANTI* APPROACH β - 2nd ISOMER - TS

S14.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.1508	Debye
Energy	:	-1342.89773926	a.u.
Number of imaginary frequencies	:	1	

S14.2. Cartesian Co-ordinates (XYZ format)

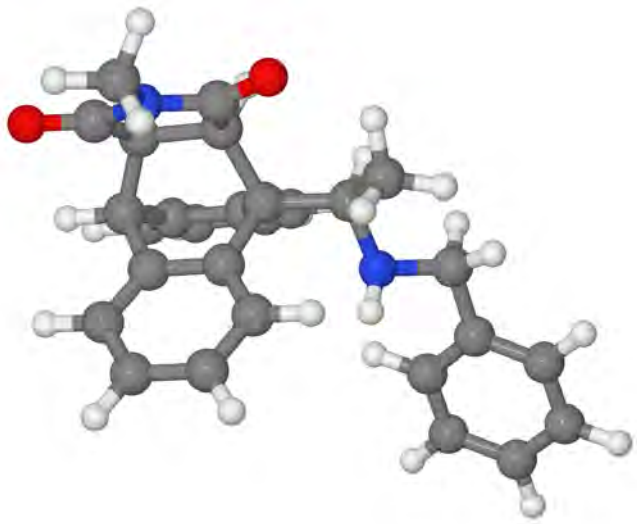
58

C	0.41557828	1.60710585	2.71058416
C	0.46724334	0.56961966	1.80421972
C	-0.70438910	0.11637290	1.13716745
C	-1.92737591	0.79125291	1.44288969
C	-1.94416463	1.87936747	2.34056282
C	-0.79160440	2.27745891	2.98063231
C	-0.76152939	-0.97789025	0.18219818
C	-3.11591053	0.37663823	0.75646156
C	-3.22102880	-1.02351964	0.44872469
C	-2.01635361	-1.71969283	0.15988617
C	-2.11486435	-3.10634041	-0.12032566
H	-1.22342169	-3.69292450	-0.29288501
C	-3.33723378	-3.74821663	-0.13415597
C	-4.52471304	-3.03308415	0.09814569
C	-4.46269703	-1.68376327	0.37953383
H	1.32323360	1.90751541	3.22240353
H	1.39994466	0.07534803	1.58988416
H	-2.88479972	2.38300037	2.53189850
H	-0.81569731	3.09457707	3.69272804

H	-3.37834597	-4.81519270	-0.32120472
H	-5.48032045	-3.54385519	0.07436526
H	-5.36820364	-1.12153602	0.58160579
C	0.47127962	-1.70209122	-0.40936476
H	-4.03242874	0.91125536	0.98440778
C	-1.59414804	0.51848638	-1.67016327
C	-2.76086450	1.10191250	-1.16169262
C	-0.51659214	1.52019536	-1.63651586
H	-3.75643325	0.86131543	-1.50658739
H	-1.54882276	-0.32780764	-2.33134913
O	0.64377737	1.42631042	-2.00138760
C	-2.43933415	2.54033351	-0.86774468
O	-3.18523812	3.42162657	-0.49826068
N	-1.07327724	2.68707776	-1.08839011
C	-0.32915136	3.90333962	-0.81493407
H	-0.86577582	4.76241207	-1.21898580
H	-0.19544995	4.04012537	0.26083112
H	0.64460272	3.81074142	-1.29276800
C	0.27734205	-2.12839913	-1.89038193
H	0.98067796	-2.92528081	-2.14118052
H	-0.72329009	-2.49383521	-2.11607432
H	0.49203202	-1.27625835	-2.53771639
H	0.57399666	-2.61709142	0.19174074
C	2.93895435	-1.77927804	-0.50169623
H	2.86716890	-2.68969941	0.10523699
H	3.03227663	-2.10527635	-1.54826617
N	1.73660815	-0.98066467	-0.24011262
H	1.73406315	-0.15201320	-0.83154696
C	4.19092607	-1.01685715	-0.12028731
C	5.05876827	-0.53137374	-1.10050702
C	4.49561024	-0.77358150	1.22427630
C	6.20714760	0.18014336	-0.75082874
H	4.83404684	-0.71012896	-2.14723134
C	5.64079666	-0.06686138	1.57839096
H	3.82901955	-1.14500916	1.99568141
C	6.50106287	0.41333434	0.58965600
H	6.86901379	0.55087119	-1.52569354
H	5.86590958	0.10798770	2.62481499
H	7.39359665	0.96409810	0.86479056

S15. BnNH - *ANTI* APPROACH γ - PRODUCT

S15.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	0.9656	Debye
Energy	:	-1342.95155522	a.u.
Number of imaginary frequencies	:	0	

S15.2. Cartesian Co-ordinates (XYZ format)

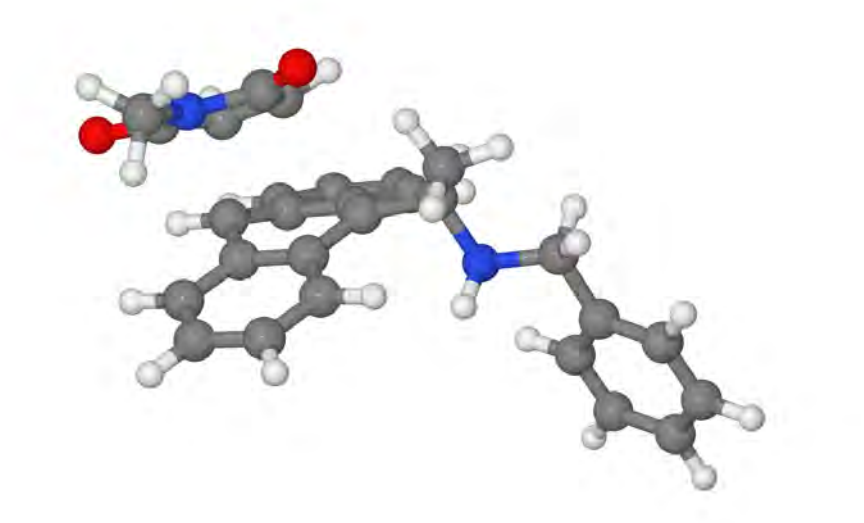
58

C	-0.96525317	0.92648697	3.27242756
C	-0.28921425	1.26644599	2.09851837
C	-0.07710627	0.31314909	1.10082614
C	-0.58056933	-0.98474401	1.30121255
C	-1.26295006	-1.32134664	2.46517968
C	-1.45091069	-0.36339086	3.46057892
C	0.62436485	0.50886804	-0.25701693
C	-0.33472529	-1.93241489	0.15177311
C	1.13760304	-1.93146110	-0.16073222
C	1.65181518	-0.65285498	-0.41160315
C	2.98226118	-0.54690647	-0.82020158
H	3.42646551	0.41362098	-1.03056669
C	3.77669716	-1.68853641	-0.94349021
C	3.25783920	-2.95011115	-0.66471881
C	1.92458570	-3.07224202	-0.27879015
H	-1.11072838	1.67935991	4.03879118
H	0.05534015	2.28459978	1.98536015
H	-1.64671969	-2.32789254	2.59174633
H	-1.97533631	-0.62240803	4.37320375

H	4.81074190	-1.58372808	-1.25250125
H	3.88328052	-3.83118343	-0.75369662
H	1.49488389	-4.04793358	-0.07723997
C	1.35179234	1.88165891	-0.46948564
H	-0.73323274	-2.92891026	0.34018356
C	-0.48721132	0.13536845	-1.36036587
C	-0.99983722	-1.31339502	-1.11361766
C	-1.79561412	0.94830936	-1.43305922
H	-0.80052614	-1.96244359	-1.96914947
H	-0.01139262	0.22712177	-2.33950615
O	-1.96428847	2.09325004	-1.78545725
C	-2.50438476	-1.21208882	-0.94512087
O	-3.27218843	-2.11858869	-0.71182746
N	-2.86290741	0.11462548	-1.11122453
C	-4.24021339	0.58743429	-1.08248031
H	-4.48611784	1.07400453	-2.02694392
H	-4.88072348	-0.27759010	-0.92384547
H	-4.37484980	1.30381322	-0.27079883
C	0.49137932	3.15009165	-0.61504877
H	1.15039563	4.02162600	-0.61401784
H	-0.06939155	3.15436196	-1.54524672
H	-0.23017292	3.27571130	0.19268820
H	1.88326180	1.77426159	-1.42207932
C	3.48152852	2.94648075	0.24720380
H	3.92594504	2.63649487	-0.70915568
H	3.14543128	3.98444462	0.09613533
N	2.40437150	2.01060605	0.55508530
H	2.00981951	2.22878551	1.46200061
C	4.55819321	2.94538951	1.31642592
C	5.20741034	4.13452196	1.66150820
C	4.94487095	1.76063931	1.95326126
C	6.22766638	4.14298153	2.61129093
H	4.91051197	5.06332207	1.18406534
C	5.96075010	1.76779461	2.90651202
H	4.43443298	0.83906978	1.70118237
C	6.60788727	2.95784044	3.23737907
H	6.71896887	5.07549381	2.86667395
H	6.24759722	0.84150642	3.39245558
H	7.39769220	2.96201205	3.98030424

S16. BnNH - *ANTI* APPROACH γ - TS

S16.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.8941	Debye
Energy	:	-1342.89853763	a.u.
Number of imaginary frequencies	:	1	

S16.2. Cartesian Co-ordinates (XYZ format)

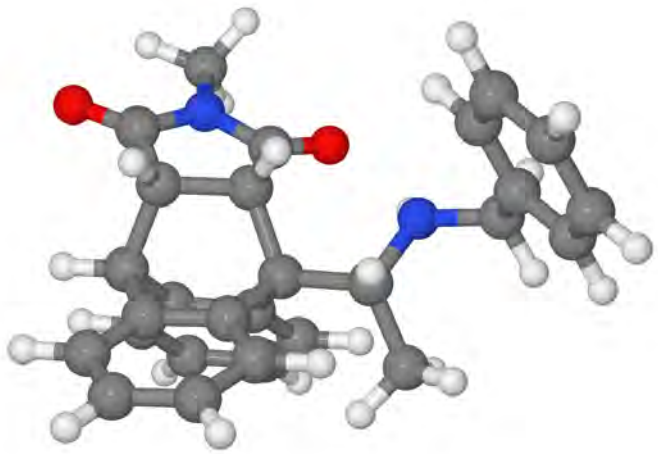
58

C	1.35212755	-2.05406499	2.61213183
C	0.63430840	-1.64490604	1.50854707
C	0.90278691	-0.40226209	0.87647480
C	1.94771683	0.39977422	1.42125165
C	2.69368672	-0.05487735	2.52536297
C	2.39533734	-1.26132667	3.12437367
C	0.17706811	0.10807229	-0.26206124
C	2.25805473	1.63652241	0.74649513
C	1.14869523	2.33890152	0.14527716
C	0.10864206	1.54882586	-0.41007581
C	-0.93801683	2.22191262	-1.09133577
H	-1.77125132	1.66134048	-1.48828161
C	-0.94319612	3.59671593	-1.20375109
C	0.10426046	4.36488104	-0.66366142
C	1.14332831	3.73759913	-0.00701837
H	1.10568798	-2.99482846	3.09097552
H	-0.16544694	-2.27463651	1.15053856
H	3.49735475	0.56488043	2.90626049
H	2.95462346	-1.59366870	3.99116683

H	-1.76778245	4.08944321	-1.70617414
H	0.08992027	5.44458485	-0.75801986
H	1.95954394	4.31666422	0.41167909
C	-0.87988770	-0.71678597	-1.01619744
H	3.03988719	2.24396920	1.19226587
C	2.39695168	0.15879351	-1.66633463
C	3.17637253	1.05960870	-0.90893990
C	2.99679136	-1.17685306	-1.55179656
H	3.39582372	2.06343865	-1.24830019
H	1.75883257	0.40907776	-2.49784350
O	2.69754744	-2.22193384	-2.09972119
C	4.33220100	0.26820400	-0.34463820
O	5.27877522	0.68012911	0.29290470
N	4.09689140	-1.05396259	-0.67344612
C	4.93420792	-2.16243863	-0.25336298
H	4.72495127	-2.43584561	0.78408492
H	4.71536398	-3.00910544	-0.90183294
H	5.98426247	-1.88204682	-0.34090191
C	-0.48218423	-2.12693739	-1.49205422
H	-1.23065436	-2.48148370	-2.20513868
H	0.48272339	-2.12295175	-1.99773598
H	-0.43086568	-2.85959363	-0.68653703
H	-1.07701206	-0.15895617	-1.93612444
C	-3.33458781	-1.10767949	-0.92558599
H	-3.39712191	-0.56189877	-1.87691474
H	-3.30597997	-2.17538023	-1.18958116
N	-2.13144326	-0.63922232	-0.23728547
H	-2.03038907	-1.12054193	0.65059215
C	-4.59166145	-0.84547740	-0.11728141
C	-5.64562654	-1.76374030	-0.14292635
C	-4.73822641	0.32247970	0.63925672
C	-6.82470131	-1.51921189	0.55917442
H	-5.54220295	-2.67987394	-0.71626395
C	-5.91361094	0.56659156	1.34593832
H	-3.91798568	1.02896881	0.67771113
C	-6.96236324	-0.35153669	1.30661929
H	-7.63103294	-2.24373794	0.52788836
H	-6.01077032	1.47579074	1.92931283
H	-7.87628031	-0.16094455	1.85806012

S17. BnNH - *SYN* APPROACH α - 1st ISOMER - PRODUCT

S17.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.5845	Debye
Energy	:	-1342.95126947	a.u.
Number of imaginary frequencies	:	0	

S17.2. Cartesian Co-ordinates (XYZ format)

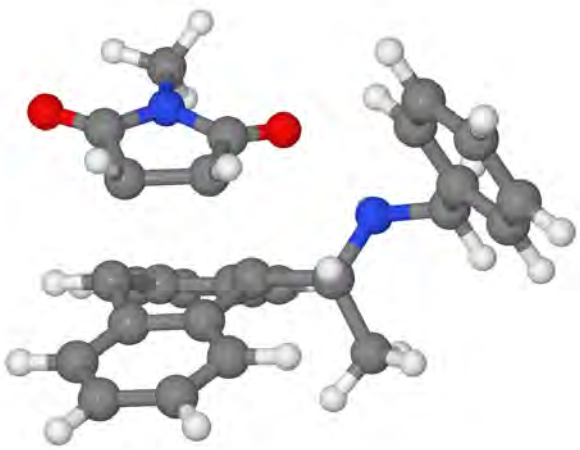
58

C	-3.82367921	-0.08389031	-1.41257071
C	-2.65466142	0.58418363	-1.03836811
C	-1.54629552	-0.13119517	-0.58003396
C	-1.64201343	-1.52892029	-0.52169675
C	-2.79894257	-2.19911194	-0.89876682
C	-3.90253019	-1.47055709	-1.34185290
C	-0.18495218	0.45365414	-0.09891637
C	-0.36438641	-2.19024730	-0.08006265
C	0.01699349	-1.59173107	1.25848877
C	0.08160537	-0.18315732	1.28070605
C	0.47136658	0.45053726	2.45836949
H	0.58236843	1.52393103	2.49792147
C	0.74405193	-0.29923168	3.60506916
C	0.65091586	-1.68718457	3.58217812
C	0.29620513	-2.33632040	2.39925742
H	-4.67461824	0.49155459	-1.75914645
H	-2.64190483	1.66266918	-1.11018729
H	-2.83708310	-3.28218174	-0.84828651
H	-4.81305695	-1.98252678	-1.63173091

H	1.03642631	0.20988582	4.51655197
H	0.86209512	-2.26359105	4.47566223
H	0.23881653	-3.41914248	2.36383462
C	-0.23002361	2.01095700	-0.24657725
H	-0.43497521	-3.27743316	-0.04841430
C	0.94902307	-0.22353077	-0.99109381
H	1.00144613	0.28731716	-1.95487797
C	0.67960083	-1.73833883	-1.16010904
H	0.28960577	-1.99884033	-2.14450026
C	2.37654948	-0.20726749	-0.38973194
C	2.01329374	-2.43004990	-0.97102398
O	2.25575233	-3.60567546	-1.13157618
O	3.00247097	0.69305390	0.12370625
C	-1.09283483	2.70931554	0.83977574
H	-1.87996674	2.05964565	1.22493315
H	-0.48617125	3.03834867	1.68494534
H	-1.57415736	3.59851432	0.42481261
N	2.92248607	-1.47970009	-0.53671753
C	4.28657103	-1.79392886	-0.13415445
H	4.46630144	-2.83990431	-0.37364066
H	4.98969603	-1.15736425	-0.67198467
H	4.41014528	-1.62923932	0.93734026
H	-0.74665219	2.16638255	-1.19739270
C	1.10679233	4.04423428	-0.72693223
H	2.15839744	4.34855223	-0.69051117
H	0.58771366	4.64507961	0.03650801
N	1.08297455	2.60945702	-0.46671033
H	1.76937711	2.33744216	0.22441177
C	0.54209083	4.41067457	-2.09020138
C	0.96249837	3.73001742	-3.23889136
C	-0.37980360	5.45041132	-2.23050928
C	0.47611740	4.08382845	-4.49391079
H	1.67264199	2.91767001	-3.13300848
C	-0.86935806	5.80977726	-3.48707676
H	-0.71773791	5.98575163	-1.34837723
C	-0.44259283	5.12687254	-4.62274742
H	0.81457728	3.54869366	-5.37467432
H	-1.58558393	6.61935043	-3.57599139
H	-0.82225788	5.40196371	-5.60045147

S18. BnNH - *SYN* APPROACH α - 1st ISOMER - TS

S18.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.1542	Debye
Energy	:	-1342.90721534	a.u.
Number of imaginary frequencies	:	1	

S18.2. Cartesian Co-ordinates (XYZ format)

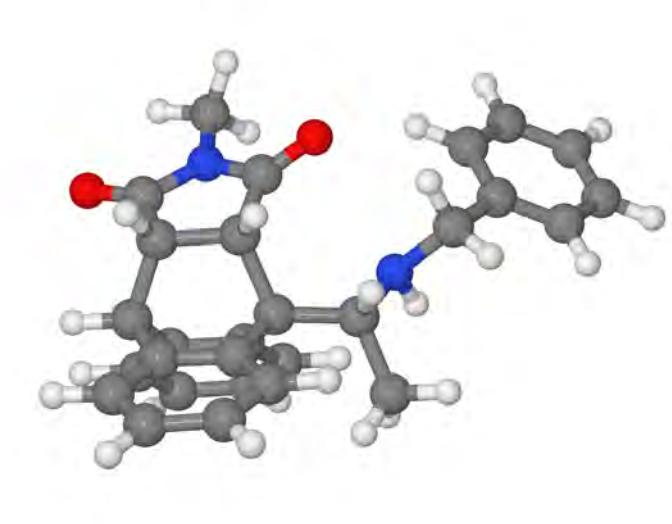
58

C	0.39542896	4.15805769	-0.37703949
C	0.62992412	2.93128943	0.21055554
C	-0.37256944	1.92739522	0.23652567
C	-1.60876119	2.21968269	-0.39781779
C	-1.81948948	3.46435094	-1.01749051
C	-0.83700901	4.43370771	-0.99380726
C	-0.19759159	0.61617303	0.83743322
C	-2.56616282	1.14305305	-0.49807933
C	-2.61397767	0.21224426	0.60251224
C	-1.38536179	-0.09508064	1.25384521
C	-1.40093899	-1.09520638	2.26290655
H	-0.46969602	-1.38205659	2.72756386
C	-2.58040833	-1.70994687	2.62602878
C	-3.79033303	-1.38933408	1.98199153
C	-3.79969549	-0.45383039	0.96803957
H	1.17178822	4.91433382	-0.36241803
H	1.59320593	2.75649714	0.66753155
H	-2.76932502	3.65533972	-1.50544810
H	-1.01142383	5.40064526	-1.45135605

H	-2.57303548	-2.45381403	3.41481519
H	-4.71029568	-1.87972569	2.27926016
H	-4.71961784	-0.21344160	0.44728574
C	1.18372297	0.29778284	1.41649675
H	-3.51310492	1.37290037	-0.97755986
C	-0.40585241	-0.37626392	-1.52721071
H	0.55061305	0.08103280	-1.72017312
C	-1.66731894	0.10627619	-1.94246614
H	-1.77753031	0.87299830	-2.69782352
C	-0.51933658	-1.82010269	-1.30082774
C	-2.57234168	-1.09493041	-2.05781746
O	-3.71201491	-1.13988411	-2.46772361
O	0.33292717	-2.62736416	-0.95829707
C	1.32883370	0.92726076	2.82300925
H	0.65626001	0.44565293	3.53380966
H	2.35208726	0.80725950	3.18545747
H	1.10546100	1.99486804	2.80803490
N	-1.85210133	-2.17571378	-1.56860292
C	-2.39784098	-3.50966501	-1.39290392
H	-1.56310236	-4.19839430	-1.27617872
H	-3.03254557	-3.55330682	-0.50414258
H	-2.99078536	-3.78011632	-2.26685262
H	1.91298902	0.79072869	0.76120788
C	2.88413072	-1.49442089	1.64815271
H	2.92676568	-2.58791566	1.64591062
H	3.21868372	-1.17890501	2.64025974
N	1.46916008	-1.14172435	1.47566533
H	1.11689925	-1.60852313	0.64504325
C	3.85788012	-0.95681721	0.60439116
C	3.68325639	-1.25900471	-0.75291771
C	4.94731569	-0.16470407	0.97588760
C	4.57763767	-0.78205037	-1.70750022
H	2.84110451	-1.87140882	-1.05972660
C	5.84620762	0.31461626	0.02185798
H	5.09890985	0.07620856	2.02388930
C	5.66307068	0.00694305	-1.32346535
H	4.43174744	-1.03023243	-2.75330663
H	6.68642187	0.92701340	0.33080691
H	6.35942554	0.37652057	-2.06793165

S19. BnNH - *SYN* APPROACH α - 2nd ISOMER - PRODUCT

S19.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.4392	Debye
Energy	:	-1342.95057190	a.u.
Number of imaginary frequencies	:	0	

S19.2. Cartesian Co-ordinates (XYZ format)

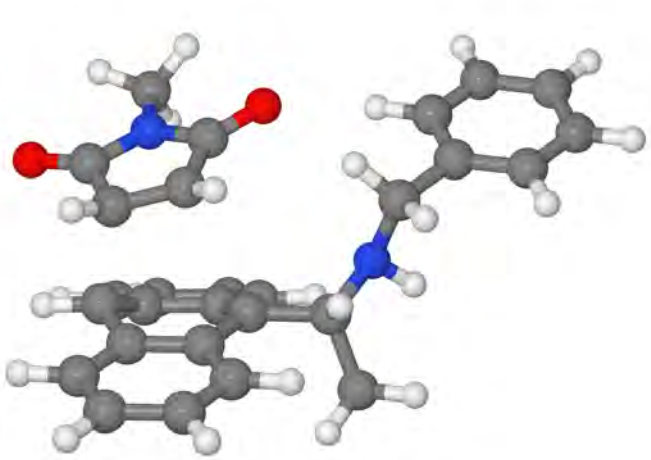
58

C	-4.27949667	0.32533199	-0.73017073
C	-3.04732656	0.92722929	-0.46156469
C	-1.91471839	0.14587827	-0.22428706
C	-2.03554225	-1.24818242	-0.33793163
C	-3.25958896	-1.85053122	-0.60426235
C	-4.39405775	-1.05988824	-0.78534591
C	-0.46309996	0.65001780	0.01919783
C	-0.71852165	-1.97587836	-0.24901916
C	-0.03046050	-1.56920409	1.02841139
C	0.14308849	-0.18212081	1.16436696
C	0.85938972	0.28486761	2.26863480
H	1.06265235	1.33511531	2.40187383
C	1.34578347	-0.60523778	3.22731590
C	1.14245725	-1.97525346	3.09103799
C	0.46080473	-2.45982552	1.97695327
H	-5.14998198	0.94950980	-0.89778721
H	-2.99848270	2.00711751	-0.45030054
H	-3.32352710	-2.93078089	-0.68302941
H	-5.35398626	-1.52173042	-0.98630577

H	1.89138412	-0.21948890	4.08114290
H	1.52296746	-2.66199207	3.83853674
H	0.31988463	-3.52607727	1.83784354
C	-0.42133349	2.19946456	0.21652628
H	-0.82013583	-3.05652738	-0.34333664
C	0.23091376	0.14978941	-1.34317291
H	-0.31338829	0.62668717	-2.16002345
C	0.14291851	-1.39984167	-1.41444862
H	-0.27852732	-1.72521996	-2.36936903
C	1.71609569	0.41730562	-1.59901404
C	1.58331931	-1.88981104	-1.36013186
O	1.95871854	-3.03908992	-1.29966640
O	2.23895741	1.43033397	-2.00087881
C	-1.24104869	2.70014334	1.42783570
H	-2.24531960	2.28507233	1.48669207
H	-0.74126750	2.45635724	2.36620498
H	-1.32791710	3.78894663	1.37110269
N	2.41327953	-0.78052408	-1.43326998
C	3.86135912	-0.86990178	-1.55592310
H	4.13110352	-1.92313671	-1.51243842
H	4.18308592	-0.43610054	-2.50381994
H	4.34043217	-0.33019993	-0.73799998
H	-0.87780344	2.61271262	-0.68952382
C	1.15399635	3.95088911	-0.54113650
H	0.33233434	4.67819643	-0.43369171
H	1.18225241	3.63110805	-1.58529198
N	0.94485897	2.74886799	0.28509083
H	1.16027999	2.99646783	1.24422085
C	2.45507240	4.63219118	-0.17923069
C	2.45749235	5.83999729	0.52411669
C	3.68270946	4.05008841	-0.52052033
C	3.65591502	6.46150255	0.87656271
H	1.51274514	6.30226374	0.79380792
C	4.87976933	4.66850519	-0.16986406
H	3.68309093	3.11431932	-1.06656599
C	4.87074471	5.87603426	0.52982199
H	3.63880467	7.40083790	1.41842246
H	5.82356215	4.21054697	-0.44594526
H	5.80445910	6.35695314	0.79981714

S20. BnNH - *SYN* APPROACH α - 2nd ISOMER - TS

S20.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)[CH][CH]C1=O
Formula	:	$C_{28}H_{26}N_2O_2$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.4487 Debye
Energy	:	-1342.89884940 a.u.
Number of imaginary frequencies	:	1

S20.2. Cartesian Co-ordinates (XYZ format)

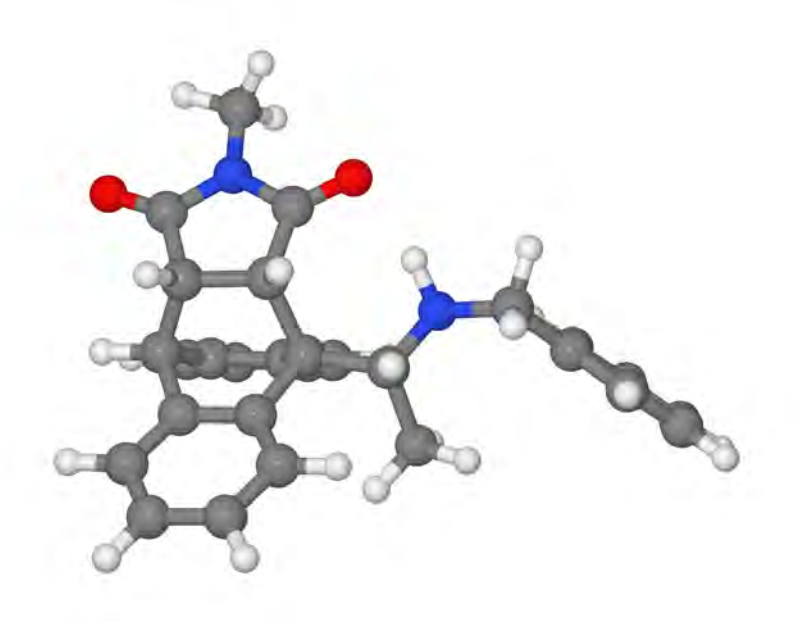
58

C	3.27517962	-3.52166128	-0.76768118
C	2.09191513	-2.97749543	-0.31064713
C	1.98239434	-1.59148812	-0.01848360
C	3.13050199	-0.78749830	-0.24558723
C	4.31999636	-1.35397553	-0.73424292
C	4.40263510	-2.71031141	-0.97908425
C	0.77438802	-0.95708382	0.48038933
C	2.97375941	0.64240867	-0.09010540
C	2.07126927	1.08329034	0.94962084
C	0.90852034	0.29527578	1.18542624
C	-0.04844414	0.79422808	2.10983419
H	-0.96847564	0.25387016	2.25909686
C	0.17365630	1.97174227	2.79122162
C	1.33770239	2.72903323	2.56350446
C	2.26334620	2.29660583	1.63611782
H	3.33307123	-4.58632803	-0.96294594
H	1.25159287	-3.64014697	-0.16219030
H	5.17627764	-0.71075505	-0.90743518
H	5.32870150	-3.14740586	-1.33409166

H	-0.56242716	2.32025743	3.50699902
H	1.50162077	3.65155697	3.10861993
H	3.15095210	2.88304949	1.42789543
C	-0.43983254	-1.87819397	0.69158137
H	3.86908817	1.24241030	-0.22586352
C	0.76095492	0.40174645	-1.80711079
H	0.54007202	-0.54346377	-2.27460456
C	2.03069830	1.02696967	-1.73763287
H	2.84001374	0.74414593	-2.39953661
C	-0.26861677	1.43127203	-1.65799141
C	1.77124321	2.51165676	-1.60672402
O	2.58575654	3.41090751	-1.61545336
O	-1.48145080	1.35243678	-1.73966420
C	-0.26521695	-2.65191460	2.02038074
H	0.71678823	-3.11938834	2.09579444
H	-0.38053852	-1.98075342	2.87420607
H	-1.02541399	-3.43532491	2.08996177
N	0.40628648	2.65573263	-1.44546103
C	-0.26220271	3.92129827	-1.20581377
H	0.37595850	4.72355556	-1.57400787
H	-1.21475947	3.92125106	-1.73441720
H	-0.44551903	4.06956100	-0.13826297
H	-0.41524860	-2.61410904	-0.11950176
C	-2.54276896	-1.45246661	-0.55503392
H	-2.51565242	-2.51050186	-0.86711472
H	-2.10263419	-0.85138398	-1.35176408
N	-1.76086652	-1.23360252	0.67563957
H	-2.30382514	-1.58869708	1.45554423
C	-3.98117876	-1.03732038	-0.34366098
C	-4.97426176	-1.99473155	-0.11670342
C	-4.33708143	0.31718409	-0.33672175
C	-6.29728317	-1.61433160	0.10932224
H	-4.71173716	-3.04845357	-0.12473751
C	-5.65691328	0.69892472	-0.11070240
H	-3.57151771	1.06006789	-0.52570611
C	-6.64093828	-0.26479304	0.11374780
H	-7.05631304	-2.37048626	0.27792132
H	-5.92109013	1.75095987	-0.11530902
H	-7.66875124	0.03517568	0.28606603

S21. BnNH - *SYN* APPROACH α - 3rd ISOMER - PRODUCT

S21.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.9362	Debye
Energy	:	-1342.95494042	a.u.
Number of imaginary frequencies	:	0	

S21.2. Cartesian Co-ordinates (XYZ format)

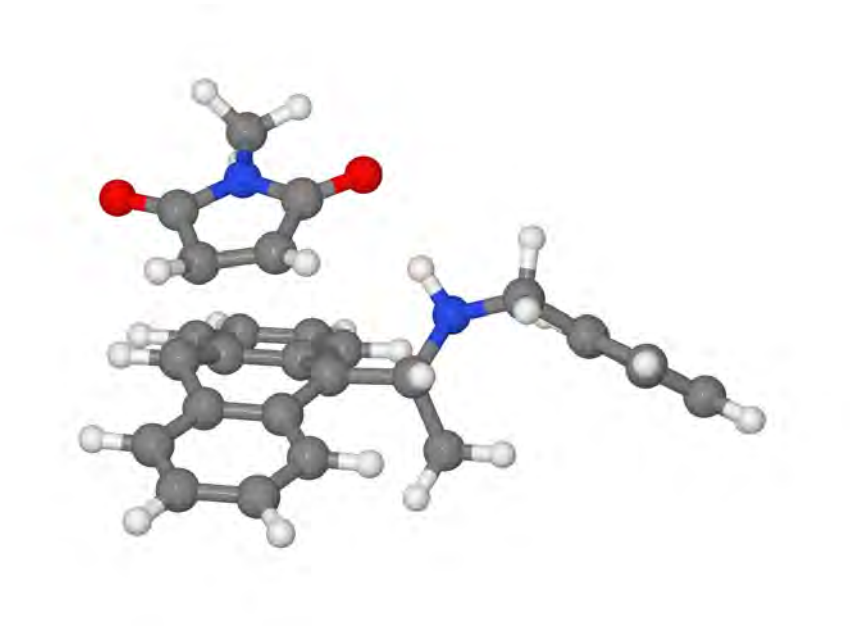
58

C	-4.11652470	-1.32555962	-0.98199648
C	-3.20478511	-0.28877780	-0.77061927
C	-1.90219581	-0.56504703	-0.34698138
C	-1.52699471	-1.90875173	-0.20700309
C	-2.43084550	-2.94445205	-0.41464242
C	-3.74088669	-2.65131664	-0.78968471
C	-0.75803608	0.46363461	-0.09228714
C	-0.05600917	-2.09377217	0.05321613
C	0.33036682	-1.28923190	1.27013028
C	-0.03020075	0.06662133	1.20197773
C	0.36213535	0.92241740	2.23175001
H	0.15558533	1.98006475	2.15844297
C	1.05429602	0.41600475	3.33361244
C	1.37915754	-0.93608391	3.40849090
C	1.02741134	-1.79105687	2.36459923
H	-5.12613773	-1.08731818	-1.29712856
H	-3.53798842	0.72515851	-0.93992198
H	-2.10802293	-3.97352409	-0.29691809
H	-4.45563078	-3.45112467	-0.94645274

H	1.34530497	1.08755279	4.13372040
H	1.91588926	-1.32173562	4.26795149
H	1.29959548	-2.84062243	2.39697647
C	-1.34669435	1.91342378	-0.13476327
H	0.23672774	-3.14058590	0.13040666
C	0.28248411	0.08670543	-1.26170790
H	-0.18543127	0.34380370	-2.21562505
C	0.62394100	-1.43014550	-1.18828332
H	0.30125740	-1.96123791	-2.08624220
C	1.67074835	0.74815208	-1.26481128
C	2.13611603	-1.52096725	-1.11465144
O	2.80444241	-2.52531981	-1.03541505
O	1.94763315	1.92320013	-1.40340579
C	-2.39546633	2.15852499	0.97603852
H	-3.03012490	1.29497099	1.16304803
H	-1.90552700	2.42648506	1.91018164
H	-3.04084063	2.99494076	0.69958270
N	2.64411116	-0.22842896	-1.15844929
C	4.06805277	0.08136227	-1.13578713
H	4.60726595	-0.86284101	-1.10093832
H	4.34212637	0.64069510	-2.03085876
H	4.30616903	0.68067360	-0.25624773
H	-1.86963046	1.97366881	-1.10568035
C	-0.81447220	4.29259825	-0.52296323
H	-1.61243916	4.20151663	-1.27867460
H	0.02679067	4.77815294	-1.03078222
N	-0.33919579	2.98016548	-0.07260141
H	0.46705002	2.73425698	-0.63390380
C	-1.28967929	5.23041534	0.57667899
C	-2.41193151	6.04038525	0.38680714
C	-0.57840413	5.34531450	1.77522910
C	-2.81886482	6.94377756	1.36879051
H	-2.97730708	5.96111727	-0.53712922
C	-0.98108035	6.24483347	2.75878787
H	0.29053709	4.71609592	1.92967117
C	-2.10413170	7.04850531	2.55951905
H	-3.69602919	7.56037235	1.20473015
H	-0.41805759	6.32074594	3.68296814
H	-2.41934824	7.74713087	3.32654691

S22. BnNH - *SYN* APPROACH α - 3rd ISOMER - TS

S22.1. General Information



SMILES	: CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	: $C_{28}H_{26}N_2O_2$	
Charge	: 0	
Multiplicity	: 1	
Dipole	: 1.9362	Debye
Energy	: -1342.90486587	a.u.
Number of imaginary frequencies	: 1	

S22.2. Cartesian Co-ordinates (XYZ format)

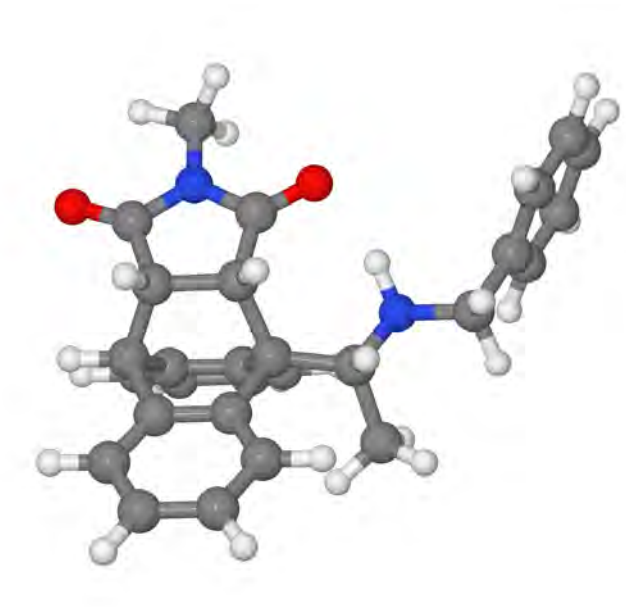
58

C	-1.52061057	4.29119349	-0.66453528
C	-0.64562601	3.24615288	-0.44617403
C	-1.09698153	2.01074314	0.08589617
C	-2.48603678	1.87986147	0.34902257
C	-3.36766648	2.94515848	0.09235470
C	-2.89187574	4.14677715	-0.39237744
C	-0.23611942	0.86809343	0.34118298
C	-2.95863867	0.57567698	0.74975115
C	-2.07350302	-0.21150418	1.57200456
C	-0.67580396	-0.09504219	1.32560098
C	0.19976830	-0.94813955	2.04826713
H	1.25809157	-0.91005975	1.83915293
C	-0.29234093	-1.82566202	2.99112701
C	-1.67538035	-1.92394793	3.23359179
C	-2.55451298	-1.13932991	2.51587558
H	-1.14384842	5.23187017	-1.04941857
H	0.40016916	3.39683509	-0.67177981
H	-4.42575169	2.81199551	0.29109305
H	-3.57040000	4.97393179	-0.56592232

H	0.39594051	-2.45060444	3.54901004
H	-2.04783463	-2.61684465	3.97942758
H	-3.62362099	-1.21997595	2.67647958
C	1.23722756	1.00645232	-0.05441327
H	-4.02104616	0.48034742	0.95331478
C	-1.50966322	-0.38880312	-1.48753130
H	-1.03019619	0.28279805	-2.18071175
C	-2.84567380	-0.31445342	-1.03492963
H	-3.58841085	0.31426084	-1.50747085
C	-1.05718076	-1.77859604	-1.35241902
C	-3.26526737	-1.72161949	-0.69127589
O	-4.35875940	-2.11645961	-0.34867409
O	0.02003784	-2.27872944	-1.63706160
C	2.00966454	1.79958951	1.02673578
H	1.53214335	2.75847054	1.23474574
H	2.06231737	1.23379755	1.95740616
H	3.02990842	1.99110293	0.69078308
N	-2.12954855	-2.50942016	-0.81341255
C	-2.06826758	-3.91578150	-0.45751333
H	-2.93528199	-4.43657684	-0.86488390
H	-1.15200901	-4.32516718	-0.87899679
H	-2.05639601	-4.03856230	0.62837428
H	1.25339997	1.61225688	-0.97290277
C	3.07727337	-0.18599355	-1.19150019
H	2.98939824	0.63456869	-1.92339885
H	3.11246610	-1.11158431	-1.77606606
N	1.89321709	-0.27865145	-0.33239740
H	1.23836696	-0.91246688	-0.77852535
C	4.40237474	-0.04402079	-0.45908898
C	5.38799286	0.82510829	-0.93349057
C	4.68344688	-0.82092100	0.66959858
C	6.62646246	0.91993225	-0.29826394
H	5.18424225	1.43728399	-1.80704260
C	5.91745567	-0.72888857	1.30730927
H	3.92116547	-1.49353278	1.04546368
C	6.89487314	0.14281222	0.82569808
H	7.37740040	1.60355723	-0.67924708
H	6.11918688	-1.33853853	2.18159318
H	7.85517502	0.21582799	1.32388997

S23. BnNH - *SYN* APPROACH α - 4th ISOMER - PRODUCT

S23.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.8668	Debye
Energy	:	-1342.95630180	a.u.
Number of imaginary frequencies	:	0	

S23.2. Cartesian Co-ordinates (XYZ format)

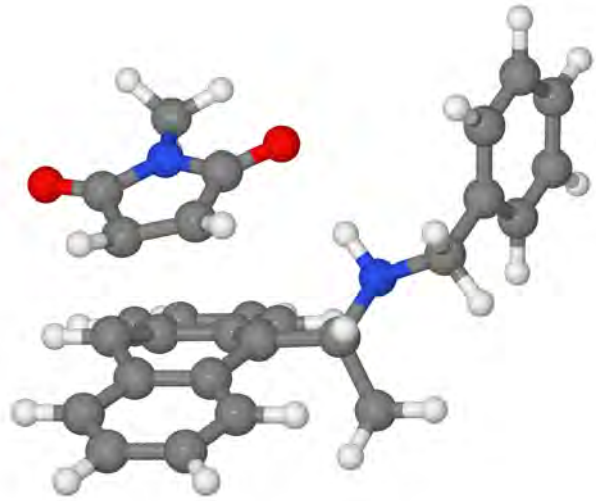
58

C	-4.15638924	-0.86171287	-0.88672292
C	-3.13998771	0.08576626	-0.74342668
C	-1.86600900	-0.30136028	-0.32150975
C	-1.62813115	-1.66582906	-0.10172683
C	-2.63650703	-2.61220908	-0.24255316
C	-3.91444588	-2.20653129	-0.62482291
C	-0.61969018	0.61581445	-0.13774417
C	-0.18269537	-1.98328459	0.17851639
C	0.28013766	-1.14440501	1.34538484
C	0.06057162	0.23364772	1.18567395
C	0.52042794	1.11167121	2.16745615
H	0.42279309	2.17736220	2.01939321
C	1.14674139	0.61068821	3.31047726
C	1.33666098	-0.75917602	3.47411966
C	0.91283274	-1.64105582	2.48032379
H	-5.14176130	-0.53883415	-1.20325708
H	-3.36958861	1.11914682	-0.96123308
H	-2.42116785	-3.66068220	-0.06524119
H	-4.70933151	-2.93605280	-0.73026270

H	1.49422073	1.29975903	4.07226038
H	1.82448149	-1.13991320	4.36441565
H	1.07861292	-2.70805550	2.58390450
C	-1.05241787	2.11181092	-0.27429774
H	0.00115244	-3.04713345	0.32623741
C	0.36221063	0.05742107	-1.28103876
H	-0.09679168	0.28459671	-2.24657607
C	0.56529433	-1.47379339	-1.09429681
H	0.20564197	-2.03609872	-1.95888424
C	1.80190229	0.58851415	-1.34761643
C	2.06395531	-1.69092059	-0.99347454
O	2.63887644	-2.74047947	-0.81980759
O	2.17741299	1.71500957	-1.60056210
C	-2.08864403	2.51722074	0.81084758
H	-2.59815979	1.66265500	1.25192797
H	-1.58453071	3.05443430	1.61467254
H	-2.85385561	3.17853522	0.39743584
N	2.68521452	-0.45791626	-1.14546692
C	4.13102770	-0.27482894	-1.14302552
H	4.58402872	-1.25213313	-0.99079973
H	4.45599794	0.14774311	-2.09450912
H	4.41933680	0.40202907	-0.33815190
H	-1.54903090	2.17193246	-1.25893044
C	-0.33780891	4.41276550	-0.69444919
H	-1.09589994	4.81471825	-0.01564524
H	-0.80026990	4.38221455	-1.69728160
N	0.05592902	3.07534122	-0.23027116
H	0.82393152	2.76105309	-0.81641185
C	0.84859186	5.35117626	-0.72341669
C	1.39716303	5.83933163	0.46812820
C	1.43193460	5.73388863	-1.93327403
C	2.49526310	6.69414186	0.44927400
H	0.95689404	5.54441500	1.41469944
C	2.53310061	6.58993387	-1.95773554
H	1.02138650	5.35794783	-2.86496973
C	3.06692576	7.07293558	-0.76600981
H	2.90548182	7.06727123	1.38139343
H	2.97240353	6.87727308	-2.90670562
H	3.92191553	7.73968267	-0.78166062

S24. BnNH - *SYN* APPROACH α - 4th ISOMER - TS

S24.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O
Formula	:	$C_{28}H_{26}N_2O_2$
Charge	:	0
Multiplicity	:	1
Dipole	:	3.2497 Debye
Energy	:	-1342.90521486 a.u.
Number of imaginary frequencies	:	1

S24.2. Cartesian Co-ordinates (XYZ format)

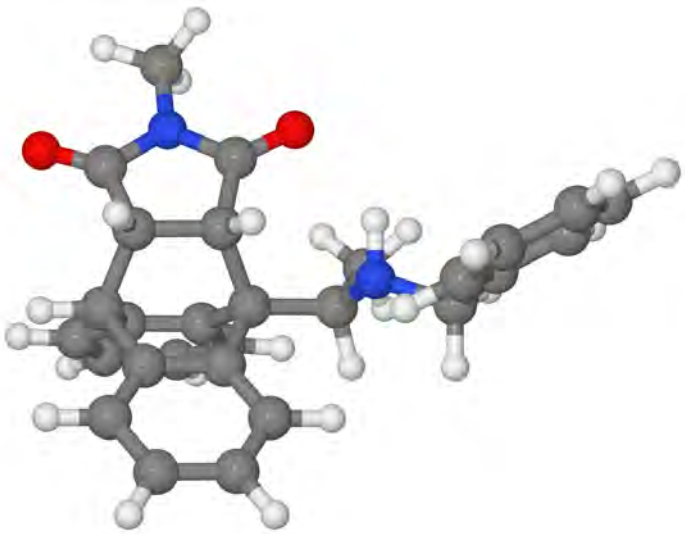
58

C	3.34974217	-3.68672085	-0.97246385
C	2.15962577	-3.15597200	-0.51683116
C	2.08375812	-1.81870925	-0.04915608
C	3.26835704	-1.03820336	-0.10569219
C	4.46567917	-1.58677328	-0.59938508
C	4.51549673	-2.90282726	-1.01244330
C	0.86740470	-1.19163847	0.44229543
C	3.14806151	0.36157912	0.22604054
C	2.20283318	0.70735037	1.25792837
C	1.00849712	-0.06414606	1.33647680
C	0.01859495	0.33648625	2.27308321
H	-0.91647208	-0.20257962	2.31021643
C	0.23550196	1.41175246	3.10857201
C	1.42539787	2.15939951	3.02972364
C	2.38678694	1.82132697	2.09978867
H	3.38283730	-4.71883726	-1.30204046
H	1.28555202	-3.79099059	-0.50722253
H	5.35202312	-0.96279997	-0.64157373
H	5.44551086	-3.32953143	-1.36977649

H	-0.52443945	1.68671489	3.83128238
H	1.58284938	3.00098896	3.69461060
H	3.29816484	2.40182066	2.01225042
C	-0.40889749	-2.03800488	0.40662238
H	4.05498028	0.95717061	0.18023525
C	0.96182764	0.35096285	-1.58144712
H	0.72244853	-0.51918381	-2.17051601
C	2.23231816	0.95396596	-1.45359159
H	3.06165147	0.71567231	-2.10595441
C	-0.05860986	1.36790383	-1.29711986
C	1.99205685	2.41385269	-1.16249800
O	2.80893159	3.30444217	-1.06752694
O	-1.27500224	1.27498257	-1.31331193
C	-0.42140776	-3.01828933	1.60551500
H	0.46783862	-3.64984989	1.62140584
H	-0.46801850	-2.46865940	2.54619813
H	-1.29476523	-3.67153716	1.54929280
N	0.62326401	2.55811214	-0.98937994
C	-0.02389452	3.79156590	-0.57949388
H	0.36600551	4.62471628	-1.16507208
H	-1.09254074	3.67811561	-0.75240231
H	0.15486659	3.98647213	0.48079464
H	-0.35401791	-2.63845730	-0.51337326
C	-2.78017259	-1.98513567	-0.20744169
H	-2.91585422	-2.92370319	0.33782625
H	-2.58253241	-2.25773168	-1.25807512
N	-1.65487146	-1.25449693	0.39256221
H	-1.52881861	-0.39771363	-0.14135070
C	-4.06231070	-1.18482757	-0.13063793
C	-4.72746849	-1.02830029	1.09082758
C	-4.60026741	-0.57912612	-1.26775324
C	-5.90538502	-0.29164091	1.17087018
H	-4.31471586	-1.48789728	1.98277175
C	-5.78024960	0.16104750	-1.19262969
H	-4.08785295	-0.68123949	-2.21855927
C	-6.43645763	0.30537158	0.02673277
H	-6.41158628	-0.18367329	2.12401509
H	-6.18317032	0.62559420	-2.08585548
H	-7.35457850	0.87911016	0.08776474

S25. BnNH - *SYN* APPROACH β - 1st ISOMER - PRODUCT

S25.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.2284	Debye
Energy	:	-1342.95525683	a.u.
Number of imaginary frequencies	:	0	

S25.2. Cartesian Co-ordinates (XYZ format)

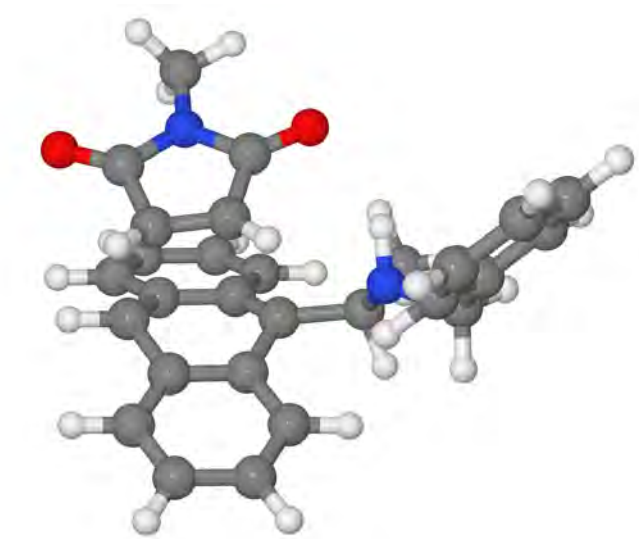
58

C	-4.02420473	-1.15852034	-0.56895876
C	-3.10571790	-0.20254298	-0.12592609
C	-1.73982251	-0.46489733	-0.18687767
C	-1.30818677	-1.69761539	-0.70623517
C	-2.21986890	-2.64392424	-1.15786791
C	-3.58745551	-2.37400079	-1.08658898
C	-0.58746737	0.46674189	0.26974124
C	0.19721919	-1.87140882	-0.70577770
C	0.66003317	-1.62224090	0.71124798
C	0.22671221	-0.39799395	1.25464785
C	0.48767537	-0.14562753	2.60223722
H	0.12803975	0.75147307	3.08201385
C	1.21060956	-1.06390536	3.36794901
C	1.68021607	-2.24451041	2.80256963
C	1.39455867	-2.52785516	1.46729326
H	-5.08559370	-0.94466084	-0.50989354
H	-3.47255182	0.74018443	0.25404537
H	-1.86659849	-3.59011674	-1.55448461
H	-4.30505514	-3.11039567	-1.43026280

H	1.40120256	-0.84904319	4.41346645
H	2.24729562	-2.94973350	3.39941764
H	1.72662985	-3.45803595	1.01911938
C	-1.10876262	1.83765078	0.81689852
H	0.51232708	-2.84498882	-1.08007073
C	0.25659087	0.63708693	-1.07392824
H	-0.41613123	1.11723709	-1.78402472
C	0.75498527	-0.72763920	-1.59210241
H	0.45214435	-0.89458507	-2.62916684
C	1.51930749	1.48562944	-1.00245738
C	2.27430272	-0.63777786	-1.57253516
O	3.06460404	-1.51697934	-1.82737827
O	1.59625173	2.68319726	-0.82713276
C	-0.10593393	2.69997764	1.64245749
H	-0.39683044	2.75588751	2.69425011
H	0.91867095	2.34082913	1.59618580
H	-0.09628878	3.71967101	1.25533032
N	2.61888814	0.66863024	-1.23552227
C	3.99041677	1.15787184	-1.20732486
H	4.62733698	0.38292170	-1.62902355
H	4.06373262	2.07411122	-1.79319954
H	4.29888725	1.36727703	-0.18142422
H	-1.93793344	1.58341551	1.48344553
C	-2.68261504	3.60491467	0.11033444
H	-3.49990630	3.08349442	0.62532061
H	-2.28148222	4.33370972	0.83208275
N	-1.70299065	2.59461617	-0.30098987
H	-0.95201898	3.06206942	-0.80379832
C	-3.23838687	4.35643387	-1.08203328
C	-3.25619078	5.75298738	-1.10147715
C	-3.75697207	3.66315269	-2.18264747
C	-3.78768182	6.44670153	-2.18893671
H	-2.84890175	6.30372715	-0.25943208
C	-4.28659010	4.35224152	-3.26977658
H	-3.73319697	2.57962275	-2.18158174
C	-4.30503941	5.74762630	-3.27613282
H	-3.79182339	7.53113985	-2.18703365
H	-4.68637037	3.80120230	-4.11413765
H	-4.71678162	6.28384495	-4.12386703

S26. BnNH - *SYN* APPROACH β - 1st ISOMER - TS

S26.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.9008	Debye
Energy	:	-1342.89486934	a.u.
Number of imaginary frequencies	:	1	

S26.2. Cartesian Co-ordinates (XYZ format)

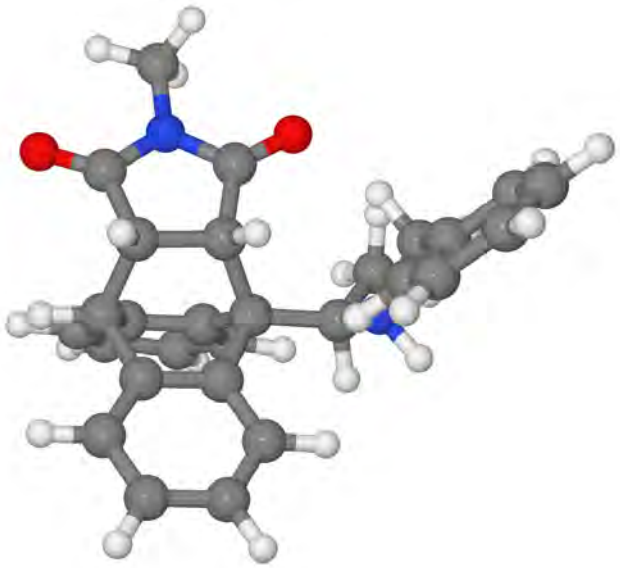
58

C	0.62545091	3.86044502	0.10386099
C	0.55526459	2.63211703	0.73054588
C	-0.50375891	1.73017383	0.46164277
C	-1.47282338	2.13069344	-0.49594906
C	-1.36368454	3.36881948	-1.15651548
C	-0.33378890	4.23510218	-0.85282683
C	-0.63394183	0.41686094	1.08266532
C	-2.50001931	1.17803335	-0.82521492
C	-2.94765806	0.32364771	0.23666221
C	-1.98923004	-0.09153993	1.21390092
C	-2.46341038	-0.97467494	2.22273326
H	-1.81282544	-1.30260527	3.01114917
C	-3.77484965	-1.39910018	2.25777149
C	-4.69305754	-0.99919349	1.27157438
C	-4.27334166	-0.15569383	0.26790851
H	1.43132842	4.54146481	0.35333630
H	1.31716692	2.37843752	1.45149922
H	-2.11239338	3.63901901	-1.89362359
H	-0.26579902	5.19932222	-1.34317243

H	-4.09862900	-2.04717755	3.06447029
H	-5.72023296	-1.34299445	1.30753648
H	-4.96047068	0.16631855	-0.50606132
C	0.59688687	-0.04817724	1.90977895
H	-3.24206781	1.47622883	-1.55913210
C	-0.29782510	-0.58174837	-1.19406402
H	0.68792361	-0.15307115	-1.14515114
C	-1.38075840	-0.11541079	-1.95352590
H	-1.27813423	0.58871382	-2.76770091
C	-0.53396708	-1.99103105	-0.85492283
C	-2.30806303	-1.28461957	-2.15161824
O	-3.31935382	-1.34114242	-2.81785297
O	0.18036839	-2.76811361	-0.24349537
C	0.49193799	-1.30009353	2.80083799
H	-0.09487163	-1.12824929	3.70444489
H	0.09539624	-2.15727806	2.25775146
H	1.49819934	-1.55937886	3.13700056
N	-1.78751624	-2.32959056	-1.39499366
C	-2.42848420	-3.62272239	-1.24026406
H	-1.69099152	-4.31247759	-0.83321249
H	-3.27966547	-3.55506539	-0.55825776
H	-2.77907777	-3.97837591	-2.20970583
H	0.81671757	0.78851777	2.58400774
C	3.06653428	0.04895396	1.64430642
H	3.07451081	1.06048727	2.06998372
H	3.26222944	-0.63808709	2.48209858
N	1.76354742	-0.15340316	1.00346744
H	1.74141085	-1.07330489	0.56741947
C	4.19224024	-0.08279871	0.63963223
C	5.19975567	-1.03391778	0.81387126
C	4.24304008	0.75100219	-0.48444721
C	6.24212837	-1.14866126	-0.10661013
H	5.16886139	-1.69226420	1.67623937
C	5.28088951	0.63929909	-1.40464211
H	3.45967889	1.48547685	-0.63424081
C	6.28531742	-0.31170473	-1.21802843
H	7.01531839	-1.89387572	0.04425707
H	5.30836153	1.29406750	-2.26883554
H	7.09321308	-0.39918599	-1.93588448

S27. BnNH - *SYN* APPROACH β - 2nd ISOMER - PRODUCT

S27.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.9144	Debye
Energy	:	-1342.94869186	a.u.
Number of imaginary frequencies	:	0	

S27.2. Cartesian Co-ordinates (XYZ format)

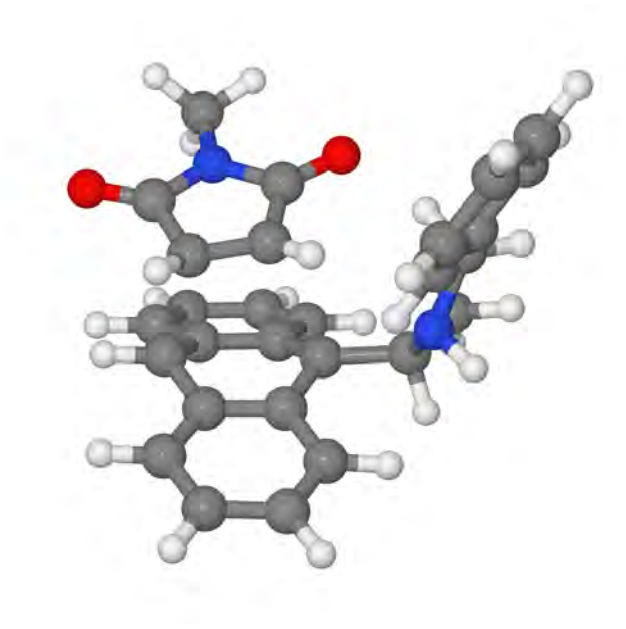
58

C	0.53792840	3.75830197	-0.46301630
C	0.56853086	2.51574421	0.17574690
C	-0.39532909	1.54966402	-0.11198130
C	-1.39988017	1.87069488	-1.04004693
C	-1.42533767	3.09969521	-1.68785584
C	-0.44747517	4.05161285	-1.39998174
C	-0.54945058	0.14065628	0.53765696
C	-2.43075585	0.78130627	-1.22466028
C	-2.97089386	0.46601185	0.15349163
C	-1.98237205	0.18149076	1.11695921
C	-2.37692642	0.07552811	2.45113659
H	-1.65194130	-0.05330527	3.24062943
C	-3.72662592	0.16827367	2.80227995
C	-4.69885588	0.37557808	1.83043230
C	-4.31466484	0.53990060	0.49944851
H	1.29478276	4.49667215	-0.22268589
H	1.35627341	2.32475424	0.88785297
H	-2.21297216	3.31766891	-2.40159917
H	-0.46289775	5.01599693	-1.89497876

H	-4.01034689	0.08209232	3.84516501
H	-5.74521255	0.43763226	2.10680223
H	-5.05570936	0.74888247	-0.26459774
C	0.61402452	-0.13378923	1.56067967
H	-3.21899796	1.05610347	-1.92509723
C	-0.56683475	-0.86037737	-0.70667320
H	0.43086156	-0.81764865	-1.14503074
C	-1.64676297	-0.45116892	-1.73770082
H	-1.21208763	-0.21879035	-2.71256399
C	-0.88247186	-2.33874321	-0.44048947
C	-2.55121517	-1.65872169	-1.90743256
O	-3.53567863	-1.74098694	-2.60632110
O	-0.23445056	-3.15168691	0.18253204
C	0.51973796	-1.36334920	2.48694301
H	-0.45273274	-1.47591794	2.95836926
H	0.71839035	-2.28922009	1.95767772
H	1.26308215	-1.24899220	3.28201079
N	-2.04713702	-2.68090320	-1.11678231
C	-2.62160921	-4.01820803	-1.06222618
H	-3.45318890	-4.04723930	-1.76326621
H	-1.86797535	-4.75720310	-1.33606029
H	-2.97820115	-4.23399496	-0.05395186
H	0.58264941	0.74177563	2.21647453
C	2.64110875	-1.29583108	0.53843713
H	3.00770140	-1.83949935	1.42191172
H	1.94862735	-1.98115993	0.04330143
N	1.92623723	-0.06148194	0.87121129
H	2.55118608	0.53673309	1.39841843
C	3.82249689	-1.03499091	-0.38074395
C	3.82706380	0.02162625	-1.29727244
C	4.92806721	-1.89229035	-0.34513092
C	4.90567684	0.20879802	-2.16088700
H	2.98250222	0.69925338	-1.31929874
C	6.00469017	-1.70996153	-1.20987093
H	4.94541740	-2.71047544	0.36853382
C	5.99717426	-0.65649879	-2.12303400
H	4.89271307	1.03449881	-2.86433291
H	6.85193062	-2.38567805	-1.16590691
H	6.83621168	-0.50899047	-2.79386997

S28. BnNH - *SYN* APPROACH β - 2nd ISOMER - TS

S28.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.6870	Debye
Energy	:	-1342.88632367	a.u.
Number of imaginary frequencies	:	1	

S28.2. Cartesian Co-ordinates (XYZ format)

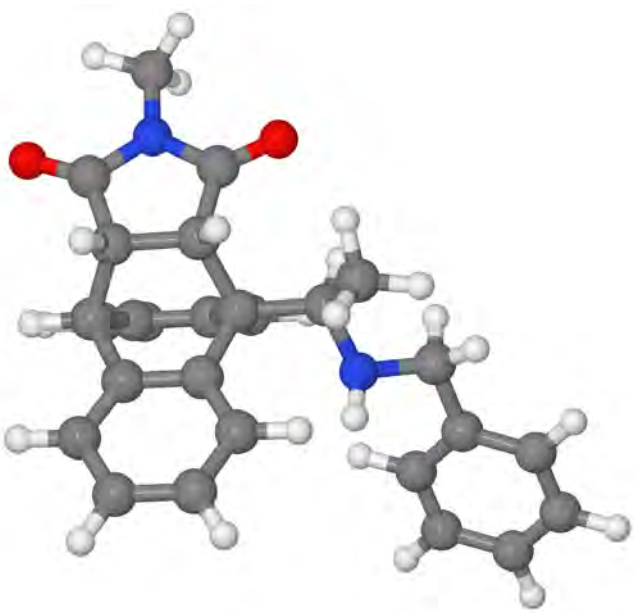
58

C	0.36307684	4.15044594	0.03186349
C	0.28439012	2.98752189	0.77095109
C	-0.59509701	1.93649852	0.40398186
C	-1.38868225	2.13768244	-0.75557381
C	-1.26204336	3.30933404	-1.52691603
C	-0.40219215	4.31343555	-1.13598979
C	-0.72627836	0.67846131	1.13476610
C	-2.26282740	1.06664777	-1.14445829
C	-2.83406258	0.28540018	-0.08678773
C	-2.04125667	0.05622261	1.08257353
C	-2.61576843	-0.78342539	2.07513022
H	-2.08812356	-0.99291682	2.98626256
C	-3.87549806	-1.32540298	1.92742169
C	-4.63239527	-1.09667337	0.76575416
C	-4.10350370	-0.31063834	-0.23347706
H	1.02299798	4.94606829	0.35869372
H	0.89108175	2.91011071	1.65929866
H	-1.87066138	3.41906524	-2.41814518
H	-0.32532325	5.22658682	-1.71482182

H	-4.28409910	-1.93526590	2.72538400
H	-5.62074566	-1.52894557	0.66128862
H	-4.66191530	-0.12520370	-1.14402330
C	0.34690037	0.47050929	2.24751306
H	-2.86651611	1.20943344	-2.03501368
C	0.02886581	-0.61743039	-0.85460061
H	0.99476200	-0.19844638	-0.63248634
C	-0.82627547	-0.21848100	-1.89262080
H	-0.53352785	0.45037377	-2.68931746
C	-0.32626849	-2.00065255	-0.47752675
C	-1.68628502	-1.39862669	-2.24189138
O	-2.49348664	-1.50660598	-3.14053106
O	0.17275402	-2.73689890	0.35527658
C	0.21481045	-0.70359802	3.23369479
H	-0.59559894	-0.54145020	3.94346261
H	0.07969929	-1.66488457	2.73879123
H	1.13053262	-0.75168151	3.82660627
N	-1.39896595	-2.38006568	-1.30101717
C	-2.08671021	-3.65532422	-1.21622407
H	-3.04708648	-3.54569292	-0.70567971
H	-2.26041508	-4.03967667	-2.22133350
H	-1.45504081	-4.34091568	-0.65394282
H	0.24116836	1.37018120	2.86457491
C	2.51485062	-0.65023834	1.52538538
H	2.83248854	-1.07605696	2.48936462
H	1.90077674	-1.42134416	1.05378628
N	1.71488392	0.56834954	1.66874349
H	2.25046945	1.24209142	2.20400953
C	3.76262212	-0.42150244	0.68837535
C	3.89584017	0.66560411	-0.18010505
C	4.81291389	-1.34521401	0.76587546
C	5.04603481	0.82097083	-0.95544088
H	3.09361506	1.39043939	-0.24162133
C	5.95805836	-1.19505918	-0.01015839
H	4.72964621	-2.19114208	1.44161940
C	6.07987642	-0.10772453	-0.87602210
H	5.13132668	1.67196274	-1.62276518
H	6.75838280	-1.92333281	0.06376024
H	6.97326469	0.01372193	-1.47833788

S29. BnNH - *SYN* APPROACH γ - PRODUCT

S29.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NCc6ccccc6	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.9443	Debye
Energy	:	-1342.96216351	a.u.
Number of imaginary frequencies	:	0	

S29.2. Cartesian Co-ordinates (XYZ format)

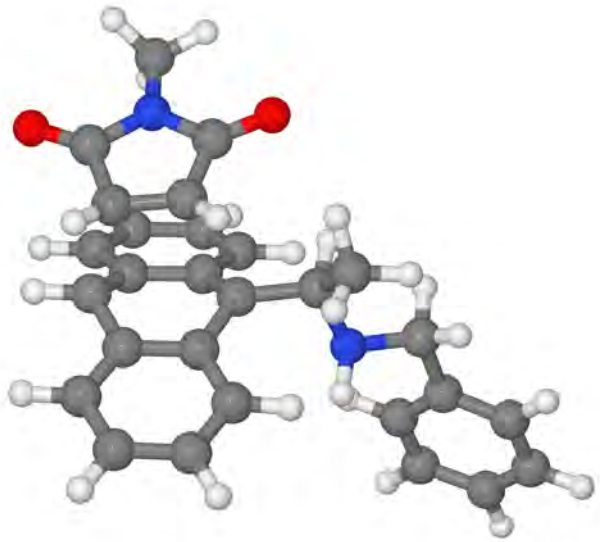
58

C	0.29211757	4.07203245	-0.58370227
C	0.40848860	2.71147346	-0.88109207
C	-0.50975239	1.79287827	-0.37131140
C	-1.56499565	2.27810287	0.42226842
C	-1.68645096	3.63125062	0.71385813
C	-0.74806559	4.53479719	0.21465285
C	-0.54425699	0.26212078	-0.58843619
C	-2.53548622	1.21248639	0.87599778
C	-1.74339867	0.12868586	1.57055676
C	-0.67898464	-0.37803134	0.80796868
C	0.09262998	-1.41391909	1.33251667
H	0.92248982	-1.81747270	0.77157807
C	-0.18773460	-1.91994321	2.60347438
C	-1.23953259	-1.40429127	3.35678148
C	-2.02610707	-0.37802657	2.83496833
H	1.02209723	4.76722479	-0.98255754
H	1.22082400	2.40048695	-1.52311552
H	-2.50973845	3.97856402	1.32928538
H	-0.83262944	5.59068108	0.44486648

H	0.42508522	-2.71921206	3.00521040
H	-1.44869530	-1.80008721	4.34420586
H	-2.85713625	0.02323502	3.40505886
C	0.61915517	-0.34311873	-1.43035471
H	-3.33945990	1.60795438	1.49625480
C	-1.95376813	0.00948993	-1.28482985
H	-1.93179703	0.45656395	-2.27895784
C	-3.10688114	0.59362787	-0.43818715
H	-3.66645265	1.36093998	-0.97737682
C	-2.31822658	-1.46596372	-1.44739783
C	-4.04656315	-0.57201344	-0.17082493
O	-5.07799673	-0.54713786	0.46084833
O	-1.71143520	-2.31993747	-2.05686045
C	0.57784808	0.03346474	-2.92885303
H	-0.24306387	-0.47749403	-3.43453193
H	0.47325832	1.10660100	-3.09903359
H	1.49944627	-0.29387560	-3.41513896
N	-3.51797819	-1.70125675	-0.78735071
C	-4.14612246	-3.01441383	-0.73921275
H	-5.11913347	-2.89742899	-0.26657626
H	-4.25973988	-3.40703821	-1.74996281
H	-3.53308463	-3.70527029	-0.15809515
H	0.47274190	-1.42554235	-1.39495981
C	3.00150824	-0.97375649	-1.18225658
H	2.67273998	-2.01026917	-1.02530897
H	3.25053954	-0.89854628	-2.25281739
N	1.90709877	-0.10069887	-0.76611412
H	2.19513535	0.86732888	-0.83201540
C	4.26546669	-0.72571337	-0.38030997
C	5.51826429	-0.83095437	-0.99211466
C	4.20966482	-0.42026937	0.98434293
C	6.69000483	-0.64816236	-0.25966123
H	5.57753897	-1.05674314	-2.05243230
C	5.37939072	-0.23180732	1.71720898
H	3.24183941	-0.32166579	1.46083462
C	6.62393522	-0.34765500	1.09923100
H	7.65252542	-0.73329431	-0.75209308
H	5.31872272	0.00611842	2.77368546
H	7.53357410	-0.20001380	1.67061770

S30. BnNH - *SYN* APPROACH γ - TS

S30.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NCc4ccccc4.CN1C(=O)C=CC1=O	
Formula	:	$C_{28}H_{26}N_2O_2$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.1550	Debye
Energy	:	-1342.90201288	a.u.
Number of imaginary frequencies	:	1	

S30.2. Cartesian Co-ordinates (XYZ format)

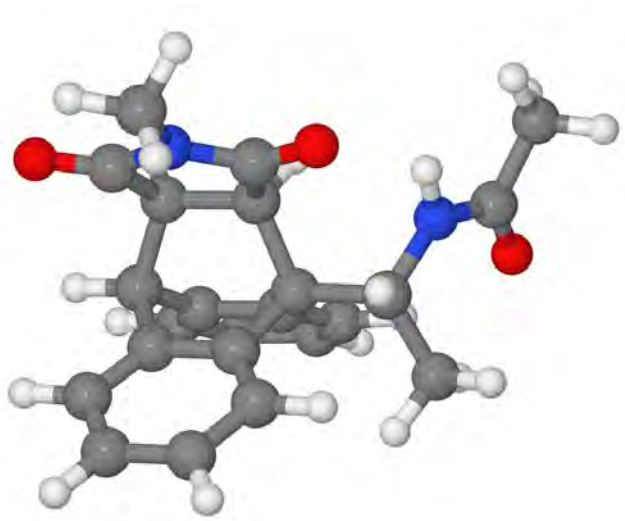
58

C	0.06929268	4.16498280	-0.56211358
C	0.33887935	2.82197213	-0.73651248
C	-0.50224847	1.82663250	-0.18002719
C	-1.63463926	2.26290679	0.56333196
C	-1.91616738	3.63639998	0.69313484
C	-1.07016790	4.58050013	0.14817701
C	-0.30370712	0.39656147	-0.32840395
C	-2.50907683	1.25099182	1.09379113
C	-1.90829408	0.01274011	1.49962640
C	-0.78357553	-0.43654072	0.75453329
C	-0.22277893	-1.69399166	1.09307873
H	0.65241736	-2.05155444	0.57062823
C	-0.74431270	-2.44530964	2.12477994
C	-1.86803591	-1.99701428	2.84611201
C	-2.45006871	-0.78967404	2.52604914
H	0.74575746	4.90405893	-0.97581035
H	1.22586560	2.54349589	-1.28683543
H	-2.79608202	3.94229794	1.24905670
H	-1.27601373	5.63708258	0.27415338

H	-0.27943081	-3.38896823	2.38702154
H	-2.26880431	-2.59879899	3.65367007
H	-3.32177448	-0.43650582	3.06491971
C	0.78252810	-0.18534613	-1.24540472
H	-3.38699913	1.58160555	1.63961446
C	-2.39154148	0.22179946	-1.59274590
H	-1.93594766	0.79843378	-2.37885594
C	-3.39289069	0.67411911	-0.72107166
H	-3.91481566	1.61329818	-0.83475518
C	-2.48585105	-1.24844527	-1.68749869
C	-4.18153000	-0.52915931	-0.29260579
O	-5.18132305	-0.57242346	0.39248499
O	-1.82972467	-2.02395868	-2.35705590
C	0.74115634	0.26518080	-2.72240734
H	-0.11448225	-0.18959968	-3.22234392
H	0.69230175	1.34503949	-2.85895562
H	1.63519585	-0.09689946	-3.23527527
N	-3.52994394	-1.63511288	-0.82919353
C	-3.91424680	-3.01145506	-0.57430536
H	-4.99879932	-3.10569954	-0.63477325
H	-3.44023228	-3.63518310	-1.33040559
H	-3.58366609	-3.32872748	0.41785148
H	0.59621203	-1.26088488	-1.28405094
C	3.17912555	-0.83739686	-1.08398354
H	2.83192897	-1.87830484	-1.12621093
H	3.46817279	-0.57330799	-2.11292911
N	2.07702637	-0.03618933	-0.55469316
H	2.35252357	0.93695581	-0.48273408
C	4.41307068	-0.75790083	-0.20457737
C	5.68679476	-0.74090785	-0.78044730
C	4.30750895	-0.73341411	1.19062376
C	6.83117151	-0.71249992	0.01512109
H	5.78441858	-0.74910033	-1.86170888
C	5.44936848	-0.69996941	1.98757493
H	3.32263756	-0.72868544	1.64178991
C	6.71560478	-0.69206583	1.40329301
H	7.81087208	-0.69932431	-0.44977769
H	5.35057211	-0.68002206	3.06750274
H	7.60377932	-0.66534704	2.02467108

S31. MEC(O)NH - *ANTI* APPROACH α - PRODUCT

S31.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.8220	Debye
Energy	:	-1225.25020450	a.u.
Number of imaginary frequencies	:	0	

S31.2. Cartesian Co-ordinates (XYZ format)

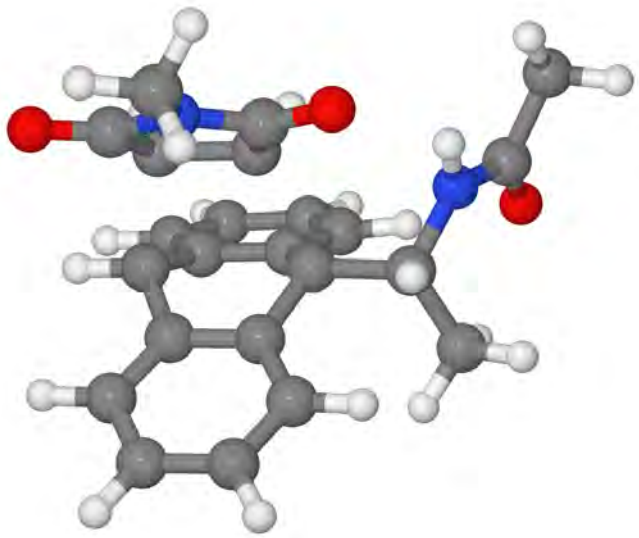
50

C	-1.50949788	-0.22940806	3.27622294
C	-0.63152975	0.43267325	2.41473031
C	-0.19948412	-0.18419556	1.23905027
C	-0.69291300	-1.46311045	0.93242592
C	-1.57372916	-2.11925292	1.78489828
C	-1.97689974	-1.50338018	2.96915579
C	0.74020642	0.40490022	0.16187435
C	-0.21977624	-1.99748456	-0.39676121
C	1.29017043	-1.93443298	-0.41479653
C	1.81686914	-0.65832651	-0.14358102
C	3.19290876	-0.46370709	-0.24843119
H	3.62860560	0.51864910	-0.13387391
C	4.02737617	-1.54222524	-0.55841041
C	3.50148892	-2.80996561	-0.78339809
C	2.12070227	-3.00377560	-0.72605938
H	-1.82535434	0.25908810	4.19102335
H	-0.29798350	1.42487633	2.68642735
H	-1.94680822	-3.10297823	1.52157402
H	-2.65661573	-2.01263618	3.64269829

H	5.09693336	-1.37861466	-0.62883651
H	4.15732956	-3.64088035	-1.01799595
H	1.69272161	-3.98007607	-0.92881131
C	1.20781529	1.84923303	0.54917693
H	-0.60640907	-2.99375844	-0.60938329
C	-0.11949805	0.42359123	-1.17951608
C	-0.68763357	-0.97927725	-1.48620248
C	-1.34523940	1.32764518	-1.14157665
H	-0.37191594	-1.34025490	-2.46755743
H	0.53325367	0.78116125	-1.97621858
O	-1.36694121	2.53663111	-1.00212312
C	-2.19852328	-0.79995817	-1.52002871
O	-3.03501153	-1.65346634	-1.69661069
N	-2.47732663	0.55424458	-1.32043695
C	-3.82604122	1.10582781	-1.31150413
H	-3.90120387	1.91362596	-2.03994966
H	-4.51180363	0.30097663	-1.56767142
H	-4.06640673	1.49652052	-0.32159665
C	2.20823669	1.94096541	1.71329415
H	2.18973494	2.95670319	2.11690593
H	1.92659986	1.25274420	2.50993681
H	3.22736430	1.72778881	1.41396046
H	0.29140320	2.32737494	0.89743084
N	1.57488072	2.68334842	-0.60760504
H	0.77017665	3.11252689	-1.04431248
C	2.79964137	3.03672814	-1.08457303
O	3.87012887	2.61757684	-0.65844166
C	2.76524091	4.03416586	-2.23430634
H	3.31875873	3.61096787	-3.07469392
H	1.75975716	4.30148649	-2.56331253
H	3.28926635	4.93983650	-1.92113090

S32. MEC(O)NH - *ANTI* APPROACH α - TS

S32.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	1.8343	Debye
Energy	:	-1225.19383794	a.u.
Number of imaginary frequencies	:	1	

S32.2. Cartesian Co-ordinates (XYZ format)

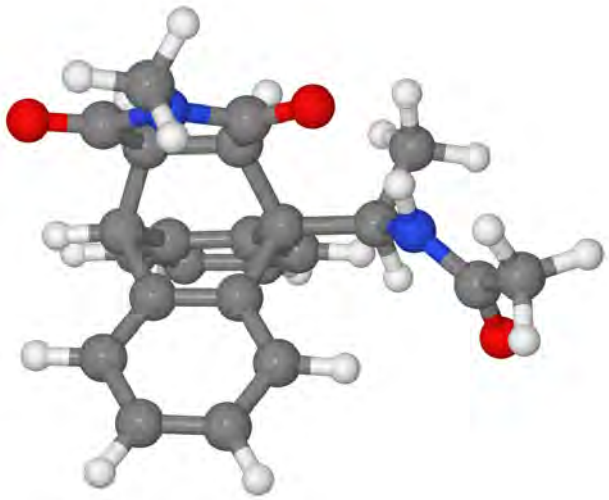
50

C	2.39812183	-0.17153253	2.91479325
C	1.12127578	-0.32020479	2.41499662
C	0.71027458	0.36767885	1.24307775
C	1.67245698	1.18424058	0.58679867
C	2.98393393	1.29205871	1.09315932
C	3.34004474	0.63787252	2.25276446
C	-0.60487437	0.25457489	0.64472133
C	1.27583385	1.79361343	-0.65147322
C	-0.10313874	2.19204593	-0.77894330
C	-1.07902730	1.38286769	-0.13339686
C	-2.44463706	1.68677950	-0.34492812
H	-3.21948576	1.08024156	0.10396510
C	-2.80963016	2.76612163	-1.12703598
C	-1.83859992	3.56362581	-1.75672865
C	-0.49988577	3.26543045	-1.59761393
H	2.67629528	-0.68284106	3.82924032
H	0.42822444	-0.94803655	2.95715761
H	3.70305324	1.90534282	0.56261909
H	4.34066343	0.74512500	2.65502143

H	-3.86112380	2.99600983	-1.25686800
H	-2.14085102	4.40681458	-2.36724901
H	0.26032782	3.86349583	-2.08887172
C	-1.55271637	-0.79507995	1.25215304
H	2.01976538	2.39307427	-1.16679871
C	0.18850809	-0.73985660	-1.42958629
C	1.20409298	0.11786718	-1.88420916
C	0.80716622	-1.93850040	-0.85108477
H	1.12538838	0.71698570	-2.78035188
H	-0.82962871	-0.75711948	-1.77829587
O	0.26499644	-2.92830539	-0.37921786
C	2.50760150	-0.58266491	-1.61902535
O	3.62884927	-0.23567852	-1.91815257
N	2.19269347	-1.75410736	-0.92715222
C	3.18036103	-2.67802548	-0.39808089
H	3.94460464	-2.86955476	-1.15180624
H	3.65680981	-2.26596618	0.49462742
H	2.66742826	-3.60349894	-0.14194183
C	-2.35380411	-0.25795874	2.45303059
H	-3.03861284	0.54063153	2.18567085
H	-2.93624306	-1.06704164	2.89806509
H	-1.65490460	0.11756138	3.20332599
H	-0.89641458	-1.57081044	1.64592397
N	-2.34756303	-1.53358376	0.25737873
H	-1.81920183	-2.28927493	-0.16237357
C	-3.68166423	-1.48245621	-0.00392234
O	-4.45384455	-0.65311611	0.46463534
C	-4.17941713	-2.55298901	-0.96392149
H	-4.68573093	-2.06124806	-1.79674399
H	-3.39357543	-3.20251942	-1.35246623
H	-4.92159653	-3.16339588	-0.44471911

S33. MEC(O)NH - *ANTI* APPROACH β - PRODUCT

S33.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.3813	Debye
Energy	:	-1225.25472618	a.u.
Number of imaginary frequencies	:	0	

S33.2. Cartesian Co-ordinates (XYZ format)

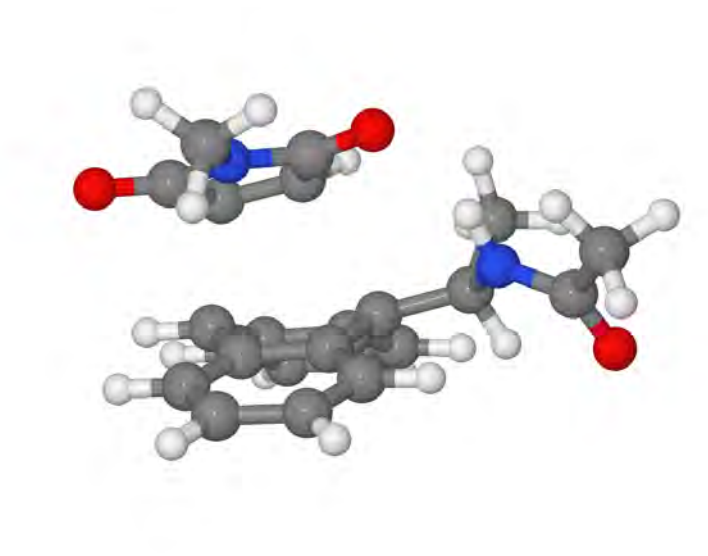
50

C	-0.81699574	0.21989405	3.41343474
C	-0.28449473	0.88191193	2.30367017
C	0.00184458	0.16959575	1.14028609
C	-0.19979677	-1.22403598	1.12872744
C	-0.74533516	-1.87644327	2.22791314
C	-1.06664932	-1.14811885	3.37388992
C	0.60525119	0.70968992	-0.17195891
C	0.30006915	-1.92135608	-0.12062627
C	1.73920536	-1.49397063	-0.30927426
C	1.91821373	-0.10052834	-0.33413330
C	3.21369123	0.40674162	-0.42118818
H	3.40278673	1.47150123	-0.40318695
C	4.30375385	-0.46306300	-0.51746118
C	4.11167812	-1.84039509	-0.52532989
C	2.82042503	-2.35912585	-0.41515917
H	-1.02955341	0.78376806	4.31473017
H	-0.06981903	1.93699777	2.37676978
H	-0.89912200	-2.94979095	2.19720578
H	-1.48565018	-1.65215814	4.23739529

H	5.30566454	-0.05405537	-0.58077538
H	4.96115780	-2.50951505	-0.60082984
H	2.65927386	-3.43181586	-0.39464059
C	0.87686270	2.24625039	-0.23704955
H	0.18254282	-3.00341058	-0.06794427
C	-0.34458190	0.19617037	-1.34619141
C	-0.46550292	-1.34432566	-1.34115422
C	-1.80032086	0.67122114	-1.30547094
H	-0.06793913	-1.79100645	-2.25497556
H	0.07174657	0.54779351	-2.29121447
O	-2.22133851	1.81261623	-1.34338021
C	-1.95277500	-1.64510298	-1.28535521
O	-2.48072457	-2.73133397	-1.25719690
N	-2.63413835	-0.42947116	-1.27574217
C	-4.08692217	-0.31932923	-1.23710644
H	-4.43563509	0.28276065	-2.07641864
H	-4.49331427	-1.32651460	-1.29935622
H	-4.40314960	0.15229742	-0.30568501
C	1.31741321	2.73432517	-1.63329470
H	1.74096107	3.73667574	-1.54162693
H	2.06353903	2.08924198	-2.09798622
H	0.45683923	2.80104947	-2.30307341
H	1.67009652	2.45742941	0.48156181
N	-0.24362001	3.07862496	0.19326383
H	-1.09836960	2.99646926	-0.34388569
C	-0.10486871	4.09421968	1.08525658
O	0.92423910	4.29612112	1.72272766
C	-1.33354664	4.96818924	1.26577914
H	-2.21401477	4.59419394	0.74104077
H	-1.55282962	5.04654598	2.33204150
H	-1.10355103	5.97347641	0.90430230

S34. MEC(O)NH - *ANTI* APPROACH β - TS

S34.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.5489	Debye
Energy	:	-1225.19050518	a.u.
Number of imaginary frequencies	:	1	

S34.2. Cartesian Co-ordinates (XYZ format)

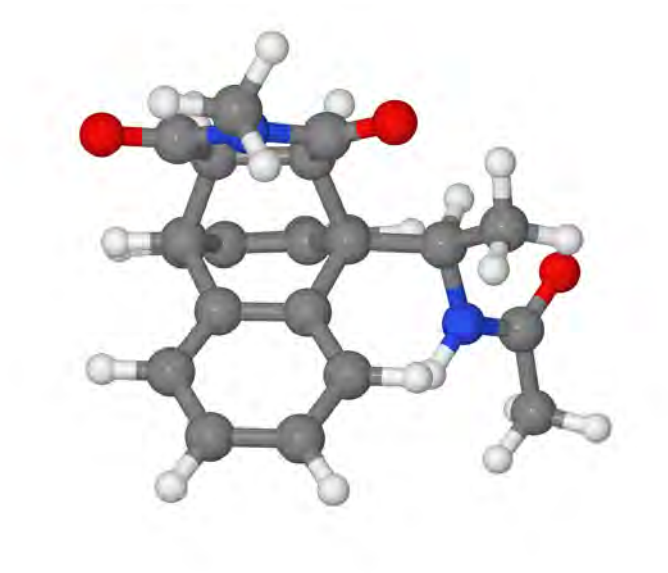
50

C	-0.91051787	-1.80636179	2.69141412
C	-1.14846599	-0.74349493	1.84629095
C	-0.09140109	-0.13367932	1.11898220
C	1.22421730	-0.65417695	1.31706035
C	1.43271875	-1.77626145	2.14652801
C	0.38222286	-2.34431505	2.83270192
C	-0.23698270	0.99464786	0.21848682
C	2.30589652	-0.03491263	0.60772783
C	2.19480133	1.37992239	0.38168108
C	0.89020717	1.91198647	0.19253403
C	0.76863962	3.31447887	0.02432073
H	-0.20872752	3.77135611	-0.04390782
C	1.88354170	4.12784386	0.00678983
C	3.17291999	3.57868385	0.12306426
C	3.32314253	2.21931267	0.30385146
H	-1.73211205	-2.22478294	3.26171446
H	-2.14533186	-0.34397557	1.77662706
H	2.43843722	-2.16578627	2.25517797
H	0.55246109	-3.18569112	3.49444151

H	1.76121378	5.20049429	-0.08926661
H	4.04224205	4.22524500	0.09474836
H	4.31016588	1.78582418	0.42414236
C	-1.59444070	1.51983523	-0.28442988
H	3.29902864	-0.44583261	0.75653762
C	0.67713231	-0.30616194	-1.74636209
C	1.96188474	-0.69385982	-1.35298157
C	-0.20066668	-1.48686588	-1.68858361
H	2.87312579	-0.25342071	-1.73085630
H	0.43097183	0.54569077	-2.35464096
O	-1.39263928	-1.58402932	-1.94500387
C	1.92581606	-2.17797303	-1.12722254
O	2.83955455	-2.92671704	-0.85936093
N	0.59258360	-2.56010008	-1.26790833
C	0.09834193	-3.90228200	-1.01573527
H	-0.89826435	-3.97712255	-1.44695115
H	0.76415712	-4.62992477	-1.48011339
H	0.04691603	-4.10011673	0.05774712
C	-1.56800783	2.15455747	-1.69797528
H	-2.46527362	2.76538515	-1.81763518
H	-0.69924700	2.78100061	-1.88881505
H	-1.60095334	1.36771786	-2.45282984
H	-1.92951918	2.28134394	0.42907637
N	-2.65901470	0.52160221	-0.29956609
H	-2.51321816	-0.28144056	-0.90290433
C	-3.90973401	0.80173337	0.16093501
O	-4.18068075	1.82695198	0.77604866
C	-4.95599079	-0.26083738	-0.12124342
H	-5.71066666	0.16117427	-0.78925490
H	-4.54538393	-1.16451836	-0.57385117
H	-5.45502090	-0.51732826	0.81498057

S35. MEC(O)NH - *ANTI* APPROACH γ - PRODUCT

S35.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C
Formula	:	$C_{23}H_{22}N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	3.8523 Debye
Energy	:	-1225.24466039 a.u.
Number of imaginary frequencies	:	0

S35.2. Cartesian Co-ordinates (XYZ format)

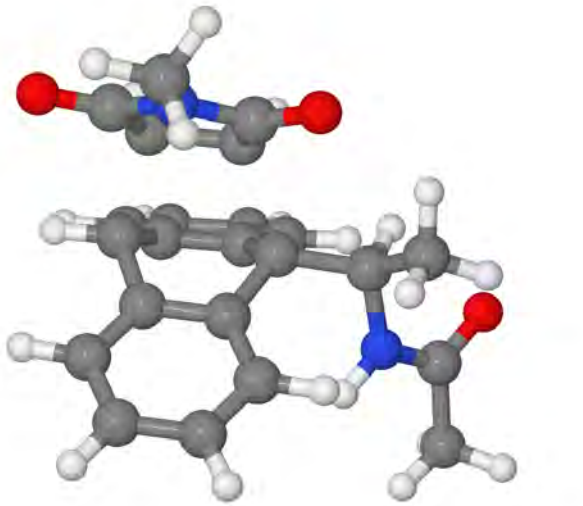
50

C	-1.05535245	1.32585979	3.14062119
C	-0.37982255	1.57374966	1.94272947
C	-0.13554832	0.53317714	1.04401863
C	-0.60255462	-0.75495929	1.36067700
C	-1.28422201	-0.99798834	2.54772305
C	-1.50592113	0.04580779	3.44617629
C	0.56278664	0.62252271	-0.32640669
C	-0.31688297	-1.79586565	0.30430391
C	1.15858757	-1.77640688	0.00430935
C	1.62946165	-0.51300097	-0.37682128
C	2.95337629	-0.39804623	-0.80615294
H	3.36118221	0.54397070	-1.14569616
C	3.78835917	-1.51824129	-0.80956453
C	3.31601310	-2.76050210	-0.39671537
C	1.98659050	-2.89289451	0.00188225
H	-1.23103571	2.14310932	3.83082294
H	-0.05808753	2.58393764	1.73016346
H	-1.64172244	-1.99787617	2.76858902
H	-2.03109145	-0.14033367	4.37590933

H	4.81564713	-1.41053891	-1.13881612
H	3.97299767	-3.62282848	-0.39696148
H	1.59277546	-3.85894966	0.29967985
C	1.25486076	1.98216629	-0.65619648
H	-0.68612415	-2.78321242	0.57976806
C	-0.54307884	0.13059187	-1.37705863
C	-0.98519683	-1.31900370	-1.02342248
C	-1.88496292	0.88955277	-1.45279670
H	-0.73136204	-2.02650738	-1.81511629
H	-0.09760261	0.17795268	-2.37357187
O	-2.09957242	2.02746272	-1.79994965
C	-2.49597311	-1.28426039	-0.88934463
O	-3.22175026	-2.21501994	-0.62046868
N	-2.91525912	0.01360018	-1.12428153
C	-4.31249380	0.42558792	-1.11135983
H	-4.57950878	0.86435115	-2.07325077
H	-4.91394329	-0.46038464	-0.91923982
H	-4.47839928	1.16593277	-0.32751906
C	0.41523293	3.23538256	-0.94191426
H	1.11078393	4.06670904	-1.07282686
H	-0.16498519	3.12189364	-1.85309219
H	-0.28097785	3.48566437	-0.14160439
H	1.84139824	1.81622207	-1.56188786
N	2.24253726	2.26862073	0.39726490
H	2.03124213	2.00771022	1.34675837
C	3.44815397	2.83875799	0.13255927
O	3.80526090	3.12975788	-1.00381660
C	4.34212399	3.07939386	1.33551848
H	3.87574506	2.82381415	2.28850675
H	5.25373173	2.48977256	1.21583450
H	4.63153172	4.13182449	1.34870088

S36. MEC(O)NH - *ANTI* APPROACH γ - TS

S36.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	4.6024	Debye
Energy	:	-1225.19003087	a.u.
Number of imaginary frequencies	:	1	

S36.2. Cartesian Co-ordinates (XYZ format)

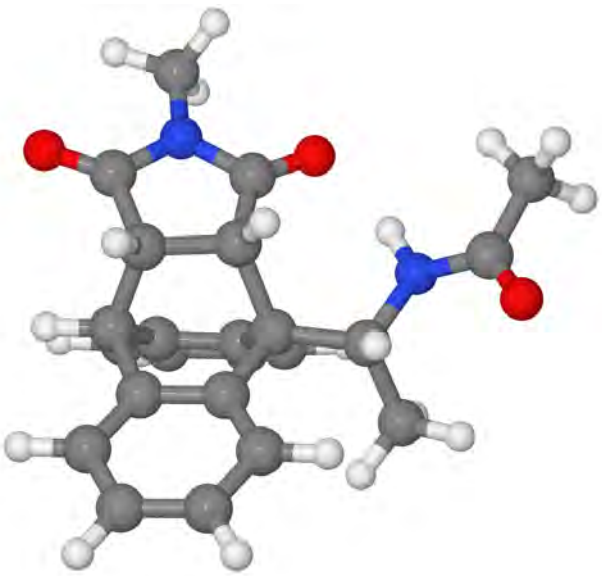
50

C	1.02518463	-1.66454768	2.87829137
C	0.13935880	-1.54469478	1.82804072
C	0.08332995	-0.36101434	1.04576969
C	0.98584926	0.68929875	1.37916577
C	1.90837300	0.53130627	2.43097234
C	1.92236948	-0.62506247	3.18328261
C	-0.83331233	-0.14540868	-0.05006924
C	0.96886629	1.86628878	0.54605305
C	-0.31162518	2.26212835	0.00941462
C	-1.21430910	1.22327268	-0.34250873
C	-2.42873096	1.59028459	-0.98003721
H	-3.15881228	0.84142888	-1.25643551
C	-2.72264266	2.91619372	-1.22671926
C	-1.81579828	3.93311143	-0.87958705
C	-0.61626345	3.60389161	-0.28147912
H	1.02789402	-2.57018018	3.47399473
H	-0.53068227	-2.36687016	1.62590039
H	2.59869504	1.33818579	2.64873505
H	2.61601591	-0.73121667	4.00911427

H	-3.66689110	3.17335391	-1.69281757
H	-2.05929804	4.96992636	-1.08111918
H	0.09818323	4.37618446	-0.01708550
C	-1.77369297	-1.25100720	-0.55478090
H	1.65219164	2.66278052	0.82465810
C	1.15830159	0.13867025	-1.69710433
C	1.81977165	1.25488698	-1.14201224
C	2.01639962	-1.04209292	-1.51451755
H	1.80315113	2.23078680	-1.60903895
H	0.40913481	0.16210221	-2.47148252
O	1.87235427	-2.18357182	-1.90933156
C	3.15630198	0.76463604	-0.63928795
O	4.06303692	1.41913724	-0.16930176
N	3.15089130	-0.61022848	-0.79310763
C	4.22607136	-1.48539817	-0.36290056
H	4.15987682	-1.68396187	0.70998752
H	4.13377380	-2.42208529	-0.91007853
H	5.18581915	-1.01532304	-0.57801718
C	-1.16702020	-2.59775448	-0.97398227
H	-1.96170902	-3.19447112	-1.42808211
H	-0.37222752	-2.45957613	-1.70567977
H	-0.75059748	-3.17078304	-0.14681824
H	-2.26433349	-0.86867863	-1.44660640
N	-2.86987400	-1.42651784	0.41235656
H	-2.63760734	-1.62646353	1.37237239
C	-4.18610048	-1.34539008	0.06689796
O	-4.55856800	-1.08775771	-1.07181001
C	-5.17561150	-1.58024395	1.19303560
H	-5.89226580	-2.33794332	0.87195414
H	-4.71120596	-1.89770925	2.12809825
H	-5.73042870	-0.65551692	1.36741817

S37. MEC(O)NH - *SYN* APPROACH α - PRODUCT

S37.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.7294	Debye
Energy	:	-1225.24824609	a.u.
Number of imaginary frequencies	:	0	

S37.2. Cartesian Co-ordinates (XYZ format)

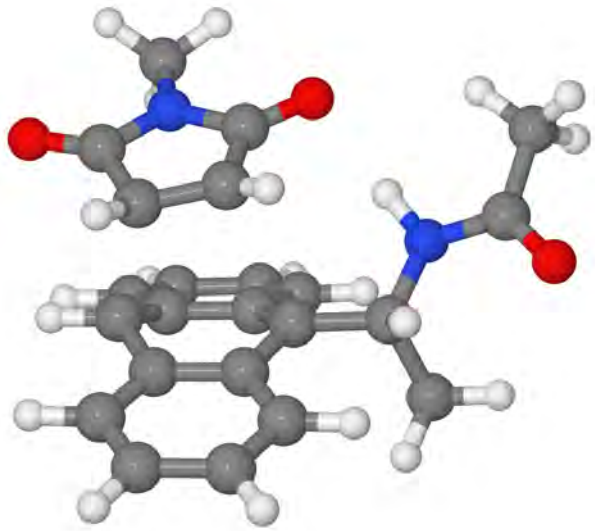
50

C	-4.19964218	0.38177660	-0.77188832
C	-3.00476885	1.00607085	-0.40530184
C	-1.84647357	0.25153109	-0.20490593
C	-1.91355276	-1.13171089	-0.42050001
C	-3.09836578	-1.75722146	-0.78857881
C	-4.25467062	-0.99606884	-0.95426828
C	-0.44129309	0.77956104	0.21208709
C	-0.57679832	-1.81398273	-0.31173110
C	0.00729778	-1.49526536	1.04693747
C	0.06514824	-0.12193166	1.35244560
C	0.66053391	0.27778468	2.54744458
H	0.77708286	1.32559657	2.78408694
C	1.13582110	-0.67812407	3.44812775
C	1.04137337	-2.03531456	3.15517545
C	0.48643470	-2.44517064	1.94261897
H	-5.08958626	0.98439896	-0.91286063
H	-3.01163459	2.07938790	-0.27914155
H	-3.11498785	-2.82949543	-0.95234007
H	-5.18655825	-1.47414541	-1.23361158

H	1.58565485	-0.35425743	4.37975740
H	1.40868819	-2.77221036	3.86020446
H	0.43109509	-3.49937844	1.69289470
C	-0.55383879	2.31418681	0.46862203
H	-0.62648606	-2.88484526	-0.50740731
C	0.53176129	0.37528419	-0.99257314
H	0.36755675	1.05723357	-1.83146334
C	0.28640786	-1.09871960	-1.40994036
H	-0.23159128	-1.18792367	-2.36537004
C	2.04647565	0.38398415	-0.68550426
C	1.65388024	-1.73470294	-1.54473448
O	1.90798593	-2.85064363	-1.93286324
O	2.72895122	1.25904822	-0.18621443
C	-1.34974897	2.69334769	1.73800361
H	-2.21437407	2.04956269	1.89821935
H	-0.72558063	2.64852309	2.62886214
H	-1.69452500	3.72254372	1.62796450
N	2.59619331	-0.81114841	-1.10563326
C	4.02195692	-1.09853876	-1.00482583
H	4.18751431	-2.08343506	-1.43603897
H	4.59196186	-0.34638292	-1.55044365
H	4.33281469	-1.09062016	0.04069304
H	-1.11390007	2.70866632	-0.38259271
N	0.71651453	3.03596091	0.43596664
H	1.58596075	2.51409769	0.46679309
C	0.75780660	4.33342600	0.02858924
O	-0.24853450	4.98299980	-0.23860462
C	2.14635086	4.94456387	-0.04935128
H	2.22750044	5.50633287	-0.98106050
H	2.26662564	5.65361834	0.77391762
H	2.94578147	4.20402050	0.00268769

S38. MEC(O)NH - *SYN* APPROACH α - TS

S38.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	3.7294	Debye
Energy	:	-1225.19621742	a.u.
Number of imaginary frequencies	:	1	

S38.2. Cartesian Co-ordinates (XYZ format)

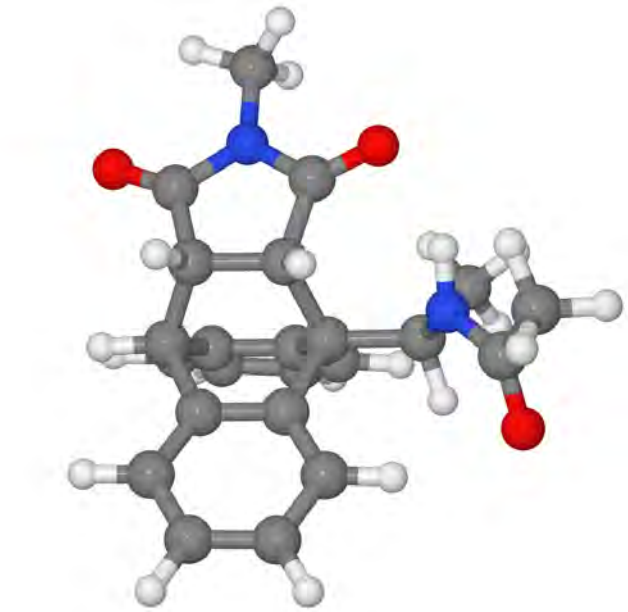
50

C	0.55660617	-4.33412838	-0.74159831
C	-0.24136490	-3.29592705	-0.30514190
C	0.31333280	-2.02615356	-0.00244747
C	1.70921803	-1.85543120	-0.19353312
C	2.50135922	-2.91473150	-0.67164528
C	1.93730450	-4.14812231	-0.92768496
C	-0.45940924	-0.88426280	0.45470366
C	2.23919821	-0.52674013	-0.00221952
C	1.63193357	0.27365667	1.03304422
C	0.23016363	0.12344529	1.23253989
C	-0.40767154	1.00035012	2.14737868
H	-1.47614992	0.94242567	2.29425383
C	0.32259181	1.92817259	2.86118865
C	1.71111166	2.05140185	2.67279887
C	2.35160184	1.24668670	1.75212538
H	0.11128151	-5.30156565	-0.94246101
H	-1.29824400	-3.48093677	-0.17598712
H	3.56302476	-2.75233650	-0.82293820
H	2.55402136	-4.97018337	-1.27190650

H	-0.18222302	2.56968617	3.57437158
H	2.27372336	2.77960706	3.24536633
H	3.41685677	1.34885240	1.57798529
C	-1.97174871	-1.08057010	0.55240059
H	3.30610061	-0.39625180	-0.15621905
C	0.10511103	0.38481188	-1.63085842
H	-0.60332763	-0.26256862	-2.12107325
C	1.51327026	0.29175329	-1.69434273
H	2.03000736	-0.37110615	-2.37453556
C	-0.23803963	1.78263831	-1.31652582
C	2.05096650	1.69078076	-1.55974019
O	3.19653225	2.07108903	-1.65733397
O	-1.33156431	2.29457498	-1.11977494
C	-2.36692524	-1.71727645	1.90661192
H	-1.83298719	-2.65750766	2.05803537
H	-2.13946438	-1.05984771	2.74544406
H	-3.43702912	-1.92134464	1.89159286
N	0.96121633	2.49961209	-1.25477397
C	1.06125808	3.90506577	-0.90163249
H	1.81332958	4.37861729	-1.53188753
H	0.08791565	4.36479950	-1.06227064
H	1.34777915	4.02156782	0.14696926
H	-2.26773119	-1.79200673	-0.22027892
N	-2.73652840	0.14047045	0.28137919
H	-2.24147177	0.96793455	-0.03604468
C	-4.05001545	0.04765605	-0.08341040
O	-4.67494535	-1.00640380	-0.05355146
C	-4.69967937	1.35741115	-0.49206698
H	-5.35552979	1.16928256	-1.34286118
H	-5.32221222	1.71351981	0.33350277
H	-3.97463560	2.13054657	-0.74730879

S39. MEC(O)NH - *SYN* APPROACH β - PRODUCT

S39.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C	
Formula	:	$C_{23}H_{22}N_2O_3$	
Charge	:	0	
Multiplicity	:	1	
Dipole	:	2.5432	Debye
Energy	:	-1225.24542527	a.u.
Number of imaginary frequencies	:	0	

S39.2. Cartesian Co-ordinates (XYZ format)

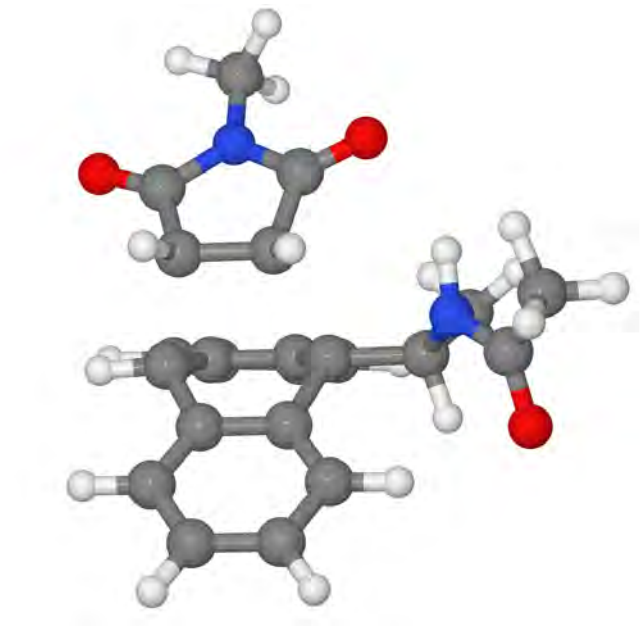
50

C	-4.11271286	0.52790481	-0.65254718
C	-2.87404609	1.11601603	-0.37350917
C	-1.73773515	0.31752062	-0.27700949
C	-1.85655856	-1.07282043	-0.46056810
C	-3.08627343	-1.65156686	-0.74472463
C	-4.22280264	-0.84537429	-0.84094739
C	-0.29071116	0.78493685	0.02372090
C	-0.55522549	-1.83499134	-0.29538995
C	0.00319306	-1.44507861	1.05296624
C	0.12638696	-0.05659293	1.25029135
C	0.49295235	0.39609635	2.51875186
H	0.53816193	1.44926345	2.74557519
C	0.78998166	-0.51193988	3.53796005
C	0.72173500	-1.88185787	3.30992508
C	0.31580707	-2.34938240	2.06071401
H	-4.99333668	1.15680206	-0.72052830
H	-2.82208610	2.18922758	-0.24107532
H	-3.16158843	-2.72560620	-0.87964386
H	-5.18732023	-1.29172063	-1.05534256

H	1.07082736	-0.13702673	4.51568317
H	0.96034157	-2.58190656	4.10239935
H	0.22390169	-3.41387606	1.87470984
C	-0.15669273	2.34125566	0.17730473
H	-0.68000984	-2.91264772	-0.39646760
C	0.49354216	0.25343475	-1.26283503
H	0.02611185	0.74173969	-2.11708975
C	0.40634698	-1.27976310	-1.37566745
H	0.05519247	-1.58345890	-2.36564541
C	1.98359525	0.54538012	-1.33774114
C	1.84172082	-1.77074122	-1.23833799
O	2.22612977	-2.91398764	-1.17276347
O	2.51008248	1.62811756	-1.50256085
C	1.12306631	2.88139844	0.87899935
H	0.89255732	3.24057174	1.88303089
H	1.92536545	2.15161514	0.95341718
H	1.50937414	3.73102307	0.31672400
N	2.67646480	-0.65058893	-1.24369335
C	4.13124561	-0.73079395	-1.23756218
H	4.40507603	-1.77704978	-1.35694683
H	4.53467751	-0.13482857	-2.05631852
H	4.52843952	-0.35330787	-0.29374689
H	-1.01764977	2.68156195	0.75081974
N	-0.28911915	2.99417806	-1.13126230
H	0.53134859	2.93882537	-1.72111166
C	-1.18213642	3.99521565	-1.38142276
O	-2.08708501	4.29657698	-0.61207426
C	-1.00289643	4.70927811	-2.70871735
H	-1.93633354	4.63742399	-3.27018261
H	-0.81945521	5.76796055	-2.51251698
H	-0.18816411	4.31099510	-3.31541467

S40. MEC(O)NH - *SYN* APPROACH β - TS

S40.1. General Information



SMILES	: CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O	
Formula	: $C_{23}H_{22}N_2O_3$	
Charge	: 0	
Multiplicity	: 1	
Dipole	: 3.8420	Debye
Energy	: -1225.19621737	a.u.
Number of imaginary frequencies	: 1	

S40.2. Cartesian Co-ordinates (XYZ format)

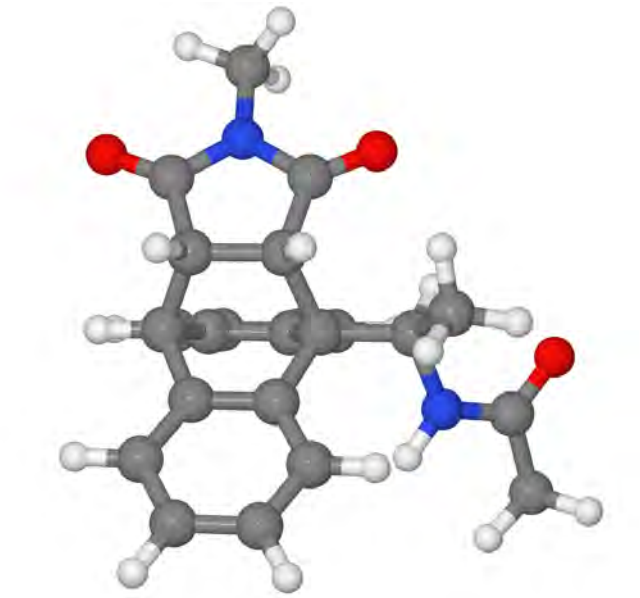
50

C	2.15449333	3.80950451	-0.31246763
C	2.09959221	2.50691128	0.14068905
C	0.87390304	1.79368508	0.16589895
C	-0.28340417	2.45694852	-0.31873432
C	-0.20223114	3.77286577	-0.80860150
C	0.99943805	4.45157862	-0.79115832
C	0.73574233	0.42122281	0.62120211
C	-1.49658179	1.67991793	-0.40420005
C	-1.70906782	0.68937373	0.62285900
C	-0.56063044	0.00609412	1.11432648
C	-0.76374620	-1.06609046	2.02089810
H	0.08098012	-1.63318706	2.38340759
C	-2.03234196	-1.39335692	2.45360708
C	-3.15768552	-0.69553649	1.97894955
C	-2.99596524	0.31915042	1.05716312
H	3.09934878	4.34020233	-0.29823071
H	3.01087761	2.05007291	0.49952120
H	-1.09938180	4.25065088	-1.18706703
H	1.05457640	5.47427940	-1.14563739

H	-2.16097045	-2.19919658	3.16710949
H	-4.14788628	-0.95831287	2.33264112
H	-3.85666847	0.84790838	0.66328865
C	2.02165794	-0.28954479	1.04129219
H	-2.37926888	2.18673992	-0.78237635
C	0.06261488	-0.31692016	-1.67670083
H	1.10355651	-0.20338789	-1.93135107
C	-0.98558754	0.57065934	-2.00694180
H	-0.86193377	1.40128767	-2.68799067
C	-0.52686030	-1.65235937	-1.47755933
C	-2.23131061	-0.25989768	-2.15803862
O	-3.33015323	0.08926974	-2.52831411
O	0.00475265	-2.69872975	-1.13246918
C	2.37601542	0.01997542	2.51576591
H	2.44719982	1.09785533	2.67438936
H	1.62884164	-0.37489453	3.20380497
H	3.34231901	-0.43090507	2.73928833
N	-1.89528763	-1.54522431	-1.74593830
C	-2.84914637	-2.63075781	-1.59825051
H	-3.38802671	-2.54648829	-0.65079969
H	-3.56356215	-2.59239030	-2.41999602
H	-2.29940987	-3.56990290	-1.61775219
H	2.83803868	0.11080343	0.43795037
N	2.00335479	-1.73148036	0.77718884
H	1.21922970	-2.12595797	0.26721618
C	3.18185663	-2.41798234	0.69494998
O	4.26376629	-1.91707289	0.97962242
C	3.05461788	-3.86778426	0.26320136
H	2.10462022	-4.08422613	-0.22591557
H	3.87985826	-4.10357189	-0.40967193
H	3.15336013	-4.50703382	1.14498353

S41. MEC(O)NH - *SYN* APPROACH γ - PRODUCT

S41.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C
Formula	:	$C_{23}H_{22}N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.9657 Debye
Energy	:	-1225.25354141 a.u.
Number of imaginary frequencies	:	0

S41.2. Cartesian Co-ordinates (XYZ format)

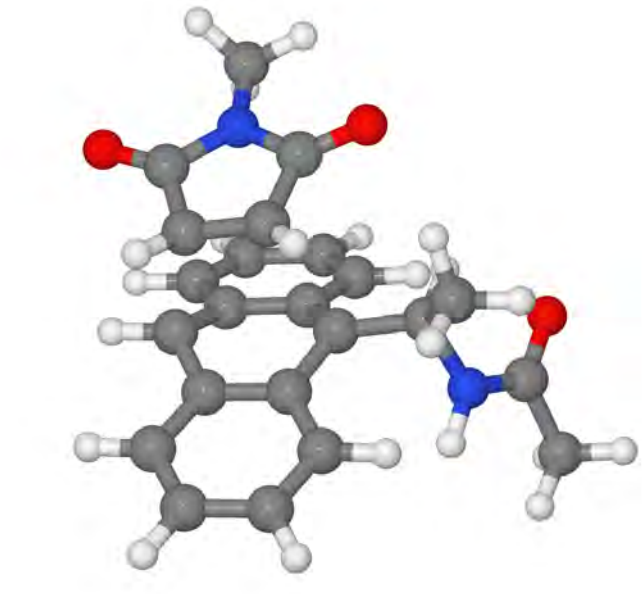
50

C	-4.39981651	0.14378646	-0.61952168
C	-3.20686388	0.85283619	-0.44951889
C	-1.99993908	0.17086814	-0.28387633
C	-2.01266456	-1.23478234	-0.31506473
C	-3.19711709	-1.93919742	-0.49108624
C	-4.39972878	-1.24656618	-0.63793445
C	-0.58992797	0.77780855	-0.08942874
C	-0.64547962	-1.86361456	-0.17917056
C	-0.00750382	-1.32044828	1.07959104
C	0.03155572	0.08187071	1.13791573
C	0.65904826	0.70008194	2.21879435
H	0.73477262	1.77740455	2.27869010
C	1.20966554	-0.07732172	3.24044752
C	1.14984238	-1.46717060	3.18484020
C	0.54736811	-2.09341908	2.09352231
H	-5.32899475	0.68887323	-0.74063504
H	-3.24459720	1.93346715	-0.45166302
H	-3.18233657	-3.02375388	-0.51297784
H	-5.32778788	-1.79092419	-0.76944810

H	1.68909705	0.41126969	4.08108997
H	1.57859492	-2.06292987	3.98259997
H	0.51586235	-3.17560148	2.02844286
C	-0.52890426	2.32512665	0.00258633
H	-0.67531437	-2.95262122	-0.19821954
C	0.23542495	0.22952093	-1.33023787
H	-0.17062828	0.67379528	-2.23941541
C	0.17950755	-1.31419992	-1.38673460
H	-0.26933405	-1.67515421	-2.31445074
C	1.72941244	0.55089200	-1.27939188
C	1.63014865	-1.77334344	-1.35693622
O	2.03225017	-2.91396451	-1.37793744
O	2.25172019	1.64249146	-1.24588835
C	-0.82177538	3.08605313	-1.30238056
H	-0.01371878	2.92905021	-2.01792789
H	-1.76615238	2.80094624	-1.76843464
H	-0.85091597	4.15305901	-1.07752240
N	2.43904710	-0.64385223	-1.30246723
C	3.89428473	-0.69557738	-1.25690937
H	4.19216299	-1.73159337	-1.40421176
H	4.31061363	-0.06502202	-2.04276276
H	4.25433683	-0.34027743	-0.29008478
H	0.49160072	2.59518552	0.27617064
N	-1.37773430	2.79154181	1.10760069
H	-2.15310454	2.22237849	1.40527475
C	-1.07449853	3.90430522	1.83254755
O	-0.09838396	4.60243368	1.59018469
C	-2.02790761	4.22867298	2.96956706
H	-1.46508825	4.23494291	3.90535402
H	-2.42080259	5.23588276	2.81732273
H	-2.86163235	3.52999258	3.05886698

S42. MEC(O)NH - *SYN* APPROACH γ - TS

S42.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{22}N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	6.1302 Debye
Energy	:	-1225.19273631 a.u.
Number of imaginary frequencies	:	1

S42.2. Cartesian Co-ordinates (XYZ format)

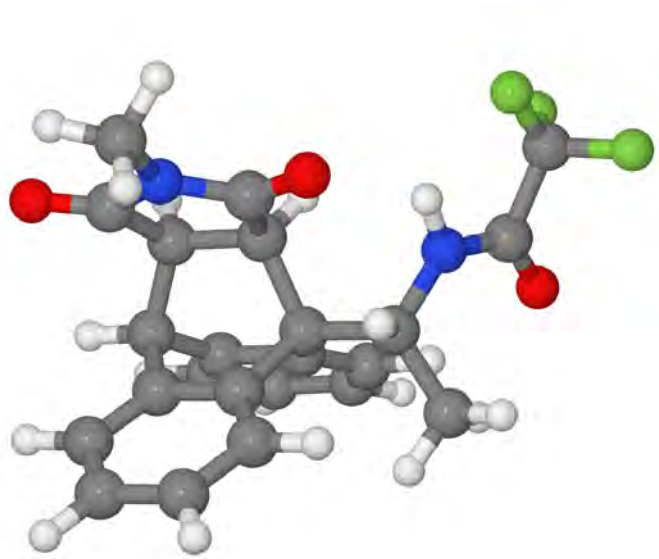
50

C	2.04643893	3.64596224	-0.54235166
C	1.98899853	2.26754069	-0.61197400
C	0.86004609	1.55618048	-0.13494034
C	-0.21425477	2.31388617	0.40747431
C	-0.15414669	3.72024131	0.43165657
C	0.96750504	4.38246155	-0.02446927
C	0.70664370	0.11280301	-0.18617129
C	-1.38076639	1.58952999	0.83763009
C	-1.17791593	0.27886078	1.38538933
C	-0.11444753	-0.49437630	0.84132916
C	0.04573882	-1.82618296	1.30475569
H	0.84402835	-2.45047975	0.92602617
C	-0.79029047	-2.33549452	2.27669597
C	-1.84293318	-1.56328905	2.80406499
C	-2.04393148	-0.27782345	2.34952450
H	2.93265676	4.16236925	-0.89289600
H	2.83601141	1.74065888	-1.02789938
H	-0.99463010	4.27559042	0.83402437
H	1.02013814	5.46395826	0.02010816

H	-0.63173640	-3.34523344	2.63789105
H	-2.49234056	-1.98023140	3.56522346
H	-2.86008692	0.32338420	2.73353601
C	1.75192368	-0.77505147	-0.87498337
H	-2.21551204	2.16617608	1.22328329
C	-1.13507950	0.35220444	-1.75348091
H	-0.44473210	0.73884851	-2.48342967
C	-2.10683060	1.09977293	-1.07128227
H	-2.35413361	2.12516856	-1.30544889
C	-1.58568704	-1.05479920	-1.81083477
C	-3.22671437	0.15969029	-0.72960877
O	-4.29353571	0.41359913	-0.21243766
O	-1.05817652	-2.01121306	-2.34387040
C	2.03828263	-0.50508738	-2.36277938
H	1.17061508	-0.79384691	-2.95592046
H	2.29283309	0.52972478	-2.59025431
H	2.87265086	-1.13880515	-2.67056870
N	-2.80420732	-1.10902524	-1.11320961
C	-3.55782413	-2.32682753	-0.87387490
H	-3.11724949	-3.11396527	-1.48333406
H	-3.50748706	-2.61088133	0.17990819
H	-4.60127974	-2.17558742	-1.15233374
H	1.38739979	-1.79868996	-0.84094507
N	2.97903705	-0.79504758	-0.06232228
H	3.38588476	0.07989664	0.22698522
C	3.54899025	-1.94969106	0.38887414
O	3.08928871	-3.05788398	0.14430119
C	4.79889011	-1.77480316	1.23204553
H	4.59512615	-2.14825392	2.23811412
H	5.59280729	-2.39142323	0.80726302
H	5.14343023	-0.74151766	1.29912817

S43. $CF_3C(O)NH$ - *ANTI* APPROACH α - PRODUCT

S43.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.4268 Debye
Energy	:	-1523.05172067 a.u.
Number of imaginary frequencies	:	0

S43.2. Cartesian Co-ordinates (XYZ format)

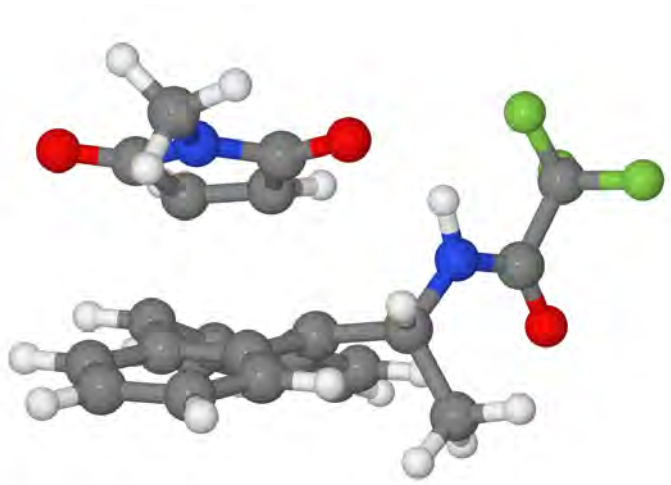
50

C	-1.51089621	-0.23590690	3.27986860
C	-0.63015580	0.42707008	2.42199302
C	-0.19906989	-0.18697140	1.24462271
C	-0.69492793	-1.46324253	0.93203229
C	-1.57846034	-2.11996675	1.78104985
C	-1.98131621	-1.50729454	2.96704364
C	0.74412107	0.40185079	0.17025800
C	-0.22145309	-1.99367571	-0.39847910
C	1.28907430	-1.93422985	-0.41455844
C	1.82065010	-0.66154146	-0.13536493
C	3.19781256	-0.47351572	-0.23628236
H	3.64282584	0.50207442	-0.10872653
C	4.02899981	-1.55263758	-0.55206609
C	3.49780011	-2.81622910	-0.78588110
C	2.11625934	-3.00448108	-0.73080474
H	-1.82669103	0.25000975	4.19594097
H	-0.29533505	1.41749358	2.69896412
H	-1.95389748	-3.10160518	1.51369095
H	-2.66336250	-2.01711464	3.63766861

H	5.09909058	-1.39257395	-0.61947948
H	4.15030718	-3.64821792	-1.02521884
H	1.68476462	-3.97773623	-0.93986094
C	1.20926130	1.84275985	0.56788999
H	-0.60964811	-2.98835206	-0.61514550
C	-0.10958003	0.42725426	-1.17451537
C	-0.68566197	-0.97071356	-1.48454070
C	-1.32819104	1.33987272	-1.13486683
H	-0.37222046	-1.32944834	-2.46732068
H	0.54544711	0.77893478	-1.97211397
O	-1.33373499	2.54831171	-0.98512322
C	-2.19568276	-0.77968955	-1.51839173
O	-3.03855062	-1.62599242	-1.69461572
N	-2.46464133	0.57804418	-1.32004666
C	-3.80967450	1.13978648	-1.31484604
H	-3.85015631	1.99955535	-1.98336911
H	-4.49288464	0.36312309	-1.65193379
H	-4.08249807	1.45836222	-0.30741933
C	2.21815944	1.94120955	1.72213924
H	2.21808052	2.96351647	2.10825920
H	1.92571342	1.27203178	2.53056908
H	3.23329210	1.70049071	1.42944658
H	0.29535457	2.32410264	0.91612154
N	1.56910503	2.67991400	-0.59397864
H	0.76141793	3.09543872	-1.04649997
C	2.78422880	3.01387239	-1.05943465
O	3.88063836	2.64992476	-0.67527074
C	2.74515271	3.99827266	-2.26194215
F	1.49242413	4.36682892	-2.62173843
F	3.42637801	5.11521721	-1.96805596
F	3.31936097	3.43065238	-3.33499479

S44. $CF_3C(O)NH$ - *ANTI* APPROACH α - TS

S44.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.8479 Debye
Energy	:	-1522.99491500 a.u.
Number of imaginary frequencies	:	1

S44.2. Cartesian Co-ordinates (XYZ format)

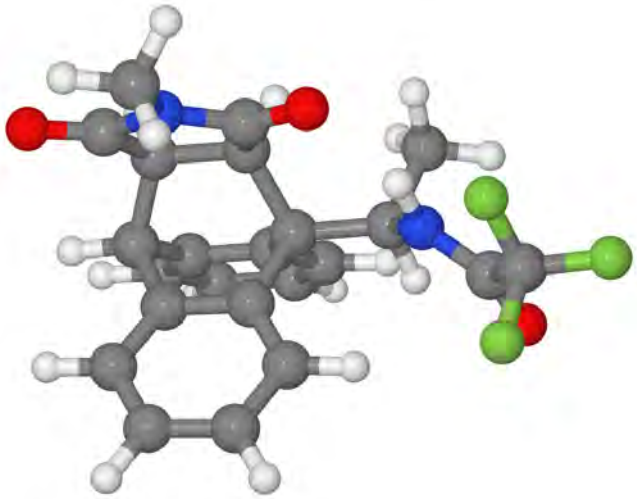
50

C	3.28060031	-0.84831405	2.63226438
C	1.96346426	-0.54094201	2.36235046
C	1.61821067	0.29506457	1.26828659
C	2.67427039	0.77161694	0.44326743
C	4.01072264	0.41337520	0.71417487
C	4.31471729	-0.37167203	1.80527639
C	0.26230982	0.65231711	0.90307122
C	2.30358887	1.53022194	-0.71808177
C	1.13788557	2.37099338	-0.61417598
C	0.06998616	1.90909672	0.20458508
C	-1.12623465	2.66388440	0.22713709
H	-1.97124362	2.34352303	0.81958258
C	-1.23312891	3.83414054	-0.50001556
C	-0.17176601	4.28399563	-1.30358791
C	0.99425006	3.54788280	-1.37165439
H	3.51974702	-1.46228433	3.49290586
H	1.20186913	-0.92538100	3.02641296
H	4.79439783	0.77307487	0.05768558
H	5.34534979	-0.62256837	2.02717638

H	-2.15087867	4.40867138	-0.44910613
H	-0.27065921	5.20338917	-1.86891723
H	1.81710196	3.87560773	-1.99795628
C	-0.86208308	-0.04584329	1.68626320
H	3.10766768	1.86759627	-1.36445510
C	0.31079781	-0.45335531	-1.25932491
C	1.47040200	0.02367087	-1.89154327
C	0.56866789	-1.81015348	-0.76078200
H	1.45751488	0.64692289	-2.77439857
H	-0.69384962	-0.11453491	-1.44632339
O	-0.19529112	-2.56320596	-0.17232671
C	2.48009706	-1.08892274	-1.82912314
O	3.58857441	-1.13357902	-2.31341219
N	1.89782524	-2.10906744	-1.07135630
C	2.58129549	-3.33335876	-0.69114774
H	1.82881391	-4.04790878	-0.36206451
H	3.12440825	-3.72895002	-1.54955792
H	3.28713894	-3.14681268	0.12171290
C	-1.23779142	0.67375970	2.99340916
H	-1.97524238	0.08525351	3.54254556
H	-0.34201992	0.76424539	3.61035633
H	-1.64649570	1.66684771	2.83348012
H	-0.45403436	-1.01479590	1.97056174
N	-2.01248622	-0.43528354	0.84705299
H	-1.84053493	-1.29227436	0.32664514
C	-3.25360370	0.07696191	0.82801336
O	-3.68033886	1.06238234	1.40227938
C	-4.24742889	-0.71467739	-0.06635200
F	-5.22669029	-1.23989058	0.68733937
F	-4.81015635	0.10732902	-0.96465713
F	-3.66950035	-1.72965682	-0.74980927

S45. $CF_3C(O)NH$ - *ANTI* APPROACH β - PRODUCT

S45.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.5246 Debye
Energy	:	-1523.05599356 a.u.
Number of imaginary frequencies	:	0

S45.2. Cartesian Co-ordinates (XYZ format)

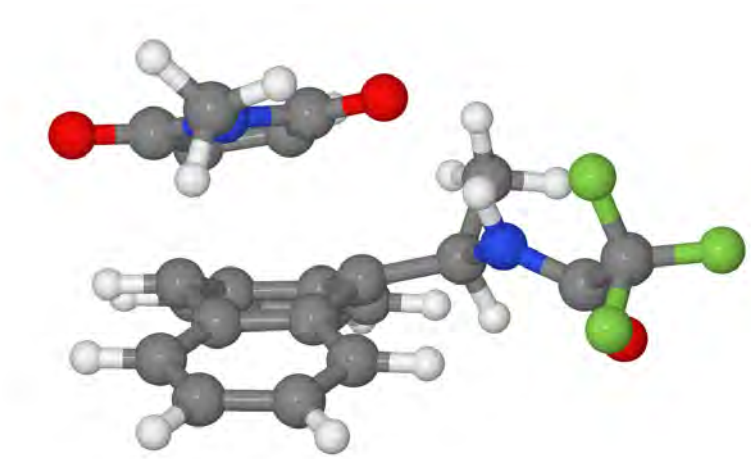
50

C	-0.87278509	0.23292199	3.39423800
C	-0.32772526	0.89203614	2.28900218
C	-0.00818719	0.17619185	1.13660944
C	-0.20445246	-1.21885777	1.12795436
C	-0.76111537	-1.86890161	2.22267056
C	-1.10497987	-1.13774312	3.36024547
C	0.60584223	0.70906264	-0.17515659
C	0.30229172	-1.92020798	-0.11614405
C	1.74169183	-1.49326301	-0.29958147
C	1.92080224	-0.10030417	-0.33070648
C	3.21619177	0.40682456	-0.42214710
H	3.40775800	1.47134948	-0.41389459
C	4.30629826	-0.46339059	-0.51254636
C	4.11438894	-1.84065270	-0.51063263
C	2.82323217	-2.35877299	-0.39878577
H	-1.11213291	0.80265576	4.28477335
H	-0.14595078	1.95293355	2.35738897
H	-0.90918201	-2.94302821	2.19423985
H	-1.53336501	-1.64057088	4.21966124

H	5.30790186	-0.05445533	-0.57933760
H	4.96395350	-2.51007557	-0.58116674
H	2.66197205	-3.43123984	-0.37299106
C	0.89108300	2.24139023	-0.25414741
H	0.18477865	-3.00200891	-0.06030460
C	-0.34490207	0.19289587	-1.34343588
C	-0.45599902	-1.34755540	-1.34485435
C	-1.80069482	0.65997994	-1.27256608
H	-0.04507353	-1.79074454	-2.25415444
H	0.05500996	0.55132395	-2.29296756
O	-2.21976185	1.80304968	-1.25238037
C	-1.94295776	-1.65504575	-1.30634201
O	-2.46614575	-2.74321270	-1.29840970
N	-2.63037109	-0.44151461	-1.28018951
C	-4.08396006	-0.33751261	-1.23186469
H	-4.43875504	0.28031281	-2.05693793
H	-4.48686647	-1.34470189	-1.31315196
H	-4.39638424	0.11412534	-0.28946087
C	1.31323922	2.72468567	-1.65667129
H	1.74462461	3.72428346	-1.57452404
H	2.04999399	2.07174826	-2.12428069
H	0.44423452	2.79255438	-2.31457520
H	1.69669664	2.44772196	0.45124751
N	-0.22021239	3.08987856	0.18827105
H	-1.11502445	2.96296716	-0.28033882
C	-0.01743578	4.13769865	1.00284493
O	1.02400327	4.45226145	1.55182064
C	-1.28745615	4.97110558	1.30504966
F	-1.69435680	4.73944950	2.56829786
F	-1.02842581	6.28030777	1.18876839
F	-2.32317495	4.68230534	0.48713985

S46. $CF_3C(O)NH$ - *ANTI* APPROACH β - TS

S46.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.3739 Debye
Energy	:	-1522.99085185 a.u.
Number of imaginary frequencies	:	1

S46.2. Cartesian Co-ordinates (XYZ format)

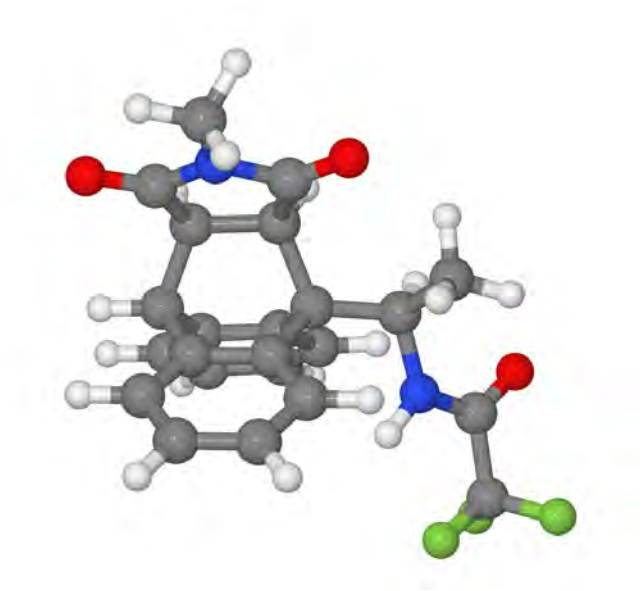
50

C	-0.42014328	-1.02414262	2.92966914
C	-0.58779854	-0.16158803	1.86728179
C	0.50118339	0.18982087	1.02532399
C	1.77407336	-0.38170710	1.33596969
C	1.90835536	-1.30076337	2.39802456
C	0.82921916	-1.61418462	3.19394946
C	0.43679807	1.08970499	-0.11211236
C	2.88774991	-0.03712993	0.50239748
C	2.89418197	1.29070985	-0.04499269
C	1.63617337	1.87816811	-0.34872332
C	1.63182104	3.20650840	-0.84320575
H	0.69737464	3.72059298	-1.02026880
C	2.81210613	3.89090109	-1.05311477
C	4.05178404	3.27311850	-0.81141865
C	4.08855486	1.98558760	-0.31765839
H	-1.26552677	-1.24183953	3.57221127
H	-1.55750465	0.27628025	1.71002221
H	2.88216901	-1.73570907	2.59145451
H	0.94406378	-2.29589176	4.02857304

H	2.77993226	4.91712570	-1.40023327
H	4.97237873	3.81571698	-0.99153960
H	5.03691912	1.50593114	-0.10100897
C	-0.87423676	1.62935925	-0.71689606
H	3.84427714	-0.49407962	0.73357195
C	1.17473865	-0.66840160	-1.72142243
C	2.42277837	-1.09754694	-1.26144791
C	0.17680448	-1.69921768	-1.38349092
H	3.36397505	-0.85338306	-1.73198581
H	1.00303972	0.03912853	-2.51258230
O	-1.02907097	-1.70551467	-1.58749473
C	2.23623037	-2.47826886	-0.70296925
O	3.07169914	-3.24434519	-0.27777341
N	0.86426950	-2.73236656	-0.74293482
C	0.23869856	-3.91809392	-0.18270238
H	0.76891214	-4.80850506	-0.52143753
H	0.25869814	-3.88408661	0.90900493
H	-0.79326791	-3.94319081	-0.52754408
C	-0.83989674	1.88460076	-2.24392247
H	-0.98639393	0.94423044	-2.77611923
H	-1.66733301	2.54781961	-2.50432181
H	0.08563685	2.34045100	-2.58836269
H	-1.09002900	2.57729888	-0.21313550
N	-2.04999590	0.79011762	-0.47182950
H	-2.01927447	-0.16008006	-0.83819813
C	-3.21868491	1.33597648	-0.08841655
O	-3.41782856	2.49795032	0.21411124
C	-4.37969255	0.31958139	0.04838533
F	-4.51621628	-0.03619216	1.34369791
F	-5.53354502	0.85984284	-0.35499778
F	-4.17840099	-0.81112832	-0.66066515

S47. $CF_3C(O)NH$ - *ANTI* APPROACH γ - PRODUCT

S47.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.3729 Debye
Energy	:	-1523.04550094 a.u.
Number of imaginary frequencies	:	0

S47.2. Cartesian Co-ordinates (XYZ format)

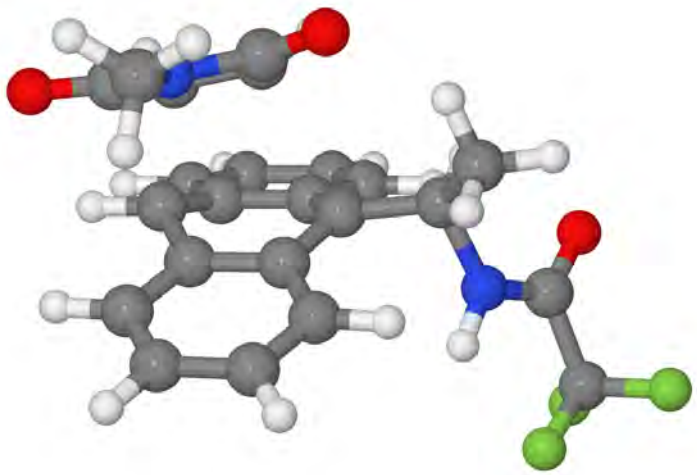
50

C	-1.04056203	1.34060836	3.13776326
C	-0.37224728	1.58413577	1.93494213
C	-0.13435869	0.54010946	1.03859317
C	-0.59840131	-0.74715686	1.36283982
C	-1.27422237	-0.98512250	2.55396223
C	-1.49043107	0.06215848	3.44971776
C	0.55873334	0.61996430	-0.33523053
C	-0.31318000	-1.79361737	0.31180191
C	1.16211486	-1.77312624	0.01044521
C	1.63074899	-0.51118362	-0.37904352
C	2.95468783	-0.39688045	-0.80766273
H	3.36373901	0.54123318	-1.15595257
C	3.79322886	-1.51427901	-0.80211604
C	3.32276893	-2.75421977	-0.38163549
C	1.99295616	-2.88706183	0.01587622
H	-1.20999968	2.16005254	3.82665491
H	-0.05391045	2.59492135	1.71956813
H	-1.63002491	-1.98409331	2.78103662
H	-2.00987601	-0.12049019	4.38323832

H	4.82107115	-1.40515971	-1.12838864
H	3.98192382	-3.61468196	-0.37419525
H	1.60158837	-3.85196018	0.32018754
C	1.24094605	1.98000336	-0.67800254
H	-0.67993402	-2.77985930	0.59400880
C	-0.54419190	0.11990997	-1.38309216
C	-0.98428357	-1.32692182	-1.01764202
C	-1.88666999	0.87723261	-1.46657550
H	-0.73176622	-2.03951812	-1.80515790
H	-0.09754775	0.15930226	-2.37941837
O	-2.09872150	2.01216340	-1.82544088
C	-2.49517250	-1.29107773	-0.88174468
O	-3.21970129	-2.21907210	-0.60246438
N	-2.91567516	0.00466899	-1.13017237
C	-4.31369543	0.41533825	-1.12212574
H	-4.57875156	0.84905893	-2.08676195
H	-4.91460896	-0.47030723	-0.92703444
H	-4.48213053	1.15901124	-0.34203723
C	0.39980653	3.23279905	-0.95638323
H	1.08797598	4.07012796	-1.08824050
H	-0.18089992	3.11499524	-1.86626995
H	-0.29647851	3.47497606	-0.15451084
H	1.82692957	1.81174672	-1.58365440
N	2.23173141	2.27243042	0.37847686
H	2.03440785	2.00506139	1.33140063
C	3.40527749	2.86570549	0.10658057
O	3.80737948	3.20903158	-0.98998690
C	4.31690645	3.09511971	1.33767200
F	4.62936640	4.39382887	1.45080197
F	3.74006462	2.71071649	2.50213480
F	5.45770311	2.40177345	1.20302963

S48. $CF_3C(O)NH$ - *ANTI* APPROACH γ - TS

S48.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	3.6592 Debye
Energy	:	-1522.98991390 a.u.
Number of imaginary frequencies	:	1

S48.2. Cartesian Co-ordinates (XYZ format)

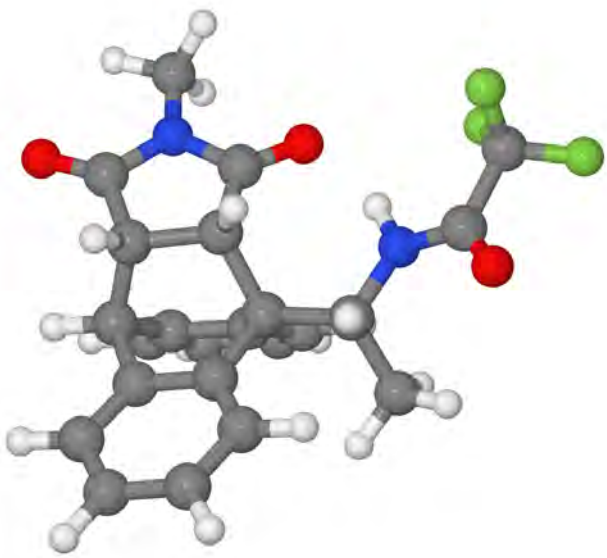
50

C	1.09962749	-2.02139926	2.68455100
C	0.32905352	-1.66422009	1.59792173
C	0.49448013	-0.40512607	0.96339881
C	1.49280417	0.46703267	1.48405755
C	2.29546809	0.06640326	2.56915760
C	2.09557509	-1.15728617	3.17397428
C	-0.28402433	0.05777718	-0.16202182
C	1.69525886	1.72192216	0.80354446
C	0.52623689	2.34835172	0.23417881
C	-0.46828616	1.48937690	-0.30514908
C	-1.56921577	2.09011459	-0.96992952
H	-2.36396194	1.48795199	-1.38856626
C	-1.67241085	3.46308303	-1.06619930
C	-0.67552370	4.29996586	-0.53465396
C	0.41944817	3.74363518	0.09478954
H	0.93295425	-2.97834420	3.16542315
H	-0.42288563	-2.35888910	1.25424731
H	3.06308389	0.74071521	2.93098617
H	2.69695783	-1.44999337	4.02653265

H	-2.53576040	3.89815545	-1.55605352
H	-0.76902217	5.37640381	-0.61888421
H	1.20161402	4.37564373	0.50149757
C	-1.30966687	-0.84444577	-0.86364144
H	2.45182562	2.37955523	1.22041726
C	1.84306800	0.24799071	-1.62019002
C	2.59726524	1.19104493	-0.89144456
C	2.52366161	-1.05531764	-1.52734482
H	2.74463058	2.20668459	-1.23371136
H	1.17518365	0.46337977	-2.43832707
O	2.26193261	-2.11258912	-2.06803846
C	3.81211472	0.46611962	-0.36463448
O	4.75369453	0.93081456	0.24142992
N	3.64089298	-0.86924446	-0.68701440
C	4.55609655	-1.92791247	-0.29948524
H	4.37432766	-2.78073144	-0.95131838
H	5.58352995	-1.58067083	-0.41024014
H	4.39038420	-2.22297883	0.73971438
C	-0.85487056	-2.20732522	-1.40194786
H	-0.00345398	-2.09223413	-2.07089567
H	-0.56472480	-2.91299939	-0.62567848
H	-1.68501079	-2.64332104	-1.96250939
H	-1.67482507	-0.29882160	-1.73014748
N	-2.49448514	-0.98388952	0.01037194
H	-2.36908174	-1.29422653	0.96262532
C	-3.74218726	-0.71549761	-0.41613892
O	-4.06502104	-0.31855315	-1.52012539
C	-4.85059881	-0.93969047	0.64352173
F	-5.73730183	-1.84246099	0.20184888
F	-4.36575794	-1.38776946	1.82742310
F	-5.50326538	0.20656626	0.88087827

S49. $CF_3C(O)NH$ - *SYN* APPROACH α - PRODUCT

S49.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.7569 Debye
Energy	:	-1523.04918556 a.u.
Number of imaginary frequencies	:	0

S49.2. Cartesian Co-ordinates (XYZ format)

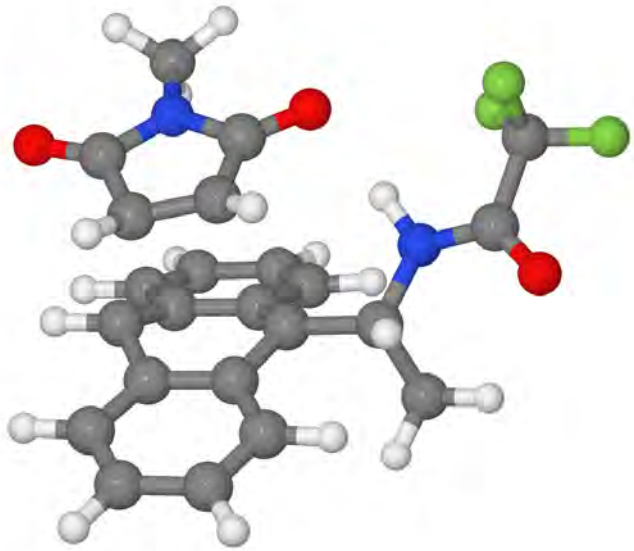
50

C	-4.20662212	0.39308223	-0.75053865
C	-3.00820518	1.01144457	-0.38561213
C	-1.84949744	0.25284183	-0.20406483
C	-1.91935062	-1.12811387	-0.43376800
C	-3.10817122	-1.74711013	-0.79973233
C	-4.26439714	-0.98233718	-0.94854116
C	-0.43867597	0.77110142	0.20638233
C	-0.58362579	-1.81525230	-0.33844107
C	0.00872571	-1.50962639	1.01980758
C	0.07269593	-0.13942920	1.33714354
C	0.67731327	0.24914907	2.53100777
H	0.79977369	1.29403210	2.77737355
C	1.15542555	-0.71561420	3.42053056
C	1.05489516	-2.06987953	3.11663961
C	0.49097371	-2.46816874	1.90442133
H	-5.09686613	0.99827778	-0.87716597
H	-3.01502967	2.08318830	-0.24525850
H	-3.12844062	-2.81749511	-0.97453690
H	-5.19892263	-1.45597279	-1.22633219

H	1.61300886	-0.40076786	4.35134649
H	1.42501855	-2.81360149	3.81286502
H	0.43157411	-3.52000213	1.64609194
C	-0.54904193	2.30209136	0.47784057
H	-0.63766479	-2.88431311	-0.54209447
C	0.52107084	0.37664619	-1.00878966
H	0.35255483	1.06356061	-1.84283829
C	0.27676076	-1.09428442	-1.43465042
H	-0.24192588	-1.17850411	-2.39007354
C	2.03251576	0.38598305	-0.70014477
C	1.64730358	-1.72502947	-1.57455182
O	1.90441835	-2.83737397	-1.96895468
O	2.70249438	1.26137304	-0.18415549
C	-1.33264446	2.66849542	1.75833464
H	-2.17074752	1.99513352	1.93265831
H	-0.69095689	2.64382553	2.63719773
H	-1.71487558	3.68476582	1.65608668
N	2.58797622	-0.80040449	-1.13012767
C	4.01503277	-1.08376300	-1.02849770
H	4.18506432	-2.06414318	-1.46805274
H	4.58278561	-0.32432601	-1.56605589
H	4.32298326	-1.08374834	0.01784107
H	-1.11107361	2.70379519	-0.36849141
N	0.72628236	3.03037715	0.44908369
H	1.60815549	2.51461983	0.44765207
C	0.72728372	4.33987474	0.14780895
O	-0.24809735	5.04158258	-0.05750588
C	2.13435769	4.97848415	0.03415269
F	2.46953082	5.12257051	-1.26427555
F	2.14424109	6.19354868	0.59745663
F	3.10214376	4.24429226	0.62230557

S50. $CF_3C(O)NH$ - *SYN* APPROACH α - TS

S50.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	6.3696 Debye
Energy	:	-1522.99527073 a.u.
Number of imaginary frequencies	:	1

S50.2. Cartesian Co-ordinates (XYZ format)

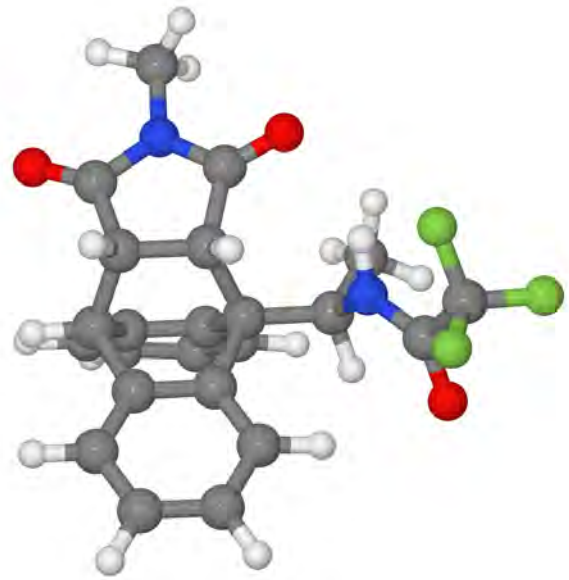
50

C	2.20668936	-4.04354143	-0.75417125
C	1.18395400	-3.23854494	-0.29389858
C	1.39974761	-1.86170232	-0.03294735
C	2.69372129	-1.33896720	-0.28996712
C	3.71491551	-2.16691828	-0.79111993
C	3.48221397	-3.50991225	-1.00606406
C	0.37586114	-0.94233954	0.43764633
C	2.86721015	0.08352420	-0.13585265
C	2.11556244	0.72656947	0.91143137
C	0.81196034	0.22119392	1.18167138
C	0.00756081	0.92496288	2.11369538
H	-1.00065017	0.59620064	2.31907153
C	0.49999151	2.02963209	2.77795053
C	1.79785252	2.50636077	2.51985264
C	2.58594370	1.87291873	1.58065271
H	2.02099848	-5.09800863	-0.92192525
H	0.21965243	-3.69222546	-0.11365995
H	4.69007778	-1.73711252	-0.99274623
H	4.27695656	-4.15144730	-1.36832368

H	-0.12404900	2.53576875	3.50536752
H	2.17381835	3.37137175	3.05358076
H	3.57899261	2.24419618	1.35365927
C	-1.02131259	-1.53591883	0.62138873
H	3.85000563	0.48916715	-0.35518402
C	0.47466969	0.34921050	-1.65222323
H	-0.06979962	-0.46266362	-2.10630512
C	1.84579599	0.63383770	-1.82009614
H	2.48319340	0.10555590	-2.51483655
C	-0.20383991	1.61652052	-1.31181562
C	2.00089121	2.12603426	-1.73512447
O	2.99361920	2.79369283	-1.91889882
O	-1.37241912	1.81643903	-1.01334953
C	-1.16210186	-2.22090411	2.00120425
H	-1.08559453	-1.50308049	2.81712008
H	-2.12860084	-2.72094369	2.05475020
H	-0.37686798	-2.96723437	2.13178635
N	0.75651586	2.62654257	-1.35726297
C	0.50284576	4.01633835	-1.01642835
H	1.11112058	4.65176392	-1.65872979
H	-0.55490905	4.22006226	-1.17237604
H	0.75765651	4.21169043	0.02850052
H	-1.15376723	-2.31371641	-0.13192640
N	-2.11078858	-0.57466108	0.38451526
H	-1.89562261	0.36990333	0.06047365
C	-3.35631108	-1.04014242	0.16409366
O	-3.72008705	-2.20000243	0.23263386
C	-4.38969231	0.04932483	-0.22725379
F	-4.43968725	0.18036509	-1.56866360
F	-5.61114931	-0.29431698	0.19727845
F	-4.09716988	1.25894117	0.29098877

S51. $CF_3C(O)NH$ - *SYN* APPROACH β - PRODUCT

S51.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.0061 Debye
Energy	:	-1523.04566634 a.u.
Number of imaginary frequencies	:	0

S51.2. Cartesian Co-ordinates (XYZ format)

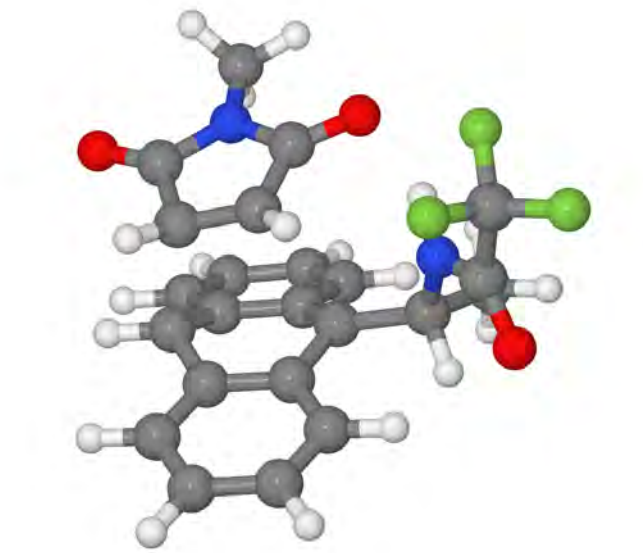
50

C	-4.07721138	0.55976808	-0.67176038
C	-2.82529688	1.13394451	-0.42510250
C	-1.69983137	0.32140517	-0.32414469
C	-1.84595609	-1.07277024	-0.45228079
C	-3.08809876	-1.63820338	-0.70568520
C	-4.21138239	-0.81589824	-0.81986123
C	-0.23874830	0.76753485	-0.04972341
C	-0.56051838	-1.85436296	-0.25029939
C	-0.00300251	-1.41579998	1.08483458
C	0.13812132	-0.02275072	1.22249091
C	0.44369057	0.48810732	2.48562646
H	0.46644688	1.55172622	2.67219853
C	0.69371915	-0.37455985	3.55551314
C	0.63177139	-1.75315678	3.38342023
C	0.26552919	-2.27508211	2.14330101
H	-4.94808960	1.20122409	-0.74444836
H	-2.76352024	2.20712852	-0.30499479
H	-3.18392015	-2.71485233	-0.79953367
H	-5.18526220	-1.25195587	-1.01101339

H	0.93032634	0.04195940	4.52791929
H	0.83632785	-2.41794729	4.21470451
H	0.16415587	-3.34589744	2.00528359
C	-0.07406438	2.31794572	0.07417279
H	-0.70908022	-2.93234515	-0.30241147
C	0.52970248	0.16589284	-1.31563830
H	0.06151425	0.61531419	-2.19178796
C	0.41209283	-1.37086642	-1.35054624
H	0.05994914	-1.71518266	-2.32678318
C	2.02742910	0.41403285	-1.43995500
C	1.83612037	-1.88436198	-1.18112779
O	2.19262409	-3.02966905	-1.04161155
O	2.57529974	1.46165204	-1.71663785
C	1.26950645	2.87825727	0.60297650
H	1.74850535	2.23878908	1.33835793
H	1.97587192	3.01347661	-0.21155412
H	1.08357549	3.85140038	1.06330967
N	2.69453764	-0.78643805	-1.26063192
C	4.14755011	-0.89855742	-1.27399993
H	4.39631844	-1.95770729	-1.28223050
H	4.54644823	-0.40683216	-2.16154146
H	4.57138300	-0.42757833	-0.38573700
H	-0.87131119	2.66103268	0.73361552
N	-0.32147554	2.97274399	-1.22218394
H	0.40501627	2.86367869	-1.91921806
C	-1.19934297	3.97971082	-1.38772571
O	-2.02535987	4.37277126	-0.58552259
C	-1.14879060	4.65285349	-2.78306770
F	-2.30323720	4.44866085	-3.43554783
F	-0.97017509	5.97458792	-2.65425682
F	-0.14891723	4.17813683	-3.56423163

S52. $CF_3C(O)NH$ - *SYN* APPROACH β - TS

S52.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.8928 Debye
Energy	:	-1522.98777967 a.u.
Number of imaginary frequencies	:	1

S52.2. Cartesian Co-ordinates (XYZ format)

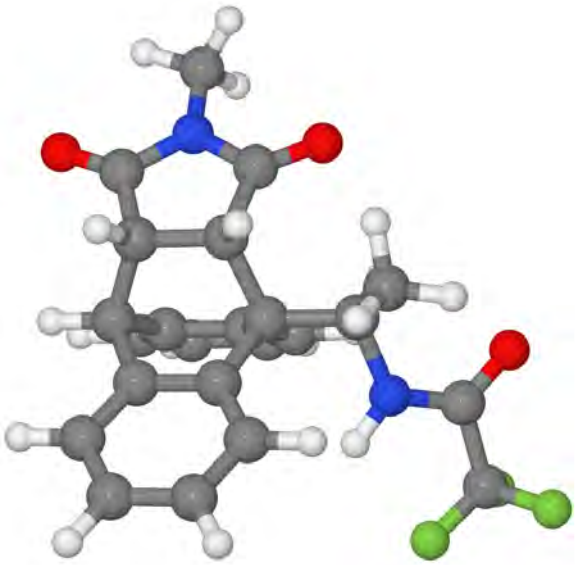
50

C	1.15356600	3.79038954	-0.71409959
C	1.09995711	2.65956879	0.07840527
C	-0.07238740	1.86378980	0.13828713
C	-1.16449785	2.25320792	-0.68365300
C	-1.08091605	3.39053869	-1.50442338
C	0.06039987	4.16747570	-1.50949907
C	-0.20564638	0.64882165	0.94067454
C	-2.30427003	1.36935604	-0.72322685
C	-2.62958002	0.68446147	0.49870360
C	-1.54932296	0.26295379	1.33507168
C	-1.90374053	-0.52820379	2.46333432
H	-1.15374553	-0.89302987	3.13733101
C	-3.21787119	-0.82493734	2.75724888
C	-4.26384592	-0.38509211	1.92911959
C	-3.96283364	0.34585601	0.80161917
H	2.05708766	4.38903904	-0.72028881
H	1.98197913	2.40368295	0.64775568
H	-1.93076456	3.65499187	-2.12452555
H	0.11507336	5.05762815	-2.12517810

H	-3.44106817	-1.40513325	3.64537024
H	-5.29288387	-0.62093407	2.17347360
H	-4.74862623	0.67714787	0.13288766
C	1.10098898	0.17926775	1.64086246
H	-3.14295363	1.67641449	-1.34058988
C	-0.36122432	-0.58809859	-1.26143241
H	0.63305324	-0.24568096	-1.48644876
C	-1.55156922	-0.10977849	-1.83963275
H	-1.56382072	0.46110311	-2.75882864
C	-0.60717702	-1.91302931	-0.69285077
C	-2.55971646	-1.22532332	-1.70769036
O	-3.68442607	-1.28053689	-2.15083981
O	0.16981572	-2.65159702	-0.09995711
C	1.08974349	-0.67448491	2.91808963
H	0.56487346	-0.17727828	3.73436880
H	0.67356950	-1.66878450	2.75540614
H	2.13000512	-0.79457504	3.22831106
N	-1.95138550	-2.21700001	-0.93885285
C	-2.62320447	-3.42211342	-0.48401123
H	-3.32390761	-3.19211650	0.32202712
H	-3.16997075	-3.87235212	-1.31289697
H	-1.86221552	-4.11008596	-0.12005620
H	1.62763107	1.09012413	1.91895020
N	1.98710787	-0.48877648	0.67246974
H	1.66734707	-1.38985240	0.31316271
C	3.26026034	-0.09765860	0.49277073
O	3.80993915	0.86611724	0.99688733
C	4.04610538	-0.95130807	-0.53465044
F	3.54662490	-2.19827247	-0.67333204
F	3.99501610	-0.36132893	-1.74751902
F	5.32957602	-1.05787826	-0.18010630

S53. $CF_3C(O)NH$ - *SYN* APPROACH γ - PRODUCT

S53.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)C(F)(F)F
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.4786 Debye
Energy	:	-1523.05465950 a.u.
Number of imaginary frequencies	:	0

S53.2. Cartesian Co-ordinates (XYZ format)

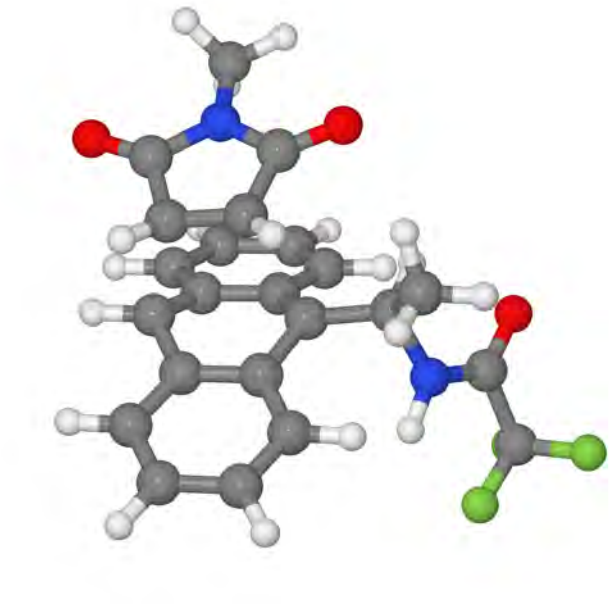
50

C	-4.36549234	0.17926495	-0.57515329
C	-3.16238499	0.86619312	-0.38670447
C	-1.96447337	0.16239694	-0.25026274
C	-1.99563646	-1.24119103	-0.32874420
C	-3.19006610	-1.92271304	-0.52420175
C	-4.38372278	-1.20923102	-0.64180249
C	-0.54488587	0.73941368	-0.03781890
C	-0.63721281	-1.89372599	-0.21484917
C	0.00696837	-1.40222192	1.06178296
C	0.06423270	-0.00317606	1.16887188
C	0.69322747	0.56835455	2.27404141
H	0.78007007	1.64143908	2.37798357
C	1.22986543	-0.25066856	3.27028155
C	1.15456367	-1.63647878	3.16453242
C	0.54856181	-2.21650505	2.04978895
H	-5.28765869	0.74060035	-0.67145246
H	-3.18921733	1.94680238	-0.35371417
H	-3.19015026	-3.00592685	-0.58259565
H	-5.31958151	-1.73628092	-0.78702778

H	1.70884669	0.20274787	4.13042021
H	1.57221913	-2.26504779	3.94259381
H	0.50285572	-3.29519916	1.94732141
C	-0.45756575	2.28125238	0.09746695
H	-0.68320203	-2.98082352	-0.26966006
C	0.27454206	0.22234859	-1.29434407
H	-0.12210030	0.70208955	-2.18948269
C	0.19681203	-1.31695533	-1.40302277
H	-0.25627667	-1.63949764	-2.34264278
C	1.77242005	0.52128232	-1.22562695
C	1.64159644	-1.79611325	-1.38923943
O	2.02846456	-2.93999267	-1.44899929
O	2.30559754	1.60543323	-1.14191365
C	-0.74650639	3.08952737	-1.17845273
H	0.06325577	2.94888735	-1.89479172
H	-1.69078970	2.82284307	-1.65412724
H	-0.76956367	4.14993477	-0.92362124
N	2.46613002	-0.67910248	-1.29568684
C	3.92075682	-0.75165266	-1.24816811
H	4.20381594	-1.79090703	-1.40124536
H	4.34862137	-0.12347182	-2.02985525
H	4.28287029	-0.40669680	-0.27855510
H	0.56639057	2.52639604	0.38159055
N	-1.30518305	2.72196031	1.22074306
H	-2.08501601	2.15233421	1.51284635
C	-1.01799130	3.82890964	1.92884254
O	-0.09190571	4.59266710	1.73619652
C	-1.98157859	4.10886621	3.10967684
F	-1.31851470	4.03076792	4.27428007
F	-2.50158787	5.33952856	3.00800228
F	-3.01405883	3.23228216	3.16896033

S54. $CF_3C(O)NH$ - *SYN* APPROACH γ - TS

S54.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)C(F)(F)F.CN1C(=O)C=CC1=O
Formula	:	$C_{23}H_{19}F_3N_2O_3$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.6268 Debye
Energy	:	-1522.99294525 a.u.
Number of imaginary frequencies	:	1

S54.2. Cartesian Co-ordinates (XYZ format)

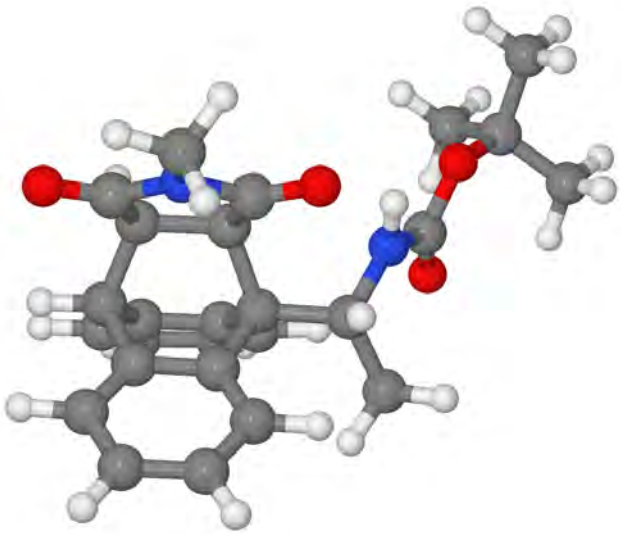
50

C	0.72837090	4.04815578	-0.45254570
C	0.90439844	2.69168758	-0.64581257
C	-0.02074157	1.75279248	-0.12622051
C	-1.13992250	2.25762367	0.59120840
C	-1.32381380	3.64536166	0.74059927
C	-0.39506939	4.53366518	0.23777805
C	0.06879260	0.31354433	-0.29766986
C	-2.10134506	1.30120730	1.07107043
C	-1.61050689	0.01411188	1.47095883
C	-0.49961880	-0.50824422	0.75124687
C	-0.05465278	-1.81642866	1.07249939
H	0.78841007	-2.25733614	0.55809969
C	-0.66591936	-2.53995800	2.07524705
C	-1.76811218	-2.01531053	2.77671647
C	-2.24484706	-0.76059532	2.46441579
H	1.46528625	4.74265766	-0.83893549
H	1.77732217	2.36377001	-1.19254637
H	-2.19528604	4.00555897	1.27653599
H	-0.52627689	5.60006762	0.37839767

H	-0.28958973	-3.52528310	2.32486749
H	-2.23854303	-2.59812641	3.56006575
H	-3.10223770	-0.34965262	2.98484635
C	1.16235399	-0.31425640	-1.17022312
H	-2.97630358	1.68367028	1.58692777
C	-1.93999028	0.31500340	-1.63763690
H	-1.42186713	0.87388688	-2.39805722
C	-2.94705963	0.81727612	-0.80116552
H	-3.39612246	1.79340315	-0.91338104
C	-2.13452458	-1.14610124	-1.77451932
C	-3.83390307	-0.33736345	-0.43561530
O	-4.86260939	-0.32545099	0.20482890
O	-1.50141907	-1.94578004	-2.43547821
C	1.23234928	0.11221189	-2.64635134
H	0.37412012	-0.30046794	-3.17608595
H	1.25910127	1.19026256	-2.79872680
H	2.13100433	-0.32104659	-3.09024024
N	-3.23721385	-1.47549331	-0.97205621
C	-3.73135090	-2.82657886	-0.77199328
H	-4.81042528	-2.85011339	-0.92688727
H	-3.23449898	-3.47183585	-1.49441016
H	-3.50860929	-3.17327857	0.23977673
H	0.99048787	-1.38737047	-1.19335961
N	2.46311307	-0.15494843	-0.48625642
H	2.72270727	0.74801242	-0.11831985
C	3.29283237	-1.19349086	-0.27089283
O	3.11149836	-2.35096335	-0.59587753
C	4.60365629	-0.82849628	0.47162852
F	5.66453266	-1.09795690	-0.30314437
F	4.67038631	0.48232892	0.81235242
F	4.71515799	-1.54564071	1.59760344

S55. tBuC(O)NH - *ANTI* APPROACH α - PRODUCT

S55.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	1.2294 Debye
Energy	:	-1418.47780922 a.u.
Number of imaginary frequencies	:	0

S55.2. Cartesian Co-ordinates (XYZ format)

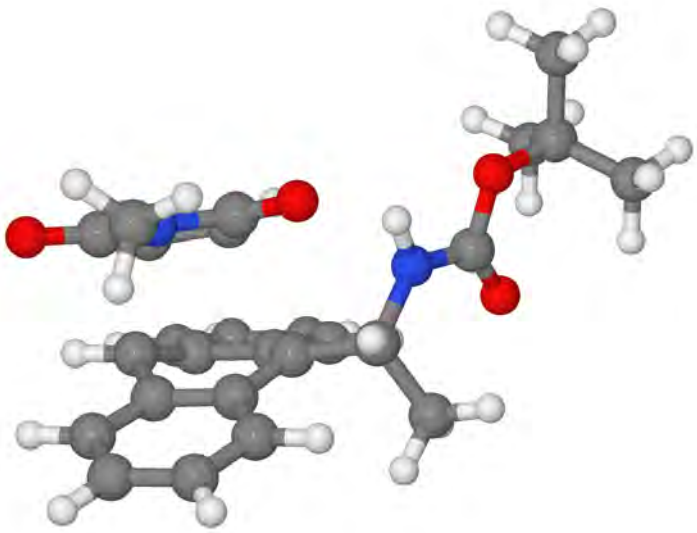
60

C	-1.64185560	-0.22172572	3.17525911
C	-0.67745286	0.41855037	2.39333963
C	-0.19383612	-0.19004814	1.23360085
C	-0.72304541	-1.43634903	0.85933107
C	-1.68906128	-2.07046413	1.63244402
C	-2.14422011	-1.46468246	2.80305862
C	0.84143686	0.38020465	0.23759748
C	-0.18511707	-1.96049738	-0.44932410
C	1.32370973	-1.96780431	-0.36474782
C	1.88721383	-0.72438860	-0.02434365
C	3.27489185	-0.59370434	-0.03035836
H	3.74759841	0.36138827	0.14552814
C	4.07926607	-1.70209265	-0.31306678
C	3.51307774	-2.93764210	-0.60813099
C	2.12428164	-3.06724048	-0.64844745
H	-1.99799430	0.25944841	4.07910061
H	-0.31972876	1.38799310	2.71232724
H	-2.08757973	-3.02885771	1.31792974
H	-2.89118242	-1.95715761	3.41506481

H	5.15748215	-1.58760238	-0.30563596
H	4.14500284	-3.79264259	-0.82072991
H	1.66717780	-4.01715517	-0.90559274
C	1.34772491	1.79326403	0.68910408
H	-0.60112226	-2.93218327	-0.71406072
C	0.07305341	0.47200736	-1.15471089
C	-0.52988219	-0.89616907	-1.54068339
C	-1.11558390	1.42554808	-1.16525114
H	-0.15938061	-1.24674988	-2.50649142
H	0.78917360	0.82614774	-1.89664602
O	-1.09971392	2.62745214	-0.98008764
C	-2.02572870	-0.65084326	-1.67614508
O	-2.88103199	-1.46295166	-1.93947458
N	-2.26276135	0.70622325	-1.45225716
C	-3.58528733	1.31397843	-1.51885390
H	-3.55624413	2.18693233	-2.17094707
H	-4.27167416	0.56754434	-1.91311908
H	-3.90970039	1.62414038	-0.52410161
C	2.26780081	1.81291521	1.92067218
H	2.27287054	2.82102895	2.34314227
H	1.89714563	1.12618649	2.68122292
H	3.29379082	1.55055928	1.69071674
H	0.43342918	2.30845904	0.98542529
N	1.83132303	2.62541914	-0.41999093
H	1.10042262	3.11873102	-0.91502112
C	3.10430193	2.93775320	-0.78340024
O	4.13181210	2.49062133	-0.30308735
C	4.27142429	4.39364004	-2.41132760
O	3.04966259	3.84444523	-1.79447448
C	5.08711386	5.16325760	-1.36905324
H	4.46475744	5.92176199	-0.88722748
H	5.48198938	4.49341583	-0.60722387
H	5.92204618	5.67016125	-1.86022699
C	3.70611787	5.34614086	-3.46591234
H	4.52087975	5.83321047	-4.00670195
H	3.08925557	4.80095243	-4.18375731
H	3.09050989	6.11632729	-2.99614930
C	5.08019161	3.27431560	-3.07247496
H	5.48463440	2.58978701	-2.32920313
H	4.45032930	2.71233773	-3.76701999
H	5.90790796	3.70844030	-3.63973999

S56. tBuC(O)NH - *ANTI* APPROACH α - TS

S56.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	0.7042 Debye
Energy	:	-1418.42117452 a.u.
Number of imaginary frequencies	:	1

S56.2. Cartesian Co-ordinates (XYZ format)

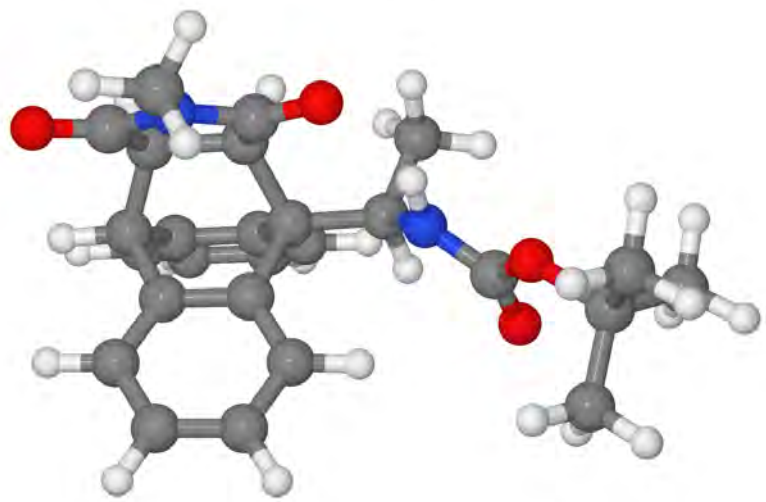
60

C	3.58272648	-0.63947147	2.63438368
C	2.27416301	-0.35954201	2.30006146
C	1.95767581	0.32362083	1.09661794
C	3.03359556	0.67350250	0.23439798
C	4.36097479	0.34349555	0.57721865
C	4.63685703	-0.28851393	1.77049220
C	0.61133796	0.63805950	0.66211390
C	2.69226575	1.26921272	-1.02636707
C	1.53398430	2.12482595	-1.06106305
C	0.44727057	1.78700340	-0.20767364
C	-0.74193650	2.54683805	-0.30943432
H	-1.59920502	2.31217098	0.30562106
C	-0.82336438	3.60864663	-1.19017446
C	0.25630966	3.93648338	-2.02824855
C	1.41560948	3.18877101	-1.97454011
H	3.79952765	-1.13387370	3.57440424
H	1.49512863	-0.64483929	2.99307132
H	5.16031122	0.60356921	-0.10701752
H	5.66061449	-0.51587814	2.04404855

H	-1.73524773	4.19333124	-1.23439658
H	0.17699848	4.77165842	-2.71470070
H	2.25273561	3.42208147	-2.62396336
C	-0.54170626	0.06195660	1.50409055
H	3.51067710	1.50570476	-1.69912660
C	0.69010216	-0.76546347	-1.30959821
C	1.85185313	-0.37838420	-1.99757040
C	0.94808161	-2.04474258	-0.63402212
H	1.84388006	0.12523107	-2.95370865
H	-0.31559914	-0.45598072	-1.53688288
O	0.18588711	-2.72263026	0.03849125
C	2.86361217	-1.46856225	-1.78353369
O	3.97376776	-1.57495415	-2.25698256
N	2.28352046	-2.37630558	-0.89589429
C	2.96795511	-3.53534579	-0.35116902
H	3.52451181	-4.03620529	-1.14359105
H	3.66226077	-3.24009371	0.43935794
H	2.21476746	-4.20558882	0.05975773
C	-0.90384018	0.95221263	2.70741987
H	-1.64764357	0.44884422	3.32824183
H	-0.00704953	1.11623049	3.30777073
H	-1.30593848	1.91798079	2.41646767
H	-0.15118057	-0.86749810	1.91778266
N	-1.68552732	-0.39854690	0.70681286
H	-1.56760788	-1.33515978	0.33955771
C	-2.94735861	0.10713810	0.64601588
O	-3.31746840	1.18275070	1.08502972
C	-5.16506243	-0.51358300	-0.26143163
O	-3.73579741	-0.78090554	-0.01138955
C	-5.91585350	-0.39876172	1.06780040
H	-5.74271011	-1.28912413	1.67774570
H	-5.59488821	0.47994870	1.62470567
H	-6.98935747	-0.32147196	0.87574387
C	-5.60331345	-1.76422381	-1.02456224
H	-6.66580009	-1.70005774	-1.27065718
H	-5.03653526	-1.86562574	-1.95267808
H	-5.43912840	-2.65896916	-0.42030412
C	-5.32866001	0.73553216	-1.13146806
H	-5.02858067	1.63243914	-0.59282571
H	-4.72471237	0.64675075	-2.03822422
H	-6.37576818	0.83694071	-1.42915130

S57. tBuC(O)NH - *ANTI* APPROACH β - PRODUCT

S57.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	1.6340 Debye
Energy	:	-1418.48152206 a.u.
Number of imaginary frequencies	:	0

S57.2. Cartesian Co-ordinates (XYZ format)

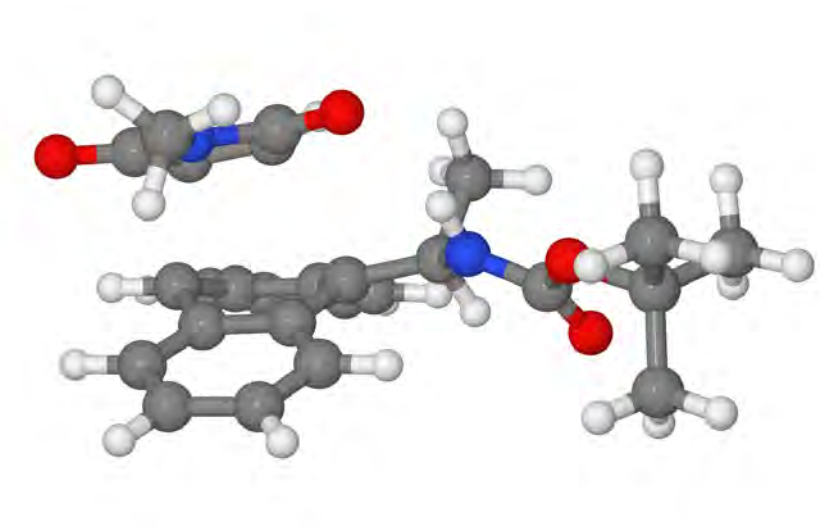
60

C	-0.59037876	0.75100017	3.35715246
C	-0.06895243	1.24839592	2.15985155
C	0.13132094	0.39259636	1.07781339
C	-0.15316255	-0.97755843	1.23483884
C	-0.68778718	-1.46640158	2.42091656
C	-0.91669917	-0.59509683	3.48626995
C	0.71052057	0.74112141	-0.30883718
C	0.24045497	-1.84087503	0.05363541
C	1.69299614	-1.53710341	-0.24089673
C	1.96002400	-0.17040397	-0.42932346
C	3.27920079	0.23235685	-0.63112396
H	3.53717923	1.27657998	-0.74533087
C	4.30474281	-0.71659273	-0.67571288
C	4.02441120	-2.06958652	-0.51840532
C	2.70963502	-2.48172855	-0.29474992
H	-0.73581833	1.42663050	4.19251728
H	0.19468144	2.29240704	2.09616065
H	-0.90649372	-2.52434659	2.51877475
H	-1.32695174	-0.97124088	4.41658831

H	5.32621813	-0.38794625	-0.82981879
H	4.82409096	-2.80052447	-0.55467808
H	2.48052955	-3.53187728	-0.14707270
C	1.07774186	2.23852491	-0.55932617
H	0.05696976	-2.89985824	0.23323940
C	-0.31670928	0.16617176	-1.38374579
C	-0.54707378	-1.34902573	-1.18998015
C	-1.72970915	0.75405496	-1.35453093
H	-0.23320600	-1.92661738	-2.06223702
H	0.08798851	0.37250593	-2.37530088
O	-2.06511402	1.91020691	-1.52541697
C	-2.04797554	-1.52360308	-1.03303421
O	-2.64977837	-2.55460954	-0.84561884
N	-2.63869381	-0.26764157	-1.15030241
C	-4.07599068	-0.04076050	-1.06876767
H	-4.42133904	0.47591278	-1.96458113
H	-4.55681419	-1.01291394	-0.98352289
H	-4.31079149	0.56856948	-0.19496734
C	1.46949351	2.53849745	-2.02169394
H	1.96279383	3.51198983	-2.06398129
H	2.14461851	1.79549670	-2.44763088
H	0.57710165	2.59357548	-2.64906669
H	1.92702651	2.46152830	0.08769616
N	0.04361157	3.18669224	-0.15783504
H	-0.84342879	3.14613080	-0.64559865
C	0.34782851	4.32360029	0.52381611
O	1.41922891	4.55010462	1.06208849
C	-0.71270293	6.43219423	1.25567913
O	-0.73050427	5.14423037	0.53776693
C	-0.48461789	6.20026779	2.75181460
H	0.51549023	5.81414223	2.94112587
H	-0.60613394	7.14390516	3.29042792
H	-1.21970904	5.49025106	3.13978481
C	0.34090939	7.35964870	0.64438623
H	1.34516513	6.97391415	0.81078541
H	0.17377992	7.46416616	-0.43079332
H	0.26348683	8.35108662	1.09873354
C	-2.12103343	6.97064257	1.00072324
H	-2.87161088	6.28448772	1.39901662
H	-2.24460125	7.94209671	1.48515511
H	-2.29711032	7.09055662	-0.07044963

S58. tBuC(O)NH - *ANTI* APPROACH β - TS

S58.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	1.6340 Debye
Energy	:	-1418.41722403 a.u.
Number of imaginary frequencies	:	1

S58.2. Cartesian Co-ordinates (XYZ format)

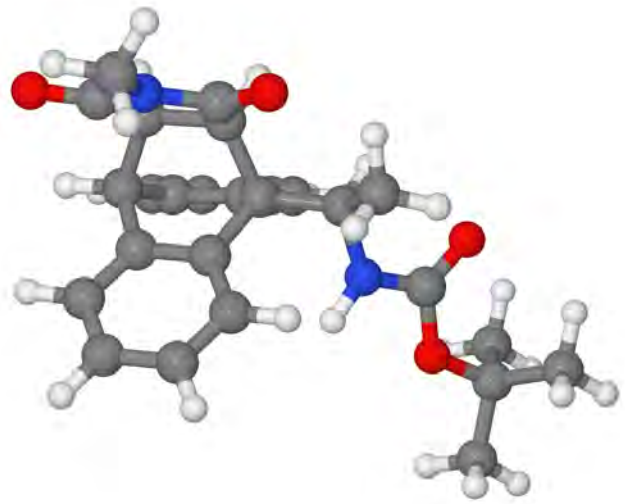
60

C	0.23969440	-1.33719897	2.71185756
C	-0.03968615	-0.51841527	1.63847828
C	0.98454934	-0.09906260	0.74661064
C	2.31004977	-0.56150007	1.01583064
C	2.56053972	-1.43841696	2.09228444
C	1.54289865	-1.81587458	2.93970776
C	0.80093735	0.77041870	-0.40190226
C	3.35758424	-0.15889697	0.12389443
C	3.24024582	1.15167224	-0.45298260
C	1.92947781	1.63469052	-0.71373051
C	1.80435824	2.94319916	-1.24449468
H	0.82676041	3.37897944	-1.39632547
C	2.91939640	3.70677066	-1.52612758
C	4.21140432	3.19085908	-1.32284689
C	4.36597776	1.92478704	-0.79700059
H	-0.55954158	-1.60934269	3.39198923
H	-1.04726923	-0.16992503	1.49446440
H	3.57298970	-1.79043067	2.25353360
H	1.74591959	-2.46425653	3.78424716

H	2.79488635	4.71620131	-1.90083838
H	5.08004665	3.79458642	-1.55855489
H	5.35627556	1.52299488	-0.61107558
C	-0.57095182	1.19662881	-0.96145517
H	4.35550308	-0.53344363	0.32710040
C	1.61461890	-0.97068435	-2.01226878
C	2.90502763	-1.29522276	-1.58140993
C	0.70576531	-2.06316233	-1.62529123
H	3.80937004	-1.00185919	-2.09464097
H	1.36664391	-0.29228908	-2.80857658
O	-0.49728662	-2.17323303	-1.80596042
C	2.83660722	-2.67100787	-0.98365164
O	3.74078393	-3.36306500	-0.56948835
N	1.48834348	-3.02369905	-0.97171581
C	0.96845484	-4.23805380	-0.36832395
H	-0.06081343	-4.35941410	-0.70109105
H	1.56824470	-5.09192801	-0.68462175
H	0.99365878	-4.16883039	0.72180307
C	-0.61406308	1.38618767	-2.49842095
H	-1.49647462	1.97997832	-2.74657798
H	0.26112261	1.88790607	-2.90740657
H	-0.71926850	0.41391268	-2.98100543
H	-0.81236255	2.15687251	-0.49329916
N	-1.67476535	0.31434286	-0.60440540
H	-1.64144695	-0.63474864	-0.96163148
C	-2.89541221	0.83184254	-0.28218246
O	-3.11026788	2.00910997	-0.05112901
C	-5.21946335	0.09373362	0.11468747
O	-3.80742288	-0.16573374	-0.22924775
C	-5.31967688	0.65532184	1.53522861
H	-4.86420012	1.64197826	1.59973860
H	-6.37138557	0.73266506	1.82366705
H	-4.82201529	-0.01337731	2.24241304
C	-5.85038376	1.02435338	-0.92422163
H	-5.40646791	2.01752019	-0.88241047
H	-5.71516562	0.61609423	-1.92910063
H	-6.92343712	1.10986757	-0.73334628
C	-5.83796167	-1.30238426	0.03849824
H	-5.35271978	-1.97577000	0.74837804
H	-6.90310144	-1.25375116	0.27663139
H	-5.72360611	-1.71813703	-0.96485990

S59. tBuC(O)NH - *ANTI* APPROACH γ - PRODUCT

S59.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	2.6055 Debye
Energy	:	-1418.47200838 a.u.
Number of imaginary frequencies	:	0

S59.2. Cartesian Co-ordinates (XYZ format)

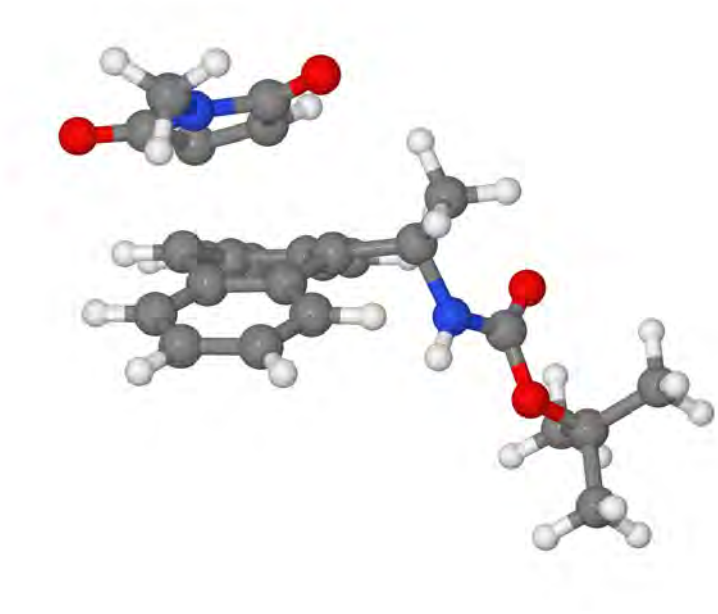
60

C	-1.04903126	1.66938901	2.99536705
C	-0.39683357	1.82490337	1.76949596
C	-0.11516695	0.71141493	0.97547042
C	-0.52018863	-0.55750364	1.42633629
C	-1.17929399	-0.70974660	2.64093161
C	-1.43918729	0.40821812	3.43356204
C	0.56626773	0.69239610	-0.40591028
C	-0.19662185	-1.68641686	0.47672987
C	1.27343452	-1.63193762	0.15544286
C	1.68319070	-0.39347687	-0.35575265
C	2.99667454	-0.26433504	-0.81169009
H	3.35961246	0.65731251	-1.24452925
C	3.88109112	-1.34152114	-0.71580863
C	3.46887589	-2.55614877	-0.17588139
C	2.15066075	-2.70590186	0.25235042
H	-1.25282252	2.54332995	3.60345244
H	-0.12305726	2.82218337	1.45400405
H	-1.48880374	-1.69717836	2.96577883
H	-1.94622254	0.29366586	4.38470268

H	4.89969635	-1.22171319	-1.06710541
H	4.16397238	-3.38455343	-0.09929526
H	1.80352962	-3.65355849	0.65049076
C	1.19041324	2.04312778	-0.88180095
H	-0.51793092	-2.65618205	0.85549867
C	-0.52365726	0.04622845	-1.38878417
C	-0.89811647	-1.37698197	-0.88249242
C	-1.89948070	0.73118633	-1.53246510
H	-0.62126857	-2.14997673	-1.60201800
H	-0.08540832	0.00906848	-2.38897514
O	-2.16867638	1.81197286	-2.00278378
C	-2.40750122	-1.39385569	-0.73157877
O	-3.08864021	-2.32162046	-0.35647523
N	-2.88659954	-0.14796464	-1.09741926
C	-4.30100775	0.20039053	-1.11363125
H	-4.59301281	0.52235001	-2.11371136
H	-4.86061239	-0.68607950	-0.82275957
H	-4.49624348	1.01143372	-0.41069978
C	0.28335905	3.21686316	-1.27864599
H	0.93172598	4.06677914	-1.50196373
H	-0.30053282	2.98416662	-2.16441941
H	-0.41561431	3.51069593	-0.49569336
H	1.77002823	1.80902648	-1.77666414
N	2.17446423	2.47486758	0.11959876
H	1.97748971	2.37786579	1.10258234
C	3.34259009	3.07891321	-0.22249764
O	3.72639394	3.23877192	-1.36919796
C	5.32263517	4.11644650	0.83290797
O	4.00528145	3.45338821	0.89758605
C	5.19719028	5.45951986	0.10934447
H	6.14633131	5.99836731	0.17233200
H	4.94314766	5.31735516	-0.93971229
H	4.42573977	6.07317829	0.58169746
C	6.34674168	3.19181204	0.16978548
H	6.11591959	3.04174066	-0.88341725
H	7.34352255	3.63328815	0.25245202
H	6.36110544	2.22151303	0.67280155
C	5.65845442	4.32477331	2.30996799
H	5.70361185	3.36640239	2.83187318
H	6.62714291	4.82030010	2.40759730
H	4.90011883	4.94583893	2.79182148

S60. tBuC(O)NH - *ANTI* APPROACH γ - TS

S60.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	4.2097 Debye
Energy	:	-1418.41743867 a.u.
Number of imaginary frequencies	:	1

S60.2. Cartesian Co-ordinates (XYZ format)

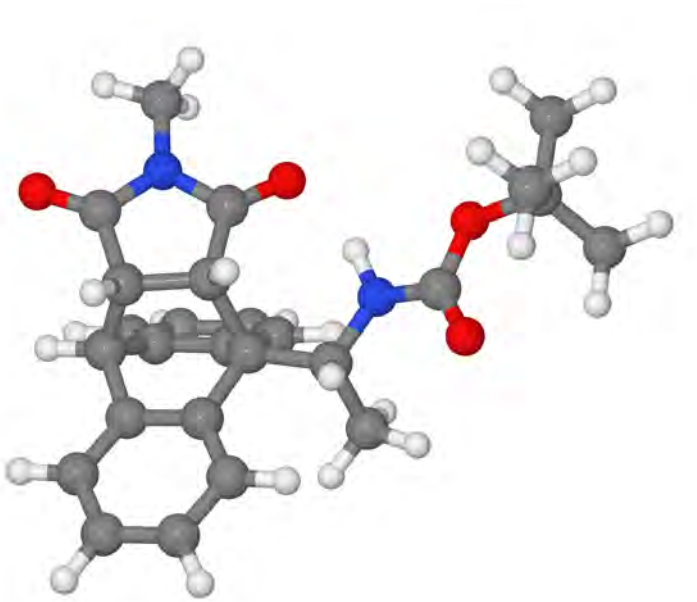
60

C	2.19788957	-2.17267156	2.44910908
C	1.28246713	-1.83349848	1.47522569
C	1.32605147	-0.56641793	0.83589435
C	2.35664201	0.33379057	1.23133850
C	3.30463147	-0.04754563	2.19994473
C	3.22235727	-1.28032911	2.81373930
C	0.38901353	-0.12478933	-0.17040212
C	2.43340206	1.59764659	0.54074192
C	1.18165731	2.18861723	0.13012704
C	0.15185370	1.30125463	-0.28223023
C	-1.04310513	1.86919665	-0.79713583
H	-1.86644053	1.24043286	-1.10774064
C	-1.19739473	3.23861194	-0.87378615
C	-0.16529508	4.10437870	-0.47086513
C	1.01676679	3.58023286	0.01184492
H	2.12404394	-3.13695407	2.93870378
H	0.51121634	-2.54669476	1.22562921
H	4.09231567	0.64819938	2.46537995
H	3.93808174	-1.55863500	3.57841396

H	-2.12864923	3.64873981	-1.24732876
H	-0.29965889	5.17782593	-0.53826708
H	1.82566357	4.23504066	0.31806812
C	-0.68989784	-1.05899346	-0.74355334
H	3.21319366	2.27828574	0.86876005
C	2.32783484	0.14724635	-1.89510512
C	3.13290238	1.11103964	-1.25123882
C	3.05729318	-1.12942243	-1.90480149
H	3.20463872	2.13288713	-1.59977329
H	1.55011141	0.34426403	-2.61468840
O	2.77103376	-2.19142890	-2.42445874
C	4.42819071	0.42517605	-0.88813353
O	5.42138100	0.91827500	-0.39617330
N	4.26433372	-0.91138929	-1.20396328
C	5.25509453	-1.94027853	-0.94565195
H	5.01464176	-2.79808044	-1.57150984
H	6.24821949	-1.56214154	-1.18977594
H	5.23786545	-2.24089217	0.10507249
C	-0.24497537	-2.39412141	-1.35732949
H	0.15744187	-3.09912729	-0.63143581
H	-1.11910427	-2.85529613	-1.82345307
H	0.51831907	-2.24200106	-2.11920094
H	-1.17496586	-0.51954430	-1.55332768
N	-1.74518669	-1.24107575	0.26103380
H	-1.51956177	-1.62377644	1.16577160
C	-3.06225324	-1.00813782	0.00026864
O	-3.49063683	-0.55688167	-1.04839933
C	-5.27107525	-1.19245934	1.09484828
O	-3.80070543	-1.34626353	1.08066380
C	-5.89945841	-2.07999921	0.01800733
H	-6.98813915	-2.05324745	0.11369495
H	-5.62656355	-1.73998034	-0.97957361
H	-5.57266331	-3.11558390	0.14243992
C	-5.64565659	0.28193694	0.92746133
H	-5.38664579	0.64255750	-0.06646687
H	-6.72185373	0.40326133	1.07650077
H	-5.12797832	0.89106202	1.67283297
C	-5.63870335	-1.69084334	2.49254107
H	-5.15288162	-1.08143139	3.25771356
H	-6.71994305	-1.63416111	2.63738990
H	-5.32457304	-2.72852039	2.62478375

S61. tBuC(O)NH - *SYN* APPROACH α - PRODUCT

S61.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	2.0663 Debye
Energy	:	-1418.47446089 a.u.
Number of imaginary frequencies	:	0

S61.2. Cartesian Co-ordinates (XYZ format)

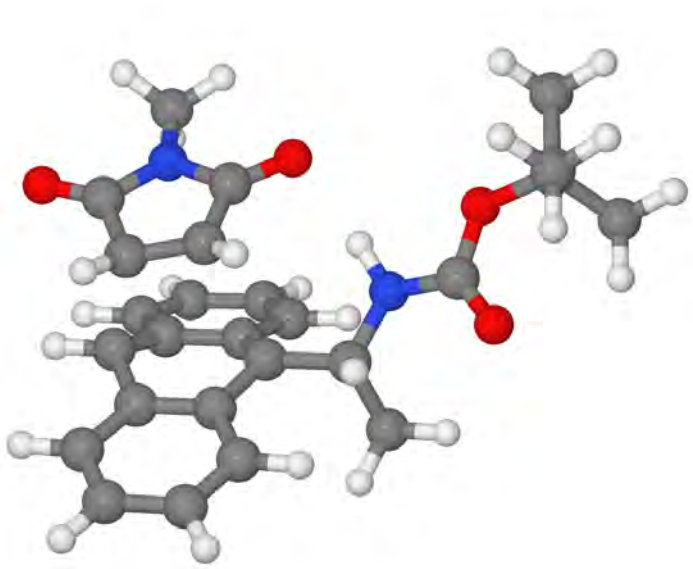
60

C	-4.06786728	0.24881589	-1.10988688
C	-2.84606838	0.87581015	-0.85359758
C	-1.74265444	0.12916034	-0.43337640
C	-1.88992441	-1.26031482	-0.32295769
C	-3.10233641	-1.88938618	-0.57848680
C	-4.20475864	-1.12755489	-0.96294147
C	-0.31648272	0.66250652	-0.10017414
C	-0.59934366	-1.97063339	-0.01652874
C	-0.01978585	-1.37883759	1.24894273
C	0.11796734	0.02181471	1.22975838
C	0.72574013	0.65490955	2.31261873
H	0.90887052	1.71980572	2.29839158
C	1.13078856	-0.09037831	3.42210698
C	0.95451152	-1.47072709	3.45050836
C	0.38948500	-2.11980057	2.35257030
H	-4.91421175	0.84847456	-1.42479444
H	-2.78923535	1.94690967	-0.98557395
H	-3.18134093	-2.96745467	-0.48685175
H	-5.15752077	-1.60659194	-1.15732121

H	1.59156668	0.41509274	4.26314831
H	1.26795530	-2.04262567	4.31638670
H	0.27344394	-3.19837785	2.35240316
C	-0.34643140	2.21959090	-0.19184156
H	-0.70939231	-3.05343819	0.03758970
C	0.64723921	-0.06037552	-1.15329897
H	0.53188229	0.41449419	-2.13157725
C	0.32422364	-1.57684946	-1.22283530
H	-0.18007492	-1.85998321	-2.14732981
C	2.15452290	-0.05825506	-0.81778163
C	1.65517080	-2.29721284	-1.16344893
O	1.84912622	-3.48569870	-1.26978290
O	2.87608671	0.87419474	-0.52274024
C	-1.17040384	2.89759922	0.92688334
H	-2.08329701	2.35332155	1.16624701
H	-0.58777016	2.99845481	1.84073877
H	-1.43890512	3.90077353	0.59288043
N	2.64145684	-1.34715974	-0.92845631
C	4.04694080	-1.67487216	-0.72252727
H	4.16200399	-2.74254870	-0.89637488
H	4.66623926	-1.10931897	-1.41896892
H	4.34354687	-1.42712235	0.29745862
H	-0.84974885	2.43984365	-1.13662374
N	0.96638757	2.85558367	-0.29609743
H	1.81517506	2.30488062	-0.19829191
C	1.07847500	4.04789495	-0.94205415
O	0.13872468	4.70382357	-1.36234915
C	2.80837536	5.64684868	-1.68500340
O	2.38608027	4.39460373	-1.03534961
C	2.23492336	6.85137081	-0.93332845
H	2.65342164	7.77354050	-1.34561694
H	1.15044606	6.88648367	-1.02063060
H	2.50409222	6.79854774	0.12479531
C	2.40291405	5.63774347	-3.16166615
H	2.79196286	4.74259806	-3.65406156
H	1.31987202	5.65889740	-3.26951098
H	2.82515812	6.51263285	-3.66337061
C	4.33025980	5.59563446	-1.54259264
H	4.77998209	6.48291922	-1.99460304
H	4.61500263	5.55867577	-0.48883602
H	4.73138952	4.70930243	-2.03890133

S62. tBuC(O)NH - *SYN* APPROACH α - TS

S62.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	2.0663 Debye
Energy	:	-1418.42173069 a.u.
Number of imaginary frequencies	:	1

S62.2. Cartesian Co-ordinates (XYZ format)

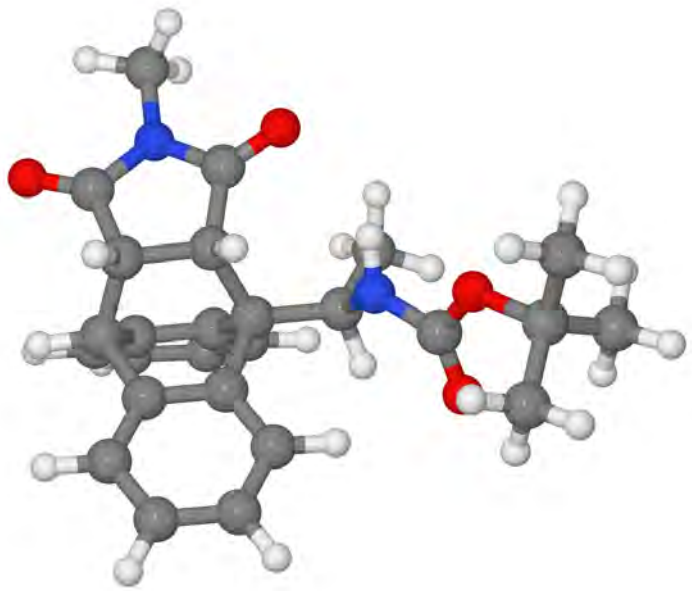
60

C	-2.32538700	3.94772816	-1.07523727
C	-1.36497664	3.11425710	-0.53804207
C	-1.65721881	1.75883496	-0.23990026
C	-2.96043015	1.28646111	-0.54363209
C	-3.91651797	2.14128828	-1.12183952
C	-3.61147356	3.46396232	-1.37055755
C	-0.70023739	0.81580299	0.31662050
C	-3.20682740	-0.12198316	-0.35567993
C	-2.53682303	-0.76127356	0.74875331
C	-1.22566116	-0.30610108	1.06633663
C	-0.50106698	-1.01074767	2.06184983
H	0.51143295	-0.71870202	2.29847169
C	-1.07607496	-2.06801820	2.73637891
C	-2.38028049	-2.49609828	2.42833281
C	-3.09145975	-1.86169386	1.43017578
H	-2.08210492	4.98570251	-1.27046704
H	-0.38884938	3.52753186	-0.32780042
H	-4.89985085	1.74862528	-1.35711467
H	-4.35737562	4.12719202	-1.79288900

H	-0.51260412	-2.57548165	3.51097846
H	-2.82143688	-3.32470345	2.97010970
H	-4.08777714	-2.19680643	1.16460228
C	0.71253574	1.35104632	0.55422765
H	-4.19919205	-0.48670733	-0.60304129
C	-0.77455485	-0.54501778	-1.76042950
H	-0.18392205	0.23650166	-2.20984793
C	-2.15258026	-0.77556366	-1.96109223
H	-2.73950219	-0.25024232	-2.70149565
C	-0.15789215	-1.82737124	-1.37112558
C	-2.37486267	-2.25716805	-1.83035541
O	-3.39195776	-2.88657808	-2.02227139
O	0.99683481	-2.07357526	-1.05982864
C	0.79139322	2.09639740	1.90861893
H	0.04577370	2.89224505	1.95480072
H	0.61955160	1.42105782	2.74664187
H	1.78155053	2.54055381	2.00569439
N	-1.16789663	-2.79597068	-1.39876378
C	-0.98472798	-4.18301344	-1.00841606
H	-1.52562869	-4.82595778	-1.70231545
H	0.08055030	-4.40383148	-1.03919625
H	-1.36011076	-4.35253620	0.00415445
H	0.92042816	2.08833957	-0.22311407
N	1.75795937	0.32764107	0.44786450
H	1.52986693	-0.58534276	0.06097922
C	3.04650879	0.73322719	0.23218107
O	3.42575312	1.89150929	0.27481574
C	5.26084709	-0.20842350	-0.31888252
O	3.82510066	-0.34345716	-0.01359382
C	5.99874258	0.40191153	0.87575406
H	7.07609940	0.37842748	0.69074178
H	5.69202900	1.43331087	1.04058146
H	5.79612970	-0.17741705	1.78027701
C	5.45148087	0.60889202	-1.59954250
H	4.87392139	0.16927992	-2.41682911
H	5.13542414	1.64100695	-1.45704949
H	6.50678873	0.60008067	-1.88511038
C	5.68774033	-1.66068292	-0.53558141
H	6.75100851	-1.70656121	-0.78293818
H	5.51379919	-2.24926567	0.36782312
H	5.11765242	-2.10817838	-1.35231245

S63. tBuC(O)NH - *SYN* APPROACH β - PRODUCT

S63.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	1.1792 Debye
Energy	:	-1418.47324399 a.u.
Number of imaginary frequencies	:	0

S63.2. Cartesian Co-ordinates (XYZ format)

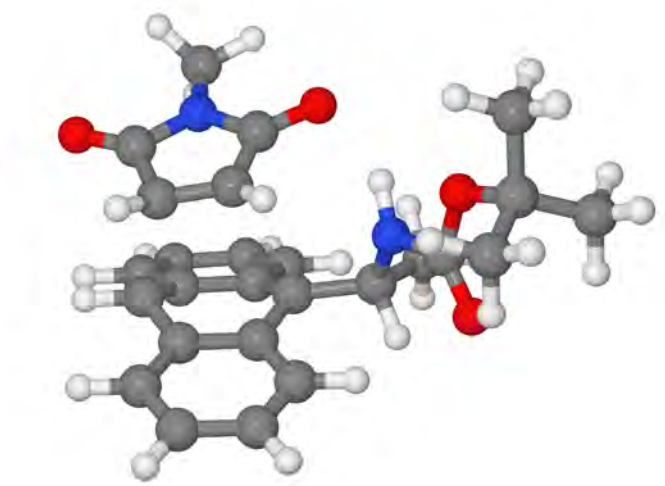
60

C	0.47477725	3.92021132	-1.09476709
C	0.64593518	2.71235800	-0.41008809
C	-0.36070725	1.75054014	-0.44144875
C	-1.54576504	2.02462149	-1.14797604
C	-1.70893979	3.22018147	-1.83511364
C	-0.68952876	4.17410278	-1.81148267
C	-0.35898969	0.36720344	0.26509416
C	-2.59250951	0.93250579	-1.04680073
C	-2.80546951	0.68173712	0.42937142
C	-1.62392724	0.42057660	1.14825428
C	-1.69536018	0.37852821	2.54183912
H	-0.80609286	0.27691668	3.14627719
C	-2.92600131	0.50369716	3.19135714
C	-4.09695721	0.68171531	2.46254992
C	-4.03241587	0.78616214	1.07329559
H	1.26271510	4.66424370	-1.05948710
H	1.56100392	2.55400872	0.14417800
H	-2.63095522	3.41394591	-2.37339139
H	-0.81254208	5.11293125	-2.33960724

H	-2.95999455	0.46779796	4.27433777
H	-5.05024195	0.76874292	2.97117519
H	-4.92972612	0.97265017	0.49337715
C	0.97499472	0.08012821	1.02983272
H	-3.51938272	1.18472075	-1.56103277
C	-0.60463232	-0.63676661	-0.95445436
H	0.23745117	-0.49228984	-1.63186634
C	-1.94630742	-0.33383930	-1.65559149
H	-1.80747008	-0.19026525	-2.73053312
C	-0.68570817	-2.13258529	-0.66368645
C	-2.79256010	-1.58547807	-1.47253776
O	-3.94899774	-1.74119365	-1.78810894
O	0.21938340	-2.87611008	-0.34886801
C	1.03428650	-1.14184749	1.97763920
H	0.10577883	-1.33831823	2.50689554
H	1.28386390	-2.04306769	1.42399085
H	1.81819427	-0.96394241	2.71826267
N	-1.98391294	-2.56370950	-0.89934927
C	-2.41357565	-3.93830180	-0.67974919
H	-3.42449927	-4.03352404	-1.07065010
H	-1.74054790	-4.62356853	-1.19604087
H	-2.40619564	-4.17028666	0.38632369
H	1.18057382	0.97336316	1.62041891
N	2.09333539	-0.03567306	0.08554562
H	2.16660047	-0.91711283	-0.40496665
C	3.28405213	0.60550117	0.28915685
O	3.44402695	1.55046511	1.04168880
C	5.61404133	0.57298005	-0.53719836
O	4.23273516	0.04860619	-0.49554533
C	5.61291265	2.02014208	-1.03543675
H	5.07649994	2.09312391	-1.98493385
H	5.14469051	2.68548203	-0.31214291
H	6.64260912	2.34841394	-1.20022023
C	6.26760292	0.43089318	0.83936220
H	6.20872974	-0.60552031	1.18149793
H	7.32311249	0.70741636	0.77215439
H	5.78279257	1.07394612	1.57187068
C	6.28381968	-0.35030097	-1.55515516
H	7.33250332	-0.07106183	-1.68025112
H	6.23794937	-1.38869345	-1.21979904
H	5.78643131	-0.27741736	-2.52478886

S64. tBuC(O)NH - *SYN* APPROACH β - TS

S64.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	0.7874 Debye
Energy	:	-1418.41433551 a.u.
Number of imaginary frequencies	:	1

S64.2. Cartesian Co-ordinates (XYZ format)

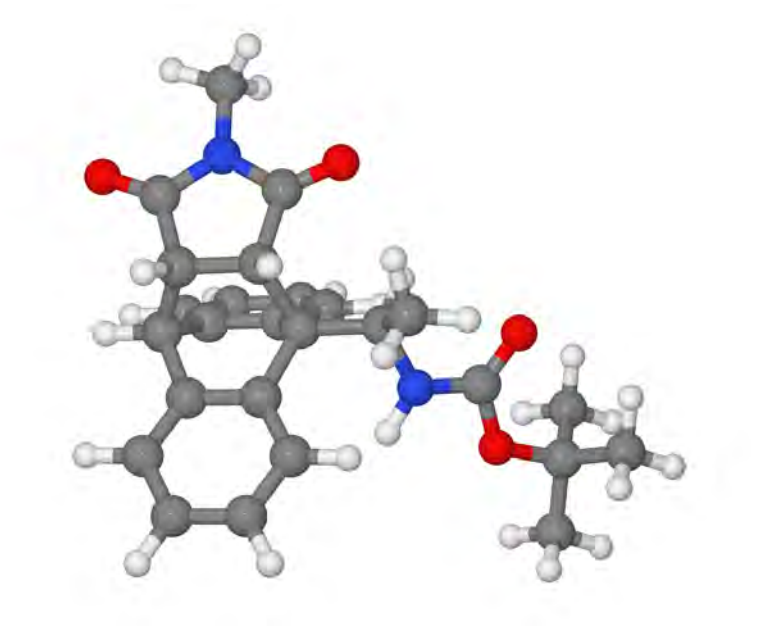
60

C	0.88769823	3.83913994	-0.46659470
C	0.80142111	2.67802572	0.27768248
C	-0.37336308	1.88427734	0.25619096
C	-1.43277621	2.30862260	-0.58993942
C	-1.31376600	3.47630692	-1.36335862
C	-0.17156298	4.24858284	-1.29238570
C	-0.53560632	0.64169300	1.00727510
C	-2.57421875	1.43431795	-0.70040673
C	-2.94322324	0.70697647	0.48269221
C	-1.89478660	0.25604260	1.34446442
C	-2.29357314	-0.55543321	2.44315243
H	-1.56896424	-0.93192917	3.13848591
C	-3.61825037	-0.85436189	2.68188977
C	-4.63154793	-0.39572486	1.82340884
C	-4.28752756	0.36249334	0.72688681
H	1.78960776	4.43798256	-0.41051549
H	1.65481746	2.39480829	0.87723923
H	-2.13809276	3.76833010	-2.00532389
H	-0.09090245	5.16196632	-1.87030959

H	-3.87605619	-1.45050406	3.54996586
H	-5.66938782	-0.63581377	2.02264142
H	-5.04757023	0.71355504	0.03865335
C	0.75044650	0.13596916	1.72102618
H	-3.38827538	1.76339018	-1.33901107
C	-0.61022758	-0.51581639	-1.23487270
H	0.39303043	-0.16313200	-1.39480698
C	-1.77587891	-0.01822064	-1.84350729
H	-1.75618148	0.59076142	-2.73758817
C	-0.87364292	-1.86603224	-0.73510075
C	-2.79119349	-1.13216901	-1.78808248
O	-3.89991283	-1.16619933	-2.27472091
O	-0.11654626	-2.63822985	-0.16396567
C	0.68999547	-0.86559093	2.88564610
H	0.25047374	-1.82001483	2.59444952
H	1.72082913	-1.05084860	3.19535756
H	0.16610792	-0.46074632	3.75240707
N	-2.21442819	-2.15286946	-1.03630710
C	-2.90172601	-3.37457967	-0.65770310
H	-2.15350103	-4.07843637	-0.29725680
H	-3.63014627	-3.17927814	0.13295202
H	-3.41981864	-3.78907323	-1.52308071
H	1.22415841	1.02594244	2.13530350
N	1.70094264	-0.37450787	0.72827578
H	1.47388327	-1.27441680	0.31505600
C	3.01483083	-0.00997860	0.75160813
O	3.46813440	0.91599768	1.40491939
C	5.17089605	-0.62954164	-0.28601009
O	3.71943450	-0.80928940	-0.08002347
C	5.45023537	0.74998879	-0.88751286
H	4.85518456	0.89531511	-1.79278755
H	5.21559525	1.54220831	-0.17882329
H	6.50664806	0.82170928	-1.15961409
C	5.91783381	-0.85328501	1.03115058
H	5.65724802	-1.82750702	1.45269668
H	6.99521732	-0.84023607	0.84602112
H	5.67703247	-0.07754101	1.75607467
C	5.49914074	-1.73503554	-1.28972399
H	6.56459999	-1.71718955	-1.53063941
H	5.25193977	-2.71480870	-0.87554997
H	4.93112278	-1.59676397	-2.21221304

S65. tBuC(O)NH - *SYN* APPROACH γ - PRODUCT

S65.1. General Information



SMILES	:	CC(C12c3ccccc3C(c4c1cccc4)C5C2C(=O)N(C5=O)C)NC(=O)OC(C)(C)C
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	3.5007 Debye
Energy	:	-1418.48123201 a.u.
Number of imaginary frequencies	:	0

S65.2. Cartesian Co-ordinates (XYZ format)

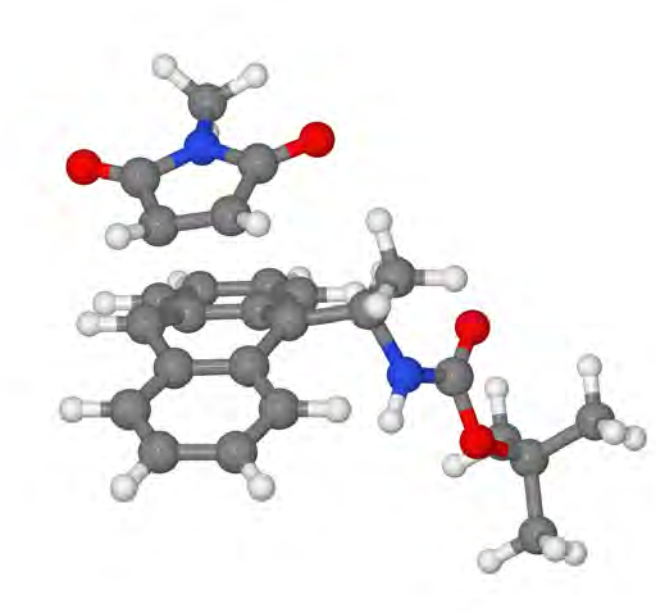
60

C	-0.09655756	4.19156933	-0.53726715
C	0.15323564	2.84200120	-0.80320346
C	-0.71767193	1.85890615	-0.33005050
C	-1.85289812	2.25930548	0.39653653
C	-2.10495925	3.60100508	0.65417194
C	-1.21851003	4.57369089	0.18982367
C	-0.61133665	0.32784736	-0.52576435
C	-2.74782753	1.11621606	0.81616199
C	-1.90138400	0.11630154	1.57121289
C	-0.76406235	-0.31247085	0.86824673
C	0.05862821	-1.28479850	1.43512225
H	0.92710507	-1.65636170	0.90839553
C	-0.23912878	-1.79629111	2.70036530
C	-1.35901535	-1.35310459	3.39875245
C	-2.20097041	-0.39868018	2.82755589
H	0.59394813	4.94173813	-0.90543908
H	1.03148437	2.58349538	-1.37836564
H	-2.98821497	3.88664818	1.21569180
H	-1.40623844	5.62164879	0.39359495

H	0.41047144	-2.54613781	3.13736844
H	-1.58209395	-1.75405943	4.38092709
H	-3.08810735	-0.06225876	3.35308146
C	0.64854532	-0.17001162	-1.28306580
H	-3.61683893	1.44455278	1.38552439
C	-1.94593728	-0.05258939	-1.29766035
H	-1.90785956	0.39024052	-2.29324675
C	-3.18889165	0.43095475	-0.51646644
H	-3.78856730	1.13664758	-1.09506559
C	-2.16626096	-1.55662513	-1.46242523
C	-4.02908897	-0.81568283	-0.27989924
O	-5.08658791	-0.88012743	0.30376706
O	-1.45259035	-2.35245562	-2.03103232
C	0.69625008	0.16015682	-2.78545761
H	-0.05836385	-0.41587055	-3.32242060
H	0.55129308	1.21994889	-3.00024867
H	1.67012644	-0.14351811	-3.17230725
N	-3.37108421	-1.89541662	-0.85850811
C	-3.87818098	-3.26072669	-0.82596511
H	-4.86491346	-3.23451543	-0.36836511
H	-3.94115376	-3.65714216	-1.83975792
H	-3.21269751	-3.89521146	-0.23867598
H	0.64977211	-1.25882065	-1.22034705
N	1.85449767	0.28603625	-0.58341950
H	1.82893193	1.10218406	0.00596118
C	3.00682282	-0.43802145	-0.58803809
O	3.15665078	-1.49123096	-1.18072653
C	5.29643440	-0.36214879	0.33899274
O	3.94118690	0.19507901	0.16280125
C	5.21890402	-1.72095871	1.03985655
H	4.65756226	-1.63260090	1.97366822
H	4.73659277	-2.46233153	0.40518630
H	6.22800970	-2.06582713	1.28074968
C	6.00946665	-0.44498670	-1.01310098
H	6.00433540	0.53172606	-1.50394416
H	7.05005646	-0.74292099	-0.85937721
H	5.52914286	-1.17174768	-1.66599679
C	5.96449661	0.67554241	1.24161065
H	6.99485254	0.38044721	1.45320129
H	5.97575283	1.65452790	0.75739282
H	5.42657804	0.76389343	2.18808079

S66. tBuC(O)NH - *SYN* APPROACH γ - TS

S66.1. General Information



SMILES	:	CC(c1c2ccccc2cc3c1cccc3)NC(=O)OC(C)(C)C.CN1C(=O)C=CC1=O
Formula	:	$C_{26}H_{28}N_2O_4$
Charge	:	0
Multiplicity	:	1
Dipole	:	5.0159 Debye
Energy	:	-1418.42037801 a.u.
Number of imaginary frequencies	:	1

S66.2. Cartesian Co-ordinates (XYZ format)

60

C	-0.47423193	4.26667595	-0.51208472
C	-0.07484134	2.96563315	-0.74796242
C	-0.80254519	1.86953676	-0.22165589
C	-1.96205342	2.15814066	0.54937088
C	-2.37584209	3.48959994	0.74387366
C	-1.63566196	4.53585196	0.23192602
C	-0.46688661	0.47305799	-0.43489343
C	-2.72707582	1.03985500	1.03393042
C	-2.00582170	-0.15192147	1.37867022
C	-0.85118800	-0.45829567	0.60550404
C	-0.17661630	-1.67808855	0.87130040
H	0.71117365	-1.94978344	0.31636456
C	-0.61659360	-2.51995707	1.87155628
C	-1.76425755	-2.20988941	2.62597132
C	-2.45936847	-1.04792154	2.36897182
H	0.11555669	5.08628845	-0.90615135
H	0.81963581	2.80313706	-1.33233595
H	-3.27398753	3.68200493	1.32096255
H	-1.94323301	5.56027555	0.40634882

H	-0.06830244	-3.43205428	2.07800794
H	-2.09827638	-2.88388610	3.40641236
H	-3.35405231	-0.80324864	2.92988515
C	0.68541622	0.06604329	-1.36543000
H	-3.62932515	1.25569367	1.59736633
C	-2.52208209	0.15984759	-1.70099795
H	-2.13482571	0.81597668	-2.46142101
C	-3.55779243	0.46793121	-0.80587351
H	-4.17024851	1.35549831	-0.87387878
C	-2.47671938	-1.30760252	-1.87286270
C	-4.22307110	-0.82697660	-0.43861717
O	-5.20972633	-1.00108182	0.24435423
O	-1.75658703	-1.97853923	-2.58623815
C	0.59662294	0.52339375	-2.83250976
H	1.53175497	0.25734350	-3.32982516
H	-0.20741993	-0.01600601	-3.33308792
H	0.43592361	1.59382772	-2.95811820
N	-3.47054172	-1.83579373	-1.03143883
C	-3.71782851	-3.25438166	-0.84594274
H	-3.34150147	-3.58926082	0.12379962
H	-4.78950071	-3.44758272	-0.89805752
H	-3.19948649	-3.78997922	-1.63947368
H	0.69900477	-1.01995659	-1.41088414
N	1.96120262	0.43195704	-0.73767382
H	2.11319566	1.36862314	-0.39926249
C	2.96095634	-0.46910203	-0.52045631
O	2.90645790	-1.64988339	-0.81557125
C	5.24514389	-0.56819898	0.41968101
O	4.00543642	0.15623060	0.06968775
C	4.94123650	-1.66893911	1.43873370
H	4.40991402	-1.25251830	2.29834509
H	4.33530331	-2.45753336	0.99620754
H	5.87883759	-2.10326934	1.79573298
C	5.90644932	-1.11374938	-0.84815514
H	6.06598043	-0.30770507	-1.56900525
H	6.88019896	-1.54190683	-0.59601307
H	5.29323196	-1.88571453	-1.31002903
C	6.10102272	0.53155398	1.04846203
H	7.06749582	0.12438422	1.35427809
H	6.27466726	1.33870173	0.33337879
H	5.60532618	0.94834358	1.92796266