Supplementary information
**Figure S1.** NMR spectra of organocatalyst 1.

**Figure S2.** The reference GC chromatogram for the aldol reaction of acetone with 4-nitrobenzaldehyde. The retention times and intensities for $R$- and $S$-enantiomers are 24.3 and 31.3 min and 49 and 51, respectively.
Figure S3. The GC chromatogram for the aldol reaction of acetone with 4-nitrobenzaldehyde catalyzed by 1 in the absence of additive. The retention times and intensities for $R$- and $S$-enantiomers are 24.1 and 32.0 min and 75 and 25, respectively.
Atomic coordinates for the TS structures in SYBYL format obtained by HF/6-31 + G(d)

@<TRIPOS>MOLECULE

Re-face catalyzed by 1

72 74

SMALL

NO_CHARGES

@<TRIPOS>ATOM

|   | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 |
|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| C1| -0.9948 | 4.3938 | 0.9298 | C  |
| C2| -0.2404 | 3.2500 | 0.7215 | C  |
| C3| 0.1923  | 2.9220 | -0.5592| C  |
| C4| -0.1511 | 3.7433 | -1.6271| C  |
| C5| -0.9106 | 4.8857 | -1.4208| C  |
| C6| -1.3303 | 5.2143 | -0.1400| C  |
| C7| 0.9978  | 1.6756 | -0.7926| C  |
| O8| 0.9302  | 0.7269 | 0.0576 | O  |
| H9| 1.0266  | 1.4030 | -1.8455| H  |
| H10| -1.3225| 4.6460 | 1.9226 | H  |
| H11| 0.0096 | 2.6044 | 1.5429 | H  |
| H12| 0.1712 | 3.4941 | -2.6245| H  |
| H13| -1.1724| 5.5141 | -2.2529| H  |
| C14| -0.9969| -2.5644| -0.3670| C  |
| C15| -0.9557| -3.9220| -0.6383| C  |
|   | C   | x    | y    | z    | N   |
|---|-----|------|------|------|--    |
| 16| C16 | 0.2900 | -4.5204 | -0.7184 | C    |
| 17| C17 | 1.4816 | -3.8264 | -0.5382 | C    |
| 18| C18 | 1.3861 | -2.4794 | -0.2738 | C    |
| 19| H19 | -1.8591 | -4.4724 | -0.7769 | H    |
| 20| H20 | 0.3376 | -5.5740 | -0.9248 | H    |
| 21| H21 | 2.4347 | -4.3035 | -0.6020 | H    |
| 22| N22 | 0.1643 | -1.9013 | -0.2075 | N    |
| 23| N23 | 2.4074 | -1.5918 | -0.0471 | N    |
| 24| H24 | 2.1068 | -0.6410 | 0.1295  | H    |
| 25| N25 | -2.1157 | -1.7910 | -0.2337 | N    |
| 26| H26 | -2.0092 | -0.8541 | 0.1039  | H    |
| 27| C27 | 3.7510 | -1.8285 | -0.1756 | C    |
| 28| C28 | 4.6561 | -0.6633 | 0.2190  | C    |
| 29| O29 | 4.2264 | -2.8697 | -0.5101 | O    |
| 30| N30 | 4.0121 | 0.6594  | 0.2405  | N    |
| 31| C31 | 5.1457 | -0.8784 | 1.6712  | C    |
| 32| H32 | 5.4886 | -0.6730 | -0.4697 | H    |
| 33| C33 | 4.0246 | 1.2319  | 1.6038  | C    |
| 34| C34 | 5.2079 | 0.5298  | 2.2562  | C    |
| 35| H35 | 4.4292 | -1.4784 | 2.2223  | H    |
| 36| H36 | 6.0906 | -1.4025 | 1.6859  | H    |
| 37| H37 | 3.0893 | 1.0158  | 2.1050  | H    |
| 38| H38 | 4.1513 | 2.3012  | 1.5519  | H    |
| 39| H39 | 5.1425 | 0.5347  | 3.3367  | H    |
| 40| H40 | 6.1321 | 1.0225  | 1.9728  | H    |
| 41| C41 | -3.4321 | -2.1861 | -0.4366 | C    |
42 C42  -4.4586  -1.0792  -0.2410 C
43 O43  -3.7357  -3.2851  -0.7805 O
44 N44  -4.0046  0.0088  0.6026 N
45 C45  -4.7574  -0.4064  -1.5967 C
46 H46  -5.3496  -1.5707  0.1314 H
47 C47  -4.2722  1.3177  -0.0094 C
48 C48  -5.1887  0.9996  -1.1888 C
49 H49  -3.8560  -0.3591  -2.2020 H
50 H50  -5.5029  -0.9554  -2.1555 H
51 H51  -3.3508  1.7917  -0.3354 H
52 H52  -4.7414  1.9726  0.7127 H
53 H53  -5.0980  1.7169  -1.9953 H
54 H54  -6.2240  0.9920  -0.8631 H
55 C55  3.6261  1.3291  -0.8340 C
56 C56  2.8169  2.4743  -0.7557 C
57 H57  2.8265  3.1086  -1.6243 H
58 H58  2.7668  3.0068  0.1739 H
59 C59  3.9551  0.7630  -2.1913 C
60 H60  3.5431  -0.2298  -2.3313 H
61 H61  3.5647  1.4036  -2.9677 H
62 H62  5.0307  0.6951  -2.3162 H
63 H63  0.1626  -0.8878  -0.0780 H
64 H64  -1.9152  6.1014  0.0240 H
65 C65  -3.8926  -0.1087  1.9983 C
66 C66  -3.4003  0.8749  2.7485 C
67 H67  -3.3513  0.7700  3.8154 H
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 68| H68| -3.0548| 1.8029| 2.3328| H |
| 69| C69| -4.3599| -1.4020| 2.6234| C |
| 70| H70| -3.8355| -2.2684| 2.2323| H |
| 71| H71| -4.1907| -1.3742| 3.6907| H |
| 72| H72| -5.4204| -1.5595| 2.4556| H |

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3 1 10 1
4 2 3 Ar
5 2 11 1
6 3 4 Ar
7 3 7 1
8 4 5 Ar
9 4 12 1
10 5 6 Ar
11 5 13 1
12 6 64 1
13 7 8 2
14 7 9 1
15 14 15 2
16 14 22 Ar
17 14 25 Ar
18 15 16 2
19 15 19 1
20 16 17 Ar
@<TRIPOS>MOLECULE

Si-face catalyzed by 1

72 74

SMALL

NO_CHARGES

@<TRIPOS>ATOM

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | C1 | -1.1596 | -2.1653 | -0.8134 C |
| 2 | C2 | -1.1816 | -3.3346 | -1.5568 C |
| 3 | H3 | -2.1103 | -3.7872 | -1.8235 H |
| 4 | C4 | 0.0360 | -3.8769 | -1.9297 C |
| 5 | H5 | 0.0352 | -4.7836 | -2.5066 H |
| 6 | C6 | 1.2600 | -3.3074 | -1.5929 C |
| 7 | H7 | 2.1909 | -3.7379 | -1.8898 H |
| 8 | C8 | 1.2266 | -2.1497 | -0.8505 C |
| 9 | N9 | 0.0310 | -1.6242 | -0.4952 N |
|10 | H10| 0.0663 | -0.7464 | 0.0243 H |
|11 | N11| -2.2392 | -1.4669 | -0.3524 N |
|12 | H12| -2.0752 | -0.6660 | 0.2259 H |
|13 | C13| -3.5795 | -1.7678 | -0.5555 C |
|14 | O14| -3.9475 | -2.7217 | -1.1663 O |
|15 | C15| -4.5486 | -0.7417 | 0.0157 C |
|     |      |      |      |     |
|-----|------|------|------|-----|
| 16  | H16  | 8.4196 | 1.3044 | 0.3298 |
| 17  | C17  | 4.9396 | 0.2609 | -1.0905 |
| 18  | H18  | 4.0943 | 0.4467 | -1.7476 |
| 19  | H19  | 5.7533 | 0.1151 | -1.6954 |
| 20  | C20  | 5.2754 | 1.5237 | -0.3023 |
| 21  | H21  | 5.2256 | 2.4210 | -0.9069 |
| 22  | H22  | 6.2771 | 1.4522 | 0.1093 |
| 23  | C23  | 5.1633 | 0.0826 | 0.8256 |
| 24  | H24  | 3.3352 | 2.0311 | 0.5365 |
| 25  | H25  | 4.6185 | 1.9777 | 1.7289 |
| 26  | N26  | 3.9896 | 0.0875 | 1.0656 |
| 27  | C27  | 3.7660 | 0.3820 | 2.3703 |
| 28  | C28  | 3.2306 | 1.7835 | 2.6888 |
| 29  | H29  | 3.9707 | 2.0323 | 3.7082 |
| 30  | H30  | 3.7770 | 2.5301 | 2.0443 |
| 31  | H31  | 5.3071 | 1.8735 | 2.5851 |
| 32  | C22  | 1.1739 | 0.3695 | 3.2963 |
| 33  | H33  | 2.8284 | 1.3677 | 3.1001 |
| 34  | H34  | 3.0390 | 0.0039 | 4.2931 |
| 35  | N35  | 4.2879 | 1.4134 | 0.8880 |
| 36  | H36  | 2.0325 | 0.6000 | 0.1559 |
| 37  | C37  | 3.6170 | 1.6307 | 0.6282 |
| 38  | O38  | 4.0460 | 2.5140 | 1.3095 |
| 39  | C39  | 4.5846 | 0.6521 | 0.0562 |
| 40  | H40  | 5.2054 | 2.453 | 0.7269 |
| 41  | C41  | 5.4193 | 1.3817 | 1.1177 |
42 H42 5.6759 -2.3853 0.8108 H
43 H43 6.3387 -0.8293 1.2773 H
44 C44 4.5270 -1.3149 2.3574 C
45 H45 3.7683 -2.0897 2.3230 H
46 H46 5.0793 -1.4416 3.2792 H
47 C47 3.8842 0.0706 2.2720 C
48 H48 2.8657 0.0886 2.6283 H
49 H49 4.4606 0.8099 2.8148 H
50 N50 3.9275 0.4097 0.8281 N
51 C51 3.5573 1.5863 0.3586 C
52 C52 3.8258 1.9110 -1.0860 C
53 H53 3.4764 1.1306 -1.7515 H
54 H54 3.3409 2.8350 -1.3582 H
55 H55 4.8948 2.0287 -1.2380 H
56 C56 2.8227 2.4951 1.1449 C
57 H57 2.8358 3.5124 0.7974 H
58 H58 2.9114 2.4032 2.2120 H
59 C59 0.9417 1.8951 0.8926 C
60 H60 0.6697 2.3178 1.8536 H
61 O61 0.8960 0.6235 0.7955 O
62 C62 0.4402 2.7443 -0.2463 C
63 C63 0.2713 2.2185 -1.5222 C
64 H64 0.5280 1.1930 -1.7142 H
65 C65 -0.2256 3.0064 -2.5508 C
66 H66 -0.3475 2.5891 -3.5346 H
67 C67 -0.5672 4.3297 -2.3118 C
68 H68  -0.9531  4.9404  -3.1079 H
69 C69  -0.4124  4.8604  -1.0381 C
70 H70  -0.6827  5.8826  -0.8433 H
71 C71   0.0863  4.0707  -0.0143 C
72 H72   0.1979  4.4900  0.9715 H

@<TRIPOS>BOND
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2 1 9 Ar
3 1 11 Ar
4 2 3 1
5 2 4 2
6 4 5 1
7 4 6 Ar
8 6 7 1
9 6 8 2
10 8 9 Ar
11 8 35 Ar
12 9 10 1
13 11 12 1
14 11 13 1
15 13 14 2
16 13 15 1
17 15 16 1
18 15 17 1
19 15 26 1
20 17 18 1
@<TRIPOS>MOLECULE

**Re-face catalyzed by 2**

78 80

SMALL

NO_CHARGES

@<TRIPOS>ATOM

|   |   |   |   |   |
|---|---|---|---|---|
| 1 | C1 | 0.2153 | 3.5767 | -0.1521 C |
| 2 | C2 | 0.6848 | 2.8293 | -0.9125 C |
| 3 | C3 | 2.0537 | 2.9233 | -0.7147 C |
| 4 | C4 | 2.5369 | 3.7984 | 0.2586 C |
| 5 | C5 | 1.6553 | 4.5461 | 1.0179 C |
| 6 | C6 | 0.2834 | 4.4323 | 0.8181 C |
| 7 | H7 | 3.5975 | 3.8879 | 0.4138 H |
| 8 | H8 | 2.0312 | 5.2220 | 1.7659 H |
| 9 | H9 | -0.3933 | 5.0173 | 1.4164 H |
| 10| N10| 3.4894 | 0.9057 | -0.8226 N |
| 11| H11| 2.8506 | 0.1224 | -0.7655 H |
| 12| N12| -2.1596 | 2.0954 | -0.2576 N |
| 13| H13| -1.5415 | 1.4325 | 0.1517 H |
| 14| C14| -3.4298 | 1.7356 | -0.5367 C |
15 C15  -3.7335  0.2406  -0.3798 C
16 O16   -4.2467  2.5193  -0.9457 O
17 N17   -5.0537  -0.0030  0.1438 N
18 C18   -3.7551  -0.4439  -1.7588 C
19 H19   -2.9846  -0.2169  0.2585 H
20 C20   -5.9727  -0.5353  -0.8549 C
21 C21   -5.2237  -0.3521  -2.1736 C
22 H22   -3.0782   0.0186  -2.4674 H
23 H23   -3.4542  -1.4792  -1.6387 H
24 H24   -6.9146  -0.0013  -0.8530 H
25 H25   -6.1835  -1.5882  -0.6720 H
26 H26   -5.4356   0.6267  -2.5847 H
27 H27   -5.4997  -1.1012  -2.9077 H
28 C28    4.6567   0.9009  -0.1840 C
29 C29    5.0865  -0.3810   0.5460 C
30 O30    5.4321  1.8299  -0.1436 O
31 N31    4.0642  -1.4329   0.6393 N
32 C32    6.2281  -1.0805  -0.2026 C
33 H33    5.3997  -0.0679  1.5300 H
34 C34    4.3032  -2.5131  -0.3463 C
35 C35    5.4929  -2.0136  -1.1642 C
36 H36    6.8801  -0.3685  -0.6877 H
37 H37    6.8183  -1.6547   0.5051 H
38 H38    3.4179  -2.6690  -0.9378 H
39 H39    4.5454  -3.4221   0.1945 H
40 H40    5.1457  -1.4660  -2.0329 H
| Atom | X    | Y    | Z    | Type |
|------|------|------|------|------|
| H41  | 6.1107 | -2.8324 | -1.5126 | H    |
| H42  | 0.3078  | 2.1595  | -1.6668 | H    |
| C43  | -1.7047 | 3.4687  | -0.3971 | C    |
| H44  | -2.2429 | 4.1065  | 0.2939  | H    |
| H45  | -1.9499 | 3.8100  | -1.3956 | H    |
| C46  | 3.0090  | 2.0792  | -1.5367 | C    |
| H47  | 2.5095  | 1.7296  | -2.4307 | H    |
| H48  | 3.8661  | 2.6645  | -1.8348 | H    |
| C49  | -5.3478 | 0.1389  | 1.4806  | C    |
| C50  | -4.4759 | 0.5640  | 2.4046  | C    |
| H51  | -4.7842 | 0.6560  | 3.4284  | H    |
| H52  | -3.4695 | 0.8590  | 2.1782  | H    |
| C53  | -6.7628 | -0.2057 | 1.8790  | C    |
| H54  | -7.4729 | 0.4556  | 1.3934  | H    |
| H55  | -7.0172 | -1.2242 | 1.6041  | H    |
| H56  | -6.8834 | -0.1035 | 2.9487  | H    |
| C57  | 3.0990  | -1.4654 | 1.5193  | C    |
| C58  | 2.0542  | -2.4256 | 1.4505  | C    |
| H59  | 2.2754  | -3.3509 | 0.9498  | H    |
| H60  | 1.5206  | -2.5671 | 2.3758  | H    |
| C61  | 3.0021  | -0.3602 | 2.5377  | C    |
| H62  | 2.1048  | -0.4764 | 3.1273  | H    |
| H63  | 3.8555  | -0.3927 | 3.2076  | H    |
| H64  | 2.9804  | 0.6140  | 2.0646  | H    |
| C65  | 0.8650  | -1.5608 | 0.2634  | C    |
| O66  | 1.4976  | -1.1309 | -0.7514 | O    |
67 C67  -0.1628  -2.6589  0.0574 C
68 C68  -1.1191  -2.9421  1.0267 C
69 C69  -0.1779  -3.3757  -1.1332 C
70 C70  -2.0652  -3.9355  0.8211 C
71 H71  -1.1344  -2.3811  1.9467 H
72 C72  -1.1201  -4.3732  -1.3404 C
73 H73  0.5402  -3.1300  -1.8928 H
74 C74  -2.0645  -4.6587  -0.3636 C
75 H75  -2.8020  -4.1384  1.5783 H
76 H76  -1.1234  -4.9215  -2.2663 H
77 H77  -2.7967  -5.4297  -0.5267 H
78 H78  0.4801  -0.8165  0.9685 H

@<TRIPOS>BOND
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2 1 6 Ar
3 1 43 1
4 2 3 Ar
5 2 42 1
6 3 4 Ar
7 3 46 1
8 4 5 2
9 4 7 1
10 5 6 Ar
11 5 8 1
12 6 9 1
13 10 11 1
|   |   |   |   |
|---|---|---|---|
| 14| 10| 28| Ar|
| 15| 10| 46| 1  |
| 16| 12| 13| 1  |
| 17| 12| 14| Ar|
| 18| 12| 43| 1  |
| 19| 14| 15| 1  |
| 20| 14| 16| 2  |
| 21| 15| 17| 1  |
| 22| 15| 18| 1  |
| 23| 15| 19| 1  |
| 24| 17| 20| 1  |
| 25| 17| 49| Ar|
| 26| 18| 21| 1  |
| 27| 18| 22| 1  |
| 28| 18| 23| 1  |
| 29| 20| 21| 1  |
| 30| 20| 24| 1  |
| 31| 20| 25| 1  |
| 32| 21| 26| 1  |
| 33| 21| 27| 1  |
| 34| 28| 29| 1  |
| 35| 28| 30| 2  |
| 36| 29| 31| 1  |
| 37| 29| 32| 1  |
| 38| 29| 33| 1  |
| 39| 31| 34| 1  |
@<TRIPOS>MOLECULE

Si-face catalyzed by 2

78 80

SMALL

NO_CHARGES

@<TRIPOS>ATOM

1 C1  -0.2078  -2.8792  -1.9946 C
2 C2  0.8015  -1.9263  -2.0321 C
| At   | X   | Y   | Z   | Type |
|------|-----|-----|-----|------|
| 3 C  | 2.1390 | -2.2757 | -1.9229 | C    |
| 4 C  | 2.4761 | -3.6220 | -1.8409 | C    |
| 5 C  | 1.4818 | -4.5891 | -1.8489 | C    |
| 6 C  | 0.1446 | -4.2201 | -1.9092 | C    |
| 7 H  | 3.5091 | -3.9158 | -1.7666 | H    |
| 8 H  | 1.7470 | -5.6301 | -1.7910 | H    |
| 9 H  | -0.6202 | -4.9768 | -1.8841 | H    |
| 10 N | 3.1122 | -0.5318 | -0.5300 | N    |
| 11 H | 2.1966 | -0.2875 | -0.1888 | H    |
| 12 N | -1.9410 | -1.5769 | -0.8687 | N    |
| 13 H | -1.2329 | -0.9389 | -0.5599 | H    |
| 14 C | -3.1696 | -1.5083 | -0.3246 | C    |
| 15 C | -3.2769 | -0.5954 | 0.8999  | C    |
| 16 O | -4.1092 | -2.1566 | -0.7128 | O    |
| 17 N | -4.5687 | 0.0523  | 1.0496  | N    |
| 18 C | -3.1378 | -1.4683 | 2.1768  | C    |
| 19 H | -2.4890 | 0.1472  | 0.8571  | H    |
| 20 C | -5.3660 | -0.5996 | 2.0669  | C    |
| 21 C | -4.3130 | -1.0557 | 3.0691  | C    |
| 22 H | -3.2217 | -2.5169 | 1.9175  | H    |
| 23 H | -2.1736 | -1.3268 | 2.6509  | H    |
| 24 H | -5.9288 | -1.4411 | 1.6651  | H    |
| 25 H | -6.0670 | 0.1054  | 2.4966  | H    |
| 26 H | -4.6553 | -1.8662 | 3.7032  | H    |
| 27 H | -4.0359 | -0.2226 | 3.7081  | H    |
| 28 C | 4.1894  | 0.0446  | 0.0040  | C    |
|   |   |   |   |
|---|---|---|---|
| 29 C29 | 4.0758 | 0.6767 | 1.4011 C |
| 30 O30 | 5.2827 | 0.0621 | -0.5104 O |
| 31 N31 | 2.8047 | 0.4897 | 2.1260 N |
| 32 C32 | 5.0704 | -0.0101 | 2.3448 C |
| 33 H33 | 4.2838 | 1.7296 | 1.2941 H |
| 34 C34 | 2.8628 | -0.7327 | 2.9590 C |
| 35 C35 | 4.2949 | -1.2496 | 2.7899 C |
| 36 H36 | 6.0043 | -0.2290 | 1.8511 H |
| 37 H37 | 5.2668 | 0.6419 | 3.1908 H |
| 38 H38 | 2.1137 | -1.4397 | 2.6290 H |
| 39 H39 | 2.6659 | -0.4772 | 3.9910 H |
| 40 H40 | 4.3358 | -2.0150 | 2.0238 H |
| 41 H41 | 4.6718 | -1.6812 | 3.7090 H |
| 42 H42 | 0.5390 | -0.8858 | -2.0949 H |
| 43 C43 | -1.6528 | -2.4317 | -2.0102 C |
| 44 H44 | -1.8688 | -1.9014 | -2.9342 H |
| 45 H45 | -2.3189 | -3.2795 | -1.9663 H |
| 46 C46 | 3.1847 | -1.1871 | -1.8325 C |
| 47 H47 | 4.1789 | -1.5913 | -1.9443 H |
| 48 H48 | 3.0432 | -0.4578 | -2.6246 H |
| 49 C49 | -5.1593 | 0.8137 | 0.0501 C |
| 50 C50 | -6.4770 | 0.9859 | -0.0673 C |
| 51 H51 | -6.8679 | 1.6461 | -0.8182 H |
| 52 H52 | -7.1921 | 0.4790 | 0.5516 H |
| 53 C53 | -4.2050 | 1.5266 | -0.8776 C |
| 54 H54 | -4.7512 | 2.1915 | -1.5333 H |
|   |   |   |   |   |
|---|---|---|---|---|
|55 | H55  | -3.4849 | 2.1154 | -0.3177 H |
|56 | H56  | -3.6519 | 0.8331 | -1.5014 H |
|57 | C57  | 1.8585  | 1.3923 | 2.2376 C  |
|58 | C58  | 1.6880  | 2.4749 | 1.3399 C  |
|59 | H59  | 1.2485  | 3.3546 | 1.7805 H  |
|60 | H60  | 2.4952  | 2.6966 | 0.6650 H  |
|61 | C61  | 0.8021  | 1.1829 | 3.2890 C  |
|62 | H62  | 0.0861  | 1.9899 | 3.2672 H  |
|63 | H63  | 0.2781  | 0.2506 | 3.1129 H  |
|64 | H64  | 1.2450  | 1.1456 | 4.2781 H  |
|65 | C65  | 0.2597  | 1.7953 | 0.2443 C  |
|66 | O66  | 0.4352  | 0.5660 | -0.0240 O |
|67 | C67  | 0.2917  | 2.8164 | -0.8730 C |
|68 | C68  | 0.9475  | 2.5430 | -2.0674 C |
|69 | C69  | -0.3604 | 4.0358 | -0.7284 C |
|70 | C70  | 0.9615  | 3.4766 | -3.0926 C |
|71 | H71  | 1.4391  | 1.5969 | -2.1899 H |
|72 | C72  | -0.3519 | 4.9714 | -1.7526 C |
|73 | H73  | -0.8870 | 4.2564 | 0.1855 H  |
|74 | C74  | 0.3127  | 4.6943 | -2.9383 C |
|75 | H75  | 1.4726  | 3.2530 | -4.0124 H |
|76 | H76  | -0.8669 | 5.9077 | -1.6282 H |
|77 | H77  | 0.3197  | 5.4160 | -3.7357 H |
|78 | H78  | -0.5382 | 2.0386 | 0.9490 H  |

`@<TRIPOS>BOND`

1 1 2 Ar
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 6 | Ar | 3 | 1 | 43 | 1 | 4 | 2 | 3 | Ar | 5 | 2 | 42 | 1 | 6 | 3 | 4 | Ar |
| 7 | 3 | 46 | 1 | 8 | 4 | 5 | Ar | 9 | 4 | 7 | 1 | 10 | 5 | 6 | Ar | 11 | 5 | 8 | 1 |
| 12 | 6 | 9 | 1 | 13 | 10 | 11 | 1 | 14 | 10 | 28 | Ar | 15 | 10 | 46 | 1 | 16 | 12 | 13 | 1 |
| 17 | 12 | 14 | Ar | 18 | 12 | 43 | 1 | 19 | 14 | 15 | 1 | 20 | 14 | 16 | 2 | 21 | 15 | 17 | 1 |
| 22 | 15 | 18 | 1 | 23 | 15 | 19 | 1 | 24 | 17 | 20 | 1 | 25 | 17 | 49 | 1 | 26 | 18 | 21 | 1 |
| 27 | 18 | 22 | 1 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |

26
28 18 23 1
29 20 21 1
30 20 24 1
31 20 25 1
32 21 26 1
33 21 27 1
34 28 29 1
35 28 30 2
36 29 31 1
37 29 32 1
38 29 33 1
39 31 34 1
40 31 57 2
41 32 35 1
42 32 36 1
43 32 37 1
44 34 35 1
45 34 38 1
46 34 39 1
47 35 40 1
48 35 41 1
49 43 44 1
50 43 45 1
51 46 47 1
52 46 48 1
53 49 50 2
@<TRIPOS>MOLECULE

Re-face catalyzed by 3

78 80

SMALL

NO_CHARGES

@<TRIPOS>ATOM

1 C1  -1.2171  -2.2823  -0.8733 C
2 C2   0.2188  -2.4528  -1.3952 C
3 C3   0.4373  -3.8374  -2.0150 C
4 C4  -0.5716  -4.1026  -3.1341 C
5 C5  -2.0031  -3.9601  -2.6165 C
6 C6  -2.2232  -2.5810  -1.9943 C
7 H7   1.4535  -3.8921  -2.3970 H
8 H8   0.3582  -1.7184  -2.1844 H
9 H9  -1.3816  -2.9732  -0.0541 H
10 H10 -0.4120  -3.4046  -3.9555 H
11 H11 -0.4097  -5.0988  -3.5370 H
12 H12 -2.7156  -4.1161  -3.4220 H
13 H13 -2.1985  -4.7323  -1.8744 H
14 H14 -2.1182  -1.8165  -2.7634 H
15 H15 -3.2258  -2.4955  -1.5948 H
|   |   |   |   |   |
|---|---|---|---|---|
| 16 | H16 | 0.3464 | -4.6006 | -1.2549 H |
| 17 | N17 | 1.2251 | -2.0862 | -0.3972 N |
| 18 | H18 | 1.3799 | -1.0935 | -0.3410 H |
| 19 | N19 | -1.3913 | -0.9265 | -0.3643 N |
| 20 | H20 | -0.7103 | -0.2323 | -0.5991 H |
| 21 | C21 | -2.4262 | -0.5715 | 0.4174 C |
| 22 | C22 | -2.4526 | 0.9020 | 0.8494 C |
| 23 | O23 | -3.2763 | -1.3468 | 0.7859 O |
| 24 | N24 | -3.7609 | 1.5117 | 0.7306 N |
| 25 | C25 | -2.1813 | 1.0261 | 2.3558 C |
| 26 | H26 | -1.7197 | 1.4559 | 0.2794 H |
| 27 | C27 | -4.5561 | 1.3258 | 1.9334 C |
| 28 | C28 | -3.5613 | 0.8412 | 2.9998 C |
| 29 | H29 | -1.4511 | 0.3092 | 2.7127 H |
| 30 | H30 | -1.7978 | 2.0224 | 2.5517 H |
| 31 | H31 | -5.3428 | 0.5951 | 1.7759 H |
| 32 | H32 | -5.0237 | 2.2688 | 2.2026 H |
| 33 | H33 | -3.7350 | -0.2031 | 3.2197 H |
| 34 | H34 | -3.6527 | 1.3994 | 3.9252 H |
| 35 | C35 | 1.7247 | -2.8575 | 0.5699 C |
| 36 | C36 | 2.7722 | -2.2154 | 1.5064 C |
| 37 | O37 | 1.4797 | -4.0240 | 0.7597 O |
| 38 | N38 | 2.9277 | -0.7582 | 1.3736 N |
| 39 | C39 | 2.3734 | -2.3769 | 2.9746 C |
| 40 | H40 | 3.7047 | -2.7170 | 1.2931 H |
| 41 | C41 | 2.1617 | -0.0452 | 2.4233 C |
| Atom | X   | Y   | Z   | Type    |
|------|-----|-----|-----|---------|
| 68   | 1.1488 | 3.6135 | -0.2686 | C       |
| 69   | 2.9803 | 3.6754 | -1.8104 | C       |
| 70   | 1.0427 | 4.9943 | -0.3412 | C       |
| 71   | 0.4711 | 3.0457 | 0.3407  | H       |
| 72   | 2.8762 | 5.0567 | -1.8873 | C       |
| 73   | 3.7294 | 3.1669 | -2.3948 | H       |
| 74   | 1.9073 | 5.7207 | -1.1490 | C       |
| 75   | 0.2818 | 5.5028 | 0.2244  | H       |
| 76   | 3.5426 | 5.6104 | -2.5249 | H       |
| 77   | 1.8212 | 6.7911 | -1.2088 | H       |
| 78   | 2.7634 | 1.0510 | -1.8001 | H       |

@<TRIPOS>BOND

```
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2 1 6 1
3 1 9 1
4 1 19 1
5 2 3 1
6 2 8 1
7 2 17 1
8 3 4 1
9 3 7 1
10 3 16 1
11 4 5 1
12 4 10 1
13 4 11 1
14 5 6 1
```
|   |     |     |   |
|---|-----|-----|---|
| 15 | 5   | 12  | 1 |
| 16 | 5   | 13  | 1 |
| 17 | 6   | 14  | 1 |
| 18 | 6   | 15  | 1 |
| 19 | 17  | 18  | 1 |
| 20 | 17  | 35  | Ar|
| 21 | 19  | 20  | 1 |
| 22 | 19  | 21  | Ar|
| 23 | 21  | 22  | 1 |
| 24 | 21  | 23  | 2 |
| 25 | 22  | 24  | 1 |
| 26 | 22  | 25  | 1 |
| 27 | 22  | 26  | 1 |
| 28 | 24  | 27  | 1 |
| 29 | 24  | 57  | 1 |
| 30 | 25  | 28  | 1 |
| 31 | 25  | 29  | 1 |
| 32 | 25  | 30  | 1 |
| 33 | 27  | 28  | 1 |
| 34 | 27  | 31  | 1 |
| 35 | 27  | 32  | 1 |
| 36 | 28  | 33  | 1 |
| 37 | 28  | 34  | 1 |
| 38 | 35  | 36  | 1 |
| 39 | 35  | 37  | 2 |
| 40 | 36  | 38  | 1 |
|   |   |   |   |
|---|---|---|---|
| 41 | 36 | 39 | 1 |
| 42 | 36 | 40 | 1 |
| 43 | 38 | 41 | 1 |
| 44 | 38 | 49 | 2 |
| 45 | 39 | 42 | 1 |
| 46 | 39 | 43 | 1 |
| 47 | 39 | 44 | 1 |
| 48 | 41 | 42 | 1 |
| 49 | 41 | 45 | 1 |
| 50 | 41 | 46 | 1 |
| 51 | 42 | 47 | 1 |
| 52 | 42 | 48 | 1 |
| 53 | 49 | 50 | Ar |
| 54 | 49 | 53 | 1 |
| 55 | 50 | 51 | 1 |
| 56 | 50 | 52 | 1 |
| 57 | 53 | 54 | 1 |
| 58 | 53 | 55 | 1 |
| 59 | 53 | 56 | 1 |
| 60 | 57 | 58 | 2 |
| 61 | 57 | 61 | 1 |
| 62 | 58 | 59 | 1 |
| 63 | 58 | 60 | 1 |
| 64 | 61 | 62 | 1 |
| 65 | 61 | 63 | 1 |
| 66 | 61 | 64 | 1 |
@<TRIPOS>MOLECULE

*Si*-face catalyzed by 3

78 80

SMALL

NO_CHARGES

@<TRIPOS>ATOM

1 C1 –1.5246  1.4585  1.5009 C
2 C2  –0.0915  1.7048  2.0018 C
3 C3  –0.0223  2.9136  2.9418 C
4 C4  -0.9832  2.7547  4.1221 C
5 C5  -2.4113  2.5073  3.6352 C
6 C6  -2.4707  1.2992  2.6992 C
7 H7  1.0001  3.0173  3.2951 H
8 H8  0.2024  0.8278  2.5715 H
9 H9  -1.8465  2.3076  0.9097 H
10 H10 -0.6656  1.9209  4.7476 H
11 H11 -0.9419  3.6437  4.7462 H
12 H12 -3.0769  2.3497  4.4797 H
13 H13 -2.7750  3.3908  3.1133 H
14 H14 -2.1900  0.3999  3.2465 H
15 H15 -3.4778  1.1485  2.3330 H
16 H16 -0.2631  3.8148  2.3925 H
17 N17  0.8976  1.7693  0.9267 N
18 H18  1.2893  0.8755  0.6867 H
19 N19 -1.5440  0.2741  0.6495 N
20 H20 -0.7188 -0.2894  0.5882 H
21 C21 -2.5881 -0.0424 -0.1321 C
22 C22 -2.4304 -1.3249 -0.9632 C
23 O23 -3.5937  0.6256 -0.2081 O
24 N24 -3.5271 -2.2577 -0.7841 N
25 C25 -2.5293 -1.0127 -2.4627 C
26 H26 -1.4879 -1.7977 -0.7246 H
27 C27 -4.6369 -1.9445 -1.6695 C
28 C28 -4.0355 -1.0449 -2.7627 C
29 H29 -2.0733 -0.0645 -2.7256 H
|   |    |    |    |    |    |    |    |    |    |
|---|----|----|----|----|----|----|----|----|----|
| 30 H30 | -2.0159 | -1.7990 | -3.0074 H |
| 31 H31 | -5.4324 | -1.4284 | -1.1417 H |
| 32 H32 | -5.0432 | -2.8685 | -2.0694 H |
| 33 H33 | -4.4538 | -0.0506 | -2.6961 H |
| 34 H34 | -4.2356 | -1.4284 | -3.7574 H |
| 35 C35 | 0.9867  | 2.7370  | 0.0117 C  |
| 36 C36 | 2.0441  | 2.4924  | -1.0943 C |
| 37 O37 | 0.3522  | 3.7632  | 0.0098 O  |
| 38 N38 | 1.5931  | 1.4682  | -2.0543 N |
| 39 C39 | 2.1967  | 3.7151  | -1.9979 C |
| 40 H40 | 2.9715  | 2.1914  | -0.6371 H |
| 41 C41 | 0.5878  | 2.1173  | -2.9203 C |
| 42 C42 | 1.0309  | 3.5939  | -2.9957 C |
| 43 H43 | 2.1709  | 4.6380  | -1.4391 H |
| 44 H44 | 3.1503  | 3.6451  | -2.5114 H |
| 45 H45 | -0.3847 | 2.0184  | -2.4563 H |
| 46 H46 | 0.5518  | 1.6449  | -3.8866 H |
| 47 H47 | 0.2150  | 4.2440  | -2.7166 H |
| 48 H48 | 1.3412  | 3.8537  | -4.0009 H |
| 49 C49 | 2.1710  | 0.3136  | -2.2933 C |
| 50 C50 | 3.1466  | -0.3002 | -1.4676 C |
| 51 H51 | 3.8168  | -0.9446 | -2.0115 H |
| 52 H52 | 3.6497  | 0.3072  | -0.7374 H |
| 53 C53 | 1.6961  | -0.4823 | -3.4851 C |
| 54 H54 | 0.6254  | -0.6408 | -3.4475 H |
| 55 H55 | 1.9325  | 0.0349  | -4.4091 H |
56 H56  2.1852  -1.4441  -3.5048 H
57 C57  -3.7321  -2.9980  0.3698 C
58 C58  -4.9236  -3.4833  0.7296 C
59 H59  -5.0072  -4.1113  1.5964 H
60 H60  -5.8271  -3.2850  0.1866 H
61 C61  -2.4998  -3.3139  1.1841 C
62 H62  -2.7561  -3.9793  1.9977 H
63 H63  -1.7444  -3.7983  0.5725 H
64 H64  -2.0561  -2.4216  1.6104 H
65 C65  2.1435  -1.5458  -0.3558 C
66 O66  1.2219  -0.9238  0.2428 O
67 C67  3.2862  -2.1253  0.4504 C
68 C68  4.0949  -3.1246  -0.0799 C
69 C69  3.5158  -1.6924  1.7505 C
70 C70  5.1264  -3.6731  0.6668 C
71 H71  3.9155  -3.4844  -1.0798 H
72 C72  4.5493  -2.2360  2.4995 C
73 H73  2.8724  -0.9439  2.1732 H
74 C74  5.3590  -3.2255  1.9599 C
75 H75  5.7407  -4.4492  0.2455 H
76 H76  4.7168  -1.8948  3.5059 H
77 H77  6.1566  -3.6501  2.5433 H
78 H78  1.8547  -2.2241  -1.1602 H

@<TRIPOS>BOND
1 1 2 1
2 1 6 1
3 1 9 1
4 1 19 1
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7 2 17 1
8 3 4 1
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11 4 5 1
12 4 10 1
13 4 11 1
14 5 6 1
15 5 12 1
16 5 13 1
17 6 14 1
18 6 15 1
19 17 18 1
20 17 35 Ar
21 19 20 1
22 19 21 Ar
23 21 22 1
24 21 23 2
25 22 24 1
26 22 25 1
27 22 26 1
28 24 27 1
|    |    |    |    |
|----|----|----|----|
| 55 | 50 | 51 | 1  |
| 56 | 50 | 52 | 1  |
| 57 | 53 | 54 | 1  |
| 58 | 53 | 55 | 1  |
| 59 | 53 | 56 | 1  |
| 60 | 57 | 58 | 2  |
| 61 | 57 | 61 | 1  |
| 62 | 58 | 59 | 1  |
| 63 | 58 | 60 | 1  |
| 64 | 61 | 62 | 1  |
| 65 | 61 | 63 | 1  |
| 66 | 61 | 64 | 1  |
| 67 | 65 | 66 | 2  |
| 68 | 65 | 67 | 1  |
| 69 | 65 | 78 | 1  |
| 70 | 67 | 68 | Ar|
| 71 | 67 | 69 | Ar|
| 72 | 68 | 70 | Ar|
| 73 | 68 | 71 | 1  |
| 74 | 69 | 72 | Ar|
| 75 | 69 | 73 | 1  |
| 76 | 70 | 74 | Ar|
| 77 | 70 | 75 | 1  |
| 78 | 72 | 74 | Ar|
| 79 | 72 | 76 | 1  |
| 80 | 74 | 77 | 1  |