

## Designing benzosiloles for better optoelectronic properties using DFT & TDDFT approaches

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### SUPPLEMENTARY MATERIAL

#### SM1

Table SM1: comparison of computed bond parameter of BS3 with crystal data

| Bond length | BS3    | Crystal Structure |
|-------------|--------|-------------------|
| 1C-2C       | 1.4178 | 1.4173            |
| 2C-3C       | 1.3903 | 1.3901            |
| 3C-4C       | 1.3997 | 1.3997            |
| 4C-5C       | 1.3928 | 1.3847            |
| 5C-6C       | 1.3951 | 1.3894            |
| 7C-8C       | 1.3973 | 1.3490            |
| 8C-15C      | 1.4695 | 1.4730            |
| 15C-16C     | 1.4052 | 1.4033            |
| 16C-18C     | 1.3889 | 1.3887            |
| 18C-22C     | 1.4012 | 1.3993            |
| 22C-20C     | 1.4045 | 1.3994            |
| 20C-17C     | 1.3863 | 1.3846            |
| 22C-33C     | 1.4830 | 1.4869            |
| 33C-34C     | 1.4032 | 1.4016            |
| 34C-36C     | 1.3914 | 1.3855            |
| 36C-40C     | 1.3934 | 1.3928            |
| 40C-38C     | 1.3933 | 1.3887            |
| 38C-35C     | 1.3914 | 1.3879            |
| 35C-33C     | 1.4031 | 1.4022            |
| Si14-29C    | 1.8852 | 1.8605            |
| Si14-25C    | 1.8887 | 1.8666            |
| 2C-14Si     | 1.8851 | 1.8766            |
| 8C-14Si     | 1.9037 | 1.8841            |

**SM2**

Table SM2 Calculated absorption maxima in dichloromethane medium from TDDFT//PBE0/6-311g(d,p) calculations along with experimentally reported absorption maxima.

| DCM | Experiment |
|-----|------------|
| 331 | 333        |
| 336 | 338        |
| 353 | ---        |
| 350 | ---        |
| 336 | 336        |
| 355 | 350        |
| 344 | 339        |
| 360 | ---        |
| 379 | ---        |
| 301 | ---        |
| 301 | ---        |
| 343 | 339        |

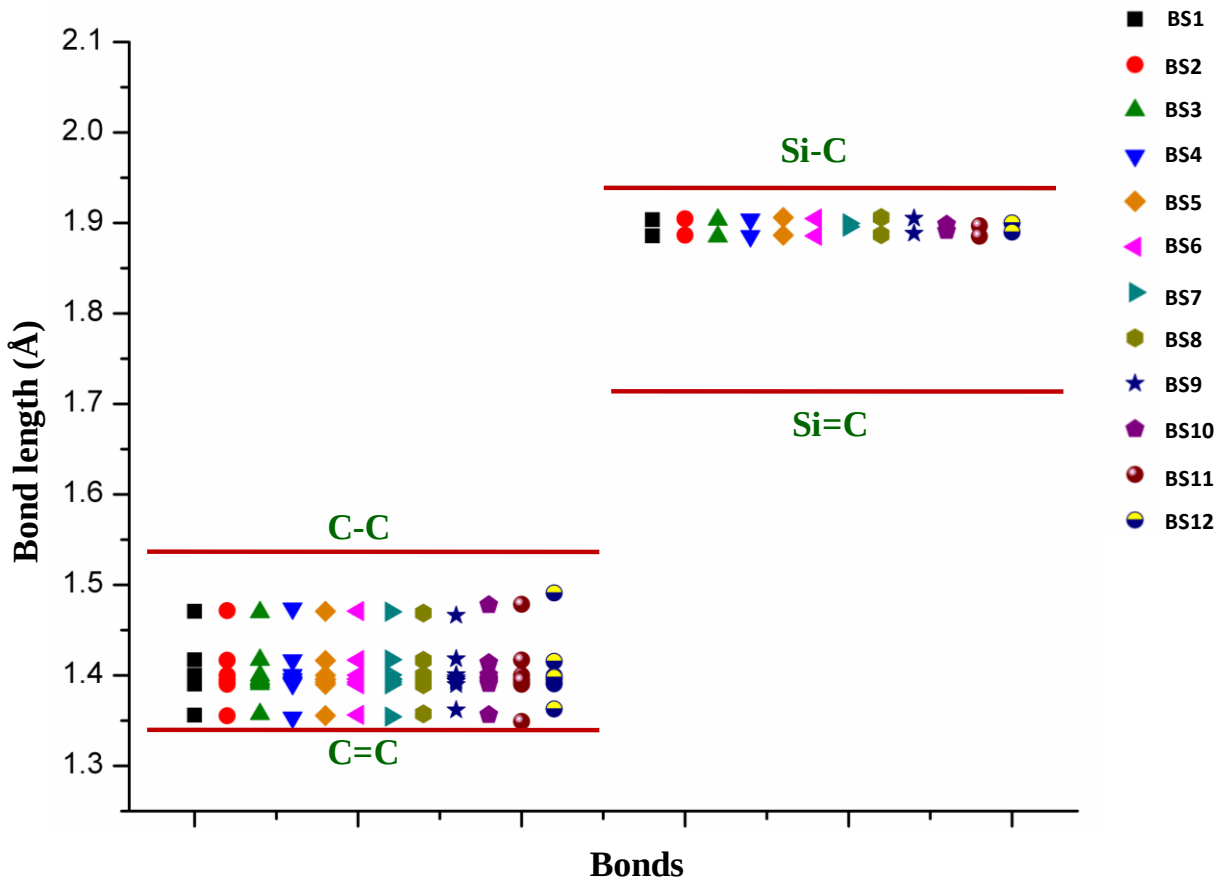
SM3

Table SM3: The computed bond parameters of optimized geometries at B3LYP/6-311g(d,p) level

|      | C1-C2  | C2-C3  | C3-C4  | C4-C5  | C5-C6  | C1-C6  | C1-C7  | C7-C8  | C8-Si14 | C2-Si14 | C2-Si14-C8 |
|------|--------|--------|--------|--------|--------|--------|--------|--------|---------|---------|------------|
| BS1  | 1.4171 | 1.3904 | 1.3999 | 1.3928 | 1.3952 | 1.3964 | 1.4707 | 1.3561 | 1.9036  | 1.8857  | 91.8       |
| BS2  | 1.4166 | 1.3902 | 1.4001 | 1.3927 | 1.3956 | 1.3959 | 1.4714 | 1.3554 | 1.9045  | 1.8864  | 91.7       |
| BS3  | 1.4171 | 1.3903 | 1.3999 | 1.3929 | 1.3951 | 1.3967 | 1.4699 | 1.3573 | 1.9037  | 1.8851  | 91.8       |
| BS4  | 1.4166 | 1.3907 | 1.4004 | 1.3924 | 1.3958 | 1.3956 | 1.4738 | 1.3535 | 1.9039  | 1.8855  | 91.8       |
| BS5  | 1.4164 | 1.3902 | 1.4000 | 1.3927 | 1.3954 | 1.3958 | 1.4708 | 1.3555 | 1.9061  | 1.8864  | 91.6       |
| BS6  | 1.4168 | 1.3901 | 1.4002 | 1.3926 | 1.3956 | 1.3962 | 1.4709 | 1.3564 | 1.9049  | 1.8858  | 91.9       |
| BS7  | 1.4173 | 1.3902 | 1.4004 | 1.3927 | 1.3952 | 1.3962 | 1.4704 | 1.3543 | 1.8995  | 1.8960  | 90.7       |
| BS8  | 1.4166 | 1.3897 | 1.4001 | 1.3928 | 1.3954 | 1.3965 | 1.4689 | 1.3576 | 1.9060  | 1.8870  | 91.4       |
| BS9  | 1.4180 | 1.3897 | 1.4004 | 1.3930 | 1.3949 | 1.3972 | 1.4663 | 1.3616 | 1.9051  | 1.8884  | 91.5       |
| BS10 | 1.4137 | 1.3905 | 1.3999 | 1.3931 | 1.3956 | 1.3952 | 1.4778 | 1.3563 | 1.8983  | 1.8912  | 92.5       |
| BS11 | 1.4168 | 1.3902 | 1.3999 | 1.3919 | 1.3964 | 1.3945 | 1.4784 | 1.3491 | 1.8968  | 1.8852  | 92.0       |
| BS12 | 1.4155 | 1.3905 | 1.3993 | 1.3919 | 1.3955 | 1.3978 | 1.4911 | 1.3629 | 1.8999  | 1.8899  | 90.6       |

SM4

Figure SM4 Illustration of  $\pi$ -delocalization from calculated C-C and Si-C bond lengths at B3LYP/6-311g(d,p) level.



SM5

Table SM5 The computed hybridization of C<sub>2</sub> & C<sub>5</sub> of the studied BSs.

| BSs | C <sub>2</sub>     | C <sub>5</sub>     |
|-----|--------------------|--------------------|
| 1   | sp <sup>2.38</sup> | sp <sup>2.56</sup> |
| 2   | sp <sup>2.37</sup> | sp <sup>2.55</sup> |
| 3   | sp <sup>2.38</sup> | sp <sup>2.56</sup> |
| 4   | sp <sup>2.37</sup> | sp <sup>2.59</sup> |
| 5   | sp <sup>2.37</sup> | sp <sup>2.52</sup> |
| 6   | sp <sup>2.37</sup> | sp <sup>2.57</sup> |
| 7   | sp <sup>2.34</sup> | sp <sup>2.53</sup> |
| 8   | sp <sup>2.38</sup> | sp <sup>2.53</sup> |
| 9   | sp <sup>2.37</sup> | sp <sup>2.49</sup> |
| 10  | sp <sup>2.37</sup> | sp <sup>2.34</sup> |
| 11  | sp <sup>2.40</sup> | sp <sup>2.57</sup> |
| 12  | sp <sup>2.33</sup> | sp <sup>2.71</sup> |

**SM6**

The bond ellipticity ( $\epsilon$ ) at the bond critical point (bcp), obtained by means of topological analysis of the electron density is used to understand the character of a chemical bond. The bond ellipticity ( $\epsilon$ ), which is defined as  $(\lambda_1/\lambda_2) - 1$ , where  $\lambda$  is the eigen value at the bcp, also provides quantitative evidence for the  $\pi$  character of a molecule. When  $\epsilon \rightarrow 0$ , the bond belongs to a typical  $\sigma$  bond, and larger is the  $\epsilon$  value, stronger will be the  $\pi$  character. The calculated ellipticity values (SM5) indicate the existence of delocalization of  $\pi$  bond throughout the molecule. It is interesting to note that the bond ellipticity of Si-C in BSs is in the order of  $\sim 10^{-9}$  and Si=C is in the order of  $\sim 10^{-1}$  and our calculated results clearly tells that the bond ellipticities lie in between the pure Si-C and Si=C.

Table SM6 The computed bond ellipticity at bond critical points of Si-C in BSs.

| Molecules | Si-C <sub>2</sub> | Si-C <sub>5</sub> |
|-----------|-------------------|-------------------|
| BS1       | 1.62329859e-002   | 2.15642737e-002   |
| BS2       | 1.50127246e-002   | 2.17464305e-002   |
| BS3       | 1.69108406e-002   | 2.08416332e-002   |
| BS4       | 1.31661781e-002   | 2.75035664e-002   |
| BS5       | 1.54020560e-002   | 2.06056860e-002   |
| BS6       | 2.13700907e-002   | 1.54395485e-002   |
| BS7       | 9.87240450e-003   | 2.05521913e-002   |
| BS8       | 1.5365097e-002    | 1.9144773e-002    |
| BS9       | 1.20438303e-002   | 1.44103386e-002   |
| BS10      | 8.63919606e-003   | 4.11768805e-003   |
| BS11      | 2.48164398e-002   | 1.12926311e-002   |
| BS12      | 7.90002774e-003   | 2.34412103e-002   |

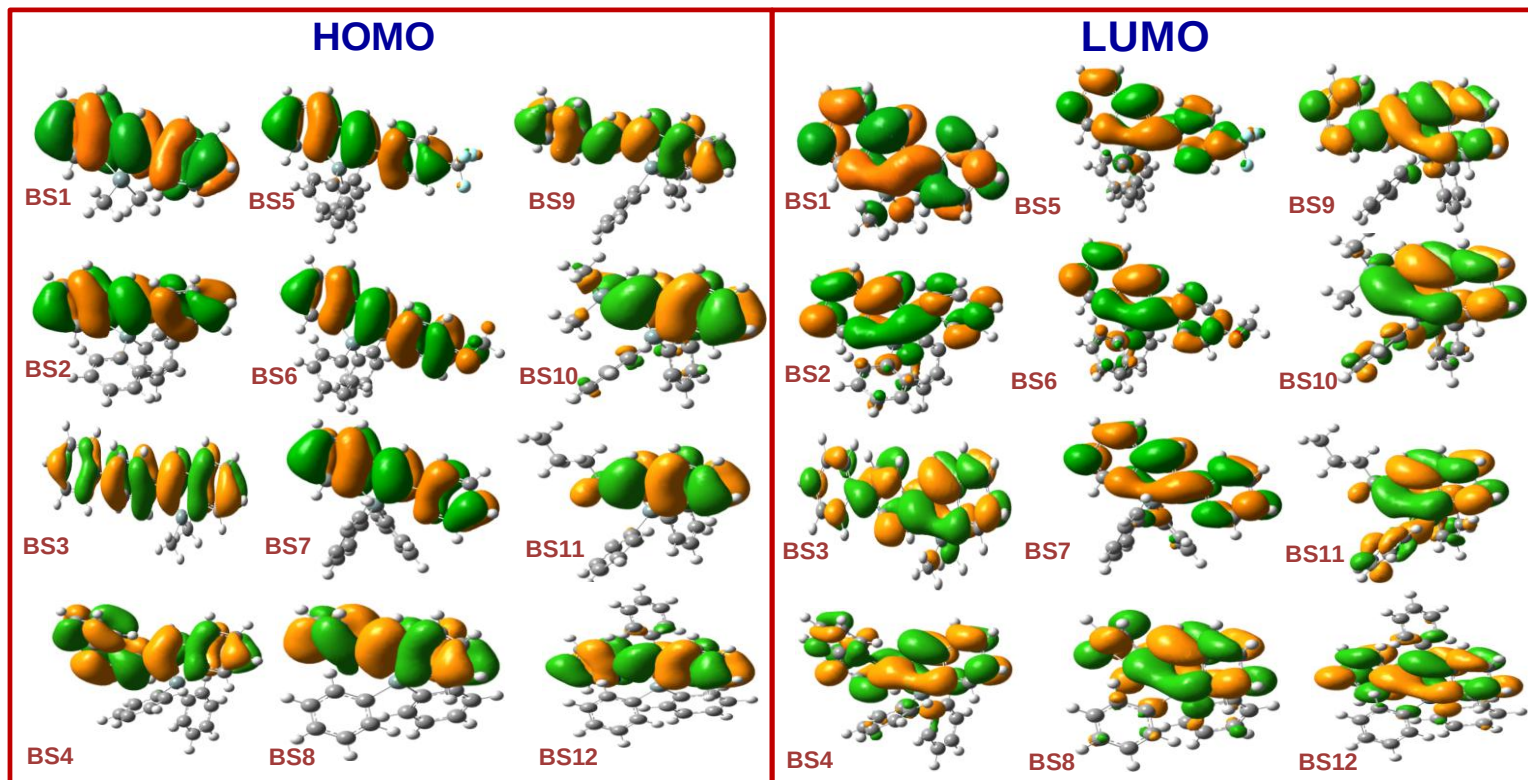
**SM7**

Table SM7: Estimated dipole moment of benzosilole derivatives at B3LYP/6-311g(d,p) level

| Molecule | Dipole moment in Debye |
|----------|------------------------|
| BS1      | 0.3858                 |
| BS2      | 0.4765                 |
| BS3      | 0.3643                 |
| BS4      | 0.6527                 |
| BS5      | 3.8635                 |
| BS6      | 1.3468                 |
| BS7      | 1.7924                 |
| BS8      | 0.3350                 |
| BS9      | 0.4411                 |
| BS10     | 0.4757                 |
| BS11     | 0.6895                 |
| BS12     | 2.3119                 |

SM8

Figure SM8: HOMO & LUMO of BSs (1-12)





SM9

Table SM9: NBO results obtained at B3LYP/6-311g(d,p) using G09 for benzosilole derivatives

| Molecules | Donor (i)             | Acceptor (j)            | E(2)<br>(kJ mol <sup>-1</sup> ) | E(j)-E(i)<br>(a.u) | F(i,j)<br>(a.u) |
|-----------|-----------------------|-------------------------|---------------------------------|--------------------|-----------------|
| BS1       | $\pi(C_{15}-C_{16})$  | $\pi^*(C_{18}-C_{22})$  | 21.61                           | 0.28               | 0.070           |
| BS2       | $\pi(C_{29}-C_{33})$  | $\pi^*(C_{26}-C_{27})$  | 22.06                           | 0.28               | 0.071           |
| BS3       | $\pi(C_{33}-C_{35})$  | $\pi^*(C_{38}-C_{40})$  | 21.50                           | 0.28               | 0.070           |
| BS4       | $\pi(C_{29}-C_{33})$  | $\pi^*(C_{26}-C_{27})$  | 21.96                           | 0.28               | 0.070           |
| BS5       | $\pi(C_{15}-C_{16})$  | $\pi^*(C_{18}-C_{22})$  | 23.97                           | 0.27               | 0.073           |
| BS6       | LP( 2)O <sub>47</sub> | $\pi^*(C_{20}-C_{22})$  | 30.41                           | 0.34               | 0.097           |
| BS7       | $\pi(C_{37}-N_{39})$  | $\pi^*(C_{42}-C_{43})$  | 28.03                           | 0.32               | 0.084           |
| BS8       | LP(2)S <sub>39</sub>  | $\pi^*(C_{40}-C_{42})$  | 22.31                           | 0.26               | 0.069           |
| BS9       | $\pi(C_{20}-C_{22})$  | $\pi^*(C_{15} -C_{17})$ | 22.19                           | 0.28               | 0.071           |
| BS10      | $\pi(C_{29}-C_{33})$  | $\pi^*(C_{26}-C_{27})$  | 22.06                           | 0.28               | 0.071           |
| BS11      | $\pi(C_{29}-C_{33})$  | $\pi^*(C_{26}-C_{27})$  | 21.97                           | 0.28               | 0.070           |
| BS12      | $\pi(C_{47}-N_{49})$  | $\pi^*(C_{52}-C_{53})$  | 28.14                           | 0.32               | 0.084           |

SM10

Table SM10: Molecular Orbital Composition (%) in the Ground State for designed candidates

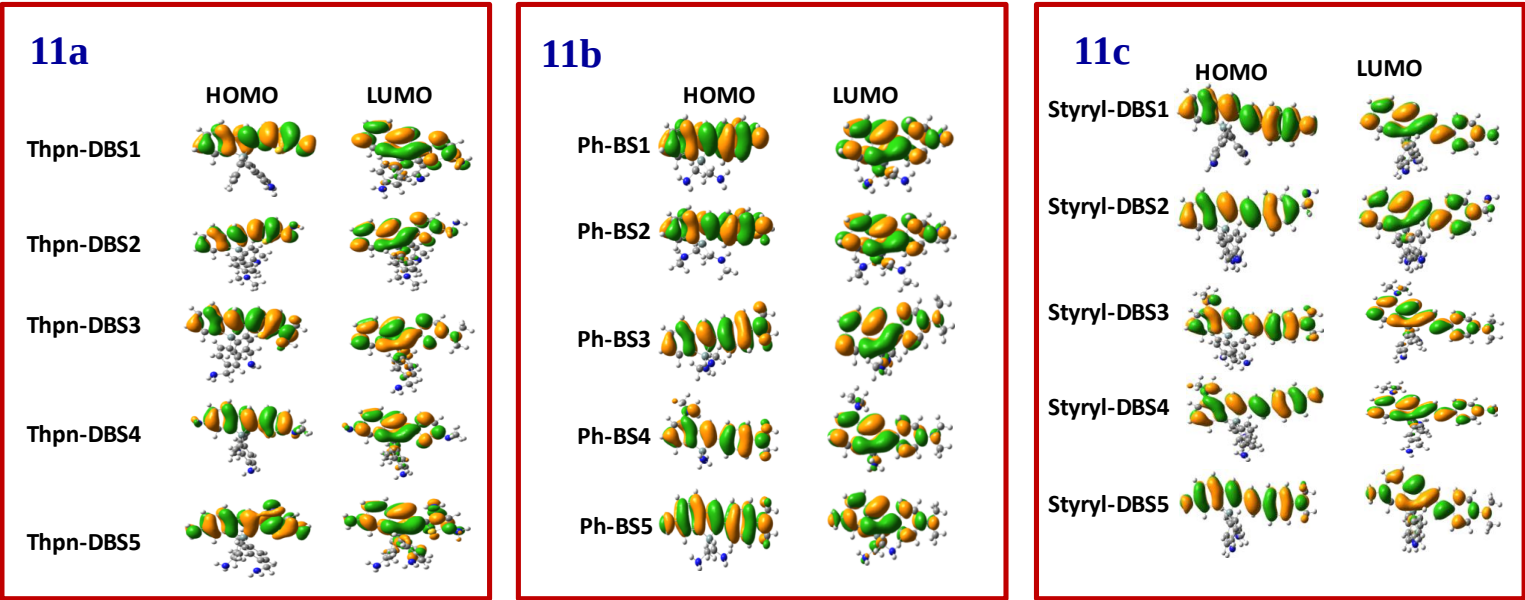
| Fragments      | Molecules |      |        |      |        |      |        |      |        |      |
|----------------|-----------|------|--------|------|--------|------|--------|------|--------|------|
|                | Ph-BS1    |      | Ph-BS2 |      | Ph-BS3 |      | Ph-BS4 |      | Ph-BS5 |      |
|                | HOMO      | LUMO | HOMO   | LUMO | HOMO   | LUMO | HOMO   | LUMO | HOMO   | LUMO |
| R              | 42%       | 65%  | 36%    | 66%  | 32%    | 69%  | 36%    | 69%  | 42%    | 60%  |
| R <sub>1</sub> | 57%       | 23%  | 63%    | 23%  | 68%    | 22%  | 56%    | 21%  | 48%    | 24%  |
| R <sub>2</sub> | 1%        | 12%  | 1%     | 11%  | -      | 9%   | 7%     | 7%   | 1%     | 13%  |
| R <sub>3</sub> | -         | -    | -      | -    | -      | -    | -      | 3%   | 9%     | 3%   |

| Fragments      | Molecules |      |           |      |           |      |           |      |           |      |
|----------------|-----------|------|-----------|------|-----------|------|-----------|------|-----------|------|
|                | Thpn-DBS1 |      | Thpn-DBS2 |      | Thpn-DBS3 |      | Thpn-DBS4 |      | Thpn-DBS5 |      |
|                | HOMO      | LUMO | HOMO      | LUMO | HOMO      | LUMO | HOMO      | LUMO | HOMO      | LUMO |
| R              | 35%       | 55%  | 46%       | 55%  | 37%       | 59%  | 38%       | 57%  | 37%       | 50%  |
| R <sub>1</sub> | 63%       | 38%  | 52%       | 37%  | 61%       | 34%  | 53%       | 33%  | 54%       | 39%  |
| R <sub>2</sub> | 2%        | 7%   | 2%        | 8%   | 2%        | 7%   | 2%        | 7%   | 1%        | 8%   |
| R <sub>3</sub> | -         | -    | -         | -    | -         | -    | 8%        | 3%   | 8%        | 3%   |

| Fragments      | Molecules   |      |             |      |             |      |             |      |             |      |
|----------------|-------------|------|-------------|------|-------------|------|-------------|------|-------------|------|
|                | Styryl-DBS1 |      | Styryl-DBS2 |      | Styryl-DBS3 |      | Styryl-DBS4 |      | Styryl-DBS5 |      |
|                | HOMO        | LUMO | HOMO        | LUMO | HOMO        | LUMO | HOMO        | LUMO | HOMO        | LUMO |
| R              | 35%         | 61%  | 33%         | 61%  | 29%         | 59%  | 36%         | 56%  | 36%         | 57%  |
| R <sub>1</sub> | 63%         | 26%  | 65%         | 27%  | 69%         | 29%  | 56%         | 27%  | 57%         | 19%  |
| R <sub>2</sub> | 2%          | 12%  | 2%          | 12%  | 2%          | 15%  | 1%          | 14%  | 1%          | 21%  |
| R <sub>3</sub> | -           | -    | -           | -    | -           | -    | 7%          | 3%   | 7%          | 3%   |

SM11

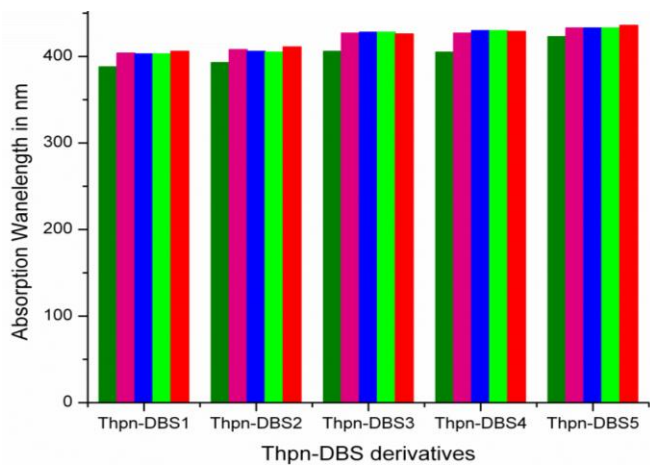
Figure SM11: Highest Occupied Molecular Orbital and Lowest Unoccupied Molecular Orbitals of designed candidates



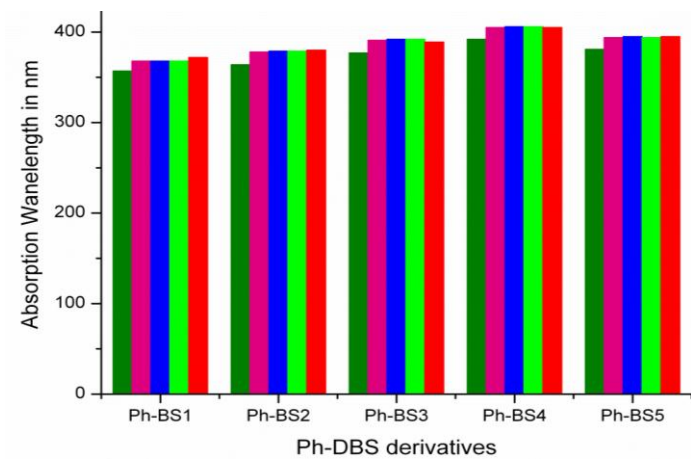
SM12

Figure SM12: The calculated absorption maxima of all the designed candidates at PBE0/6-311g(d,p) level both in gas as well as solvent phase.

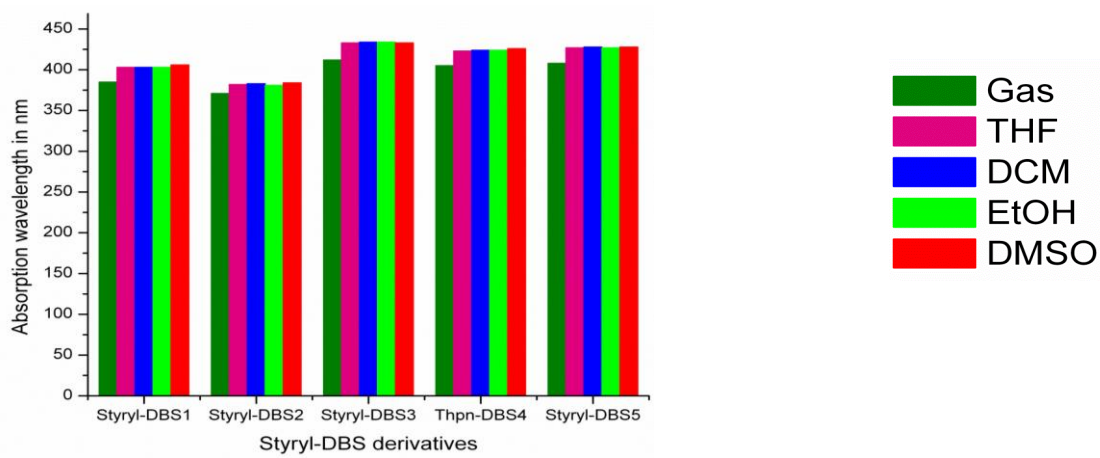
12a



12b



12c



SM13

Table SM13: NBO results obtained at B3LYP/6-311g(d,p) using G09 for designed benzosilole derivatives

| molecule  | donor    | acceptor            | E(KJ mol-1) | E(j)-E(i)(a.u) | F(i,j)(a.u) |
|-----------|----------|---------------------|-------------|----------------|-------------|
| Thpn-DBS1 | LP (N45) | $\pi^*$ (C18 - C22) | 28.03       | 0.33           | 0.091       |
| Thpn-DBS2 | LP (N45) | $\pi^*$ (C30 - C32) | 40.97       | 0.28           | 0.100       |
| Thpn-DBS3 | LP (N42) | $\pi^*$ (C38 - C40) | 37.40       | 0.29           | 0.096       |
| Thpn-DBS4 | LP (N41) | $\pi^*$ (C37 - C39) | 35.79       | 0.29           | 0.094       |
| Thpn-DBS5 | LP (N46) | $\pi^*$ (C34 - C35) | 26.55       | 0.35           | 0.092       |

| molecule   | donor             | acceptor            | E(KJ mol-1) | E(j)-E(i)(a.u) | F(i,j)(a.u) |
|------------|-------------------|---------------------|-------------|----------------|-------------|
| Stryl-DBS1 | LP (N55)          | $\pi^*$ (C30 - C32) | 27.95       | 0.33           | 0.091       |
| Stryl-DBS2 | $\pi$ (C20 - C22) | $\pi^*$ (C20 - C22) | 23.19       | 0.28           | 0.072       |
| Stryl-DBS3 | LP (N63)          | $\pi^*$ (C43 - C45) | 40.88       | 0.28           | 0.100       |
| Stryl-DBS4 | LP (N69)          | $\pi^*$ (C43 - C45) | 27.35       | 0.33           | 0.091       |
| Stryl-DBS5 | LP (N47)          | $\pi^*$ (C42 - C44) | 40.39       | 0.28           | 0.099       |

| molecule | donor     | acceptor              | E(KJ mol-1) | E(j)-E(i)(a.u) | F(i,j)(a.u) |
|----------|-----------|-----------------------|-------------|----------------|-------------|
| Ph-BS1   | LP (N 33) | $\pi^*$ (C 18 - C 22) | 27.65       | 0.33           | 0.091       |
| Ph-BS2   | LP (N 27) | $\pi^*$ (C 18 - C 21) | 18.93       | 0.29           | 0.099       |
| Ph-BS3   | LP (N 25) | $\pi^*$ (C 18 - C 22) | 40.95       | 0.28           | 0.100       |
| Ph-BS4   | LP (N 24) | $\pi^*$ (C 17 - C 21) | 40.44       | 0.28           | 0.099       |
| Ph-BS5   | LP (N 32) | $\pi^*$ (C 17 - C 21) | 40.32       | 0.28           | 0.099       |

**Coordinates of the optimized geometries**

BS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.78131200 | -1.06848800 | -0.11769900 |
| C  | -2.14457600 | 0.29169600  | 0.04423100  |
| C  | -3.49159900 | 0.63221800  | 0.09719300  |
| C  | -4.47742900 | -0.35657500 | -0.00336700 |
| C  | -4.11246100 | -1.69147000 | -0.16094800 |
| C  | -2.76624300 | -2.05308300 | -0.22027400 |
| C  | -0.33412800 | -1.32604600 | -0.16663700 |
| C  | 0.51451300  | -0.27329400 | -0.06367900 |
| H  | -3.79395300 | 1.66836500  | 0.21820300  |
| H  | -5.52603200 | -0.08373200 | 0.04143200  |
| H  | -4.87884900 | -2.45491200 | -0.23910400 |
| H  | -2.48623700 | -3.09439600 | -0.34514100 |
| H  | 0.00799100  | -2.35103200 | -0.29729000 |
| Si | -0.54947100 | 1.29453600  | 0.11948700  |
| C  | 1.98152300  | -0.39181800 | -0.05025500 |
| C  | 2.79231600  | 0.67940600  | -0.46348500 |
| C  | 2.62856000  | -1.56400800 | 0.38427100  |
| C  | 4.18028300  | 0.57860800  | -0.46844500 |
| H  | 2.32775700  | 1.59722000  | -0.80523000 |
| C  | 4.01429200  | -1.66541700 | 0.38143400  |
| H  | 2.03580200  | -2.39428800 | 0.75033700  |
| C  | 4.79960700  | -0.59556300 | -0.04800000 |
| H  | 4.77853400  | 1.41975200  | -0.80125900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.48569500  | -2.57937800 | 0.72622100  |
| H | 5.88077600  | -0.67446600 | -0.04569800 |
| C | -0.41828400 | 2.52747300  | -1.30530500 |
| H | 0.51509800  | 3.09632200  | -1.27196600 |
| H | -0.47578700 | 2.02082000  | -2.27164700 |
| H | -1.24170400 | 3.24710500  | -1.25529600 |
| C | -0.26956400 | 2.17399800  | 1.76311600  |
| H | -0.38816200 | 1.48369300  | 2.60167100  |
| H | 0.73927200  | 2.59453600  | 1.81270800  |
| H | -0.98057500 | 2.99507000  | 1.89633800  |

BS2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.60802200  | -2.23576600 | -0.49079100 |
| C | 2.04410200  | -0.93282100 | -0.14597600 |
| C | 3.40634600  | -0.67523000 | -0.04363400 |
| C | 4.33759600  | -1.69648800 | -0.26763300 |
| C | 3.90204500  | -2.97618100 | -0.60256400 |
| C | 2.53869400  | -3.25104000 | -0.71810500 |
| C | 0.14917600  | -2.40030000 | -0.58897600 |
| C | -0.64033500 | -1.32120100 | -0.36686600 |
| H | 3.76011600  | 0.31958700  | 0.20901300  |
| H | 5.39886000  | -1.49023000 | -0.18364000 |
| H | 4.62637700  | -3.76417200 | -0.77772400 |
| H | 2.20394400  | -4.24894400 | -0.98335300 |
| H | -0.25066300 | -3.37866500 | -0.84928800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 0.50631900  | 0.14365100  | 0.04130300  |
| C  | -2.11213000 | -1.35791600 | -0.38612500 |
| C  | -2.85756100 | -0.22724700 | -0.76237600 |
| C  | -2.82234200 | -2.51653600 | -0.02189000 |
| C  | -4.24850700 | -0.26069500 | -0.79802200 |
| H  | -2.33941600 | 0.67924400  | -1.05370400 |
| C  | -4.21139800 | -2.54853500 | -0.05431000 |
| H  | -2.27613600 | -3.38994500 | 0.31539200  |
| C  | -4.93318200 | -1.42133900 | -0.44589100 |
| H  | -4.79818500 | 0.62349800  | -1.10178100 |
| H  | -4.73414800 | -3.45273600 | 0.23823000  |
| H  | -6.01682100 | -1.44578500 | -0.46675800 |
| C  | 0.27112100  | 0.80847900  | 1.79115600  |
| C  | 1.12870000  | 0.42407700  | 2.83454300  |
| C  | -0.79648700 | 1.66816200  | 2.10314800  |
| C  | 0.93120300  | 0.88222700  | 4.13596600  |
| H  | 1.95996900  | -0.24187600 | 2.62958700  |
| C  | -0.99891000 | 2.12435600  | 3.40301800  |
| H  | -1.48211700 | 1.98693100  | 1.32483800  |
| C  | -0.13330800 | 1.73294000  | 4.42284300  |
| H  | 1.60833100  | 0.57359400  | 4.92506700  |
| H  | -1.83170700 | 2.78438200  | 3.62016100  |
| H  | -0.28883600 | 2.08910400  | 5.43531900  |
| C  | 0.43236000  | 1.54545900  | -1.22435600 |
| C  | 0.17133400  | 1.26754400  | -2.57721700 |



|   |             |            |             |
|---|-------------|------------|-------------|
| C | 0.70175100  | 2.87641700 | -0.86808900 |
| C | 0.17530300  | 2.27853400 | -3.53430900 |
| H | -0.04160100 | 0.24907200 | -2.88646500 |
| C | 0.70837600  | 3.89102300 | -1.82446000 |
| H | 0.90463800  | 3.12759900 | 0.16749800  |
| C | 0.44409900  | 3.59407200 | -3.15894000 |
| H | -0.03182600 | 2.04098400 | -4.57210000 |
| H | 0.91809800  | 4.91253100 | -1.52607500 |
| H | 0.44622800  | 4.38274900 | -3.90332800 |

BS3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.59694200 | -1.14815200 | -0.02147400 |
| C  | -4.05545500 | 0.19194700  | 0.02556600  |
| C  | -5.42296800 | 0.44071800  | 0.05795400  |
| C  | -6.33684700 | -0.61963100 | 0.04834800  |
| C  | -5.87877500 | -1.93423200 | 0.00179300  |
| C  | -4.51057800 | -2.20456800 | -0.03475500 |
| C  | -2.13592300 | -1.30685900 | -0.05292000 |
| C  | -1.36221900 | -0.19180900 | -0.03899600 |
| H  | -5.79717500 | 1.45977800  | 0.09205500  |
| H  | -7.40202500 | -0.41823200 | 0.07680100  |
| H  | -6.58958700 | -2.75335700 | -0.00669300 |
| H  | -4.15829700 | -3.23066600 | -0.07201200 |
| H  | -1.72528200 | -2.31371400 | -0.09723600 |
| Si | -2.53553900 | 1.30675700  | 0.00292500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.10719300  | -0.20061700 | -0.01998700 |
| C | 0.84029400  | 0.92851500  | -0.42302300 |
| C | 0.84880200  | -1.31729500 | 0.41038200  |
| C | 2.22921300  | 0.93722900  | -0.42136700 |
| H | 0.31336800  | 1.80994000  | -0.77005900 |
| C | 2.23507400  | -1.30998200 | 0.41253800  |
| H | 0.32888900  | -2.19414800 | 0.77841600  |
| C | 2.96131900  | -0.18306500 | -0.00618000 |
| H | 2.75415800  | 1.81839300  | -0.77264400 |
| H | 2.76824900  | -2.17988200 | 0.77956300  |
| C | -2.48690300 | 2.40170500  | -1.53544200 |
| H | -1.59223700 | 3.02971900  | -1.56810500 |
| H | -2.51383500 | 1.79965800  | -2.44685100 |
| H | -3.35531800 | 3.06810000  | -1.54862800 |
| C | -2.33253200 | 2.35944300  | 1.55371600  |
| H | -2.40008200 | 1.74571700  | 2.45513800  |
| H | -1.36172200 | 2.86383100  | 1.56107800  |
| H | -3.10878300 | 3.12881700  | 1.60827000  |
| C | 4.44426600  | -0.17666800 | 0.00002500  |
| C | 5.16083300  | 0.96835100  | 0.38023700  |
| C | 5.17229400  | -1.31580400 | -0.37604100 |
| C | 6.55221300  | 0.97456000  | 0.38321600  |
| H | 4.62143500  | 1.85225900  | 0.70107900  |
| C | 6.56370100  | -1.31000900 | -0.37274800 |
| H | 4.64182000  | -2.20445700 | -0.69869300 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 7.26064900 | -0.16467400 | 0.00668900  |
| H | 7.08422600 | 1.86866700  | 0.68912800  |
| H | 7.10475400 | -2.19960700 | -0.67590800 |
| H | 8.34472300 | -0.16002900 | 0.00916500  |

BS4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.92969900  | 2.36202300  | -1.24762500 |
| C  | 1.90236600  | 1.69388000  | -0.46379900 |
| C  | 3.15272600  | 2.27692800  | -0.28888700 |
| C  | 3.44123500  | 3.51871100  | -0.86759000 |
| C  | 2.47726800  | 4.17366300  | -1.62965000 |
| C  | 1.22057800  | 3.59866300  | -1.82542800 |
| C  | -0.35236000 | 1.65058200  | -1.39710400 |
| C  | -0.48655600 | 0.43745200  | -0.81195900 |
| H  | 3.91801300  | 1.77239400  | 0.29291900  |
| H  | 4.41727300  | 3.96923700  | -0.72521900 |
| H  | 2.70491700  | 5.13465900  | -2.07784500 |
| H  | 0.47467400  | 4.10913400  | -2.42644800 |
| H  | -1.14308000 | 2.11117800  | -1.98583100 |
| Si | 1.13965900  | 0.06630600  | 0.10586200  |
| C  | 2.07352900  | -1.44425600 | -0.54080800 |
| C  | 2.58457300  | -2.43021700 | 0.31627000  |
| C  | 2.31009500  | -1.58367000 | -1.91989200 |
| C  | 3.30104700  | -3.51757800 | -0.18369600 |
| H  | 2.42358200  | -2.35056000 | 1.38574000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.02434200  | -2.66724400 | -2.42199400 |
| H | 1.93239200  | -0.83581800 | -2.61045900 |
| C | 3.52128800  | -3.63845300 | -1.55275900 |
| H | 3.68669600  | -4.26853000 | 0.49735300  |
| H | 3.19551700  | -2.75462400 | -3.48945000 |
| H | 4.07819300  | -4.48347100 | -1.94258600 |
| C | 0.88265500  | -0.04914900 | 1.97041300  |
| C | 1.48741400  | 0.85894700  | 2.85354300  |
| C | 0.05284000  | -1.04416100 | 2.51695100  |
| C | 1.28060100  | 0.77246900  | 4.22939600  |
| H | 2.12066900  | 1.64914600  | 2.46472800  |
| C | -0.15781400 | -1.13098700 | 3.89068200  |
| H | -0.44395100 | -1.75587100 | 1.86507400  |
| C | 0.45859400  | -0.22335400 | 4.75047300  |
| H | 1.75864500  | 1.48517500  | 4.89270200  |
| H | -0.80593400 | -1.90372600 | 4.28949000  |
| H | 0.29479300  | -0.29012700 | 5.82044600  |
| C | -1.69978600 | -0.40426100 | -0.87430400 |
| C | -3.01000900 | 0.09649900  | -0.54519400 |
| C | -1.57506200 | -1.72795800 | -1.26768900 |
| C | -3.23661400 | 1.40015900  | -0.02635000 |
| C | -4.14468200 | -0.76740000 | -0.70319100 |
| C | -2.69505200 | -2.57104500 | -1.41389800 |
| H | -0.59139100 | -2.11660600 | -1.50297000 |
| C | -4.50295300 | 1.83962900  | 0.27781900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.38942300 | 2.04840800  | 0.15011500  |
| C | -5.44006800 | -0.27590700 | -0.39203400 |
| C | -3.95609000 | -2.09933700 | -1.15095400 |
| H | -2.55021900 | -3.59307600 | -1.74602500 |
| C | -5.62089900 | 0.99959400  | 0.08060500  |
| H | -4.64445400 | 2.83629200  | 0.68087600  |
| H | -6.28966700 | -0.93726200 | -0.52793600 |
| H | -4.82391400 | -2.73920100 | -1.27174200 |
| H | -6.61598500 | 1.35962600  | 0.31693200  |

BS5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.14915300 | 2.48885400  | -0.40699200 |
| C  | -2.83968800 | 1.27174900  | -0.18794800 |
| C  | -4.22989800 | 1.26906000  | -0.18810200 |
| C  | -4.93832700 | 2.45949400  | -0.39090900 |
| C  | -4.25277700 | 3.65343700  | -0.60096700 |
| C  | -2.85758300 | 3.67380800  | -0.61294700 |
| C  | -0.68223300 | 2.38210400  | -0.40422400 |
| C  | -0.12360900 | 1.16155400  | -0.21583500 |
| H  | -4.77809400 | 0.34490500  | -0.03380500 |
| H  | -6.02260400 | 2.45150600  | -0.38757800 |
| H  | -4.80575400 | 4.57274600  | -0.75920100 |
| H  | -2.32674600 | 4.60541600  | -0.78144200 |
| H  | -0.09225100 | 3.28183300  | -0.56967400 |
| Si | -1.54604400 | -0.08602900 | 0.01529600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.32718900  | 0.92648800  | -0.15393200 |
| C | 1.87831800  | -0.29953500 | -0.56443700 |
| C | 2.21212100  | 1.90936700  | 0.32778400  |
| C | 3.24883000  | -0.52504100 | -0.52586500 |
| H | 1.22661600  | -1.07928100 | -0.93977300 |
| C | 3.58062700  | 1.68871500  | 0.37120000  |
| H | 1.81590000  | 2.84690800  | 0.69872300  |
| C | 4.10680600  | 0.46903700  | -0.05917800 |
| H | 3.65173000  | -1.47570400 | -0.85172800 |
| H | 4.24221400  | 2.45411800  | 0.75789700  |
| C | -1.56241100 | -0.88187600 | 1.72481500  |
| C | -2.42495100 | -0.41704300 | 2.73075700  |
| C | -0.68287400 | -1.93010300 | 2.04752800  |
| C | -2.41415300 | -0.97962400 | 4.00589600  |
| H | -3.11215100 | 0.39436500  | 2.51718100  |
| C | -0.66736500 | -2.49191500 | 3.32147800  |
| H | 0.00086100  | -2.31609100 | 1.29853600  |
| C | -1.53562000 | -2.01814700 | 4.30348700  |
| H | -3.09124400 | -0.60588300 | 4.76624900  |
| H | 0.02166600  | -3.29820400 | 3.54786600  |
| H | -1.52572500 | -2.45617500 | 5.29546800  |
| C | -1.62839400 | -1.39632100 | -1.34298300 |
| C | -1.27230900 | -1.07010600 | -2.66314100 |
| C | -2.10481100 | -2.69286100 | -1.09249800 |
| C | -1.38297300 | -2.00300600 | -3.69031600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.90103000 | -0.07593700 | -2.89164200 |
| C | -2.21719100 | -3.62940300 | -2.11933800 |
| H | -2.38861900 | -2.97834600 | -0.08531700 |
| C | -1.85548400 | -3.28653400 | -3.41939600 |
| H | -1.10007600 | -1.73016000 | -4.70110900 |
| H | -2.58606800 | -4.62603600 | -1.90263800 |
| H | -1.94037800 | -4.01474600 | -4.21845000 |
| C | 5.59220500  | 0.25331100  | -0.05984500 |
| F | 6.19835300  | 0.88126400  | 0.97322700  |
| F | 6.17081100  | 0.72915300  | -1.19003200 |
| F | 5.92090600  | -1.05526100 | 0.01922000  |

BS6

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.61033300 | 2.50341100 | -0.48688100 |
| C | -2.33307300 | 1.32237900 | -0.18634800 |
| C | -3.72150100 | 1.36684600 | -0.13470600 |
| C | -4.39963100 | 2.57020400 | -0.36401900 |
| C | -3.68329600 | 3.72886700 | -0.65356700 |
| C | -2.28955400 | 3.70097200 | -0.71921600 |
| C | -0.14883500 | 2.34593400 | -0.53902300 |
| C | 0.37962000  | 1.11671500 | -0.31663800 |
| H | -4.29236400 | 0.46917200 | 0.08223100  |
| H | -5.48267700 | 2.59949500 | -0.31895700 |
| H | -4.21148900 | 4.65917100 | -0.83241500 |
| H | -1.73640200 | 4.60605000 | -0.94994200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.46180900  | 3.21779300  | -0.76701700 |
| Si | -1.07397100 | -0.06499000 | 0.02854900  |
| C  | 1.81990500  | 0.82356300  | -0.28954600 |
| C  | 2.30898900  | -0.45780200 | -0.61156300 |
| C  | 2.76913900  | 1.79448400  | 0.06282100  |
| C  | 3.66403700  | -0.74246800 | -0.60777500 |
| H  | 1.61252800  | -1.23851300 | -0.89479800 |
| C  | 4.13442300  | 1.52327700  | 0.07569000  |
| H  | 2.43484900  | 2.78154200  | 0.36097200  |
| C  | 4.59264500  | 0.24716800  | -0.26595200 |
| H  | 4.03220700  | -1.72765600 | -0.86768400 |
| H  | 4.82486300  | 2.30459900  | 0.36439500  |
| C  | -1.05372900 | -0.78261800 | 1.77432600  |
| C  | -1.81945300 | -0.20421000 | 2.79964800  |
| C  | -0.23826700 | -1.87890100 | 2.10492500  |
| C  | -1.77659400 | -0.70211000 | 4.10070600  |
| H  | -2.45656300 | 0.64555000  | 2.57980600  |
| C  | -0.19110400 | -2.37722100 | 3.40444000  |
| H  | 0.36977400  | -2.35344300 | 1.34175200  |
| C  | -0.96223500 | -1.78972700 | 4.40573900  |
| H  | -2.37887600 | -0.23988100 | 4.87536500  |
| H  | 0.44755300  | -3.22285700 | 3.63555700  |
| H  | -0.92745900 | -2.17792700 | 5.41782200  |
| C  | -1.26442300 | -1.43568900 | -1.25901800 |
| C  | -0.91595900 | -1.19870700 | -2.59995100 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.81867900 | -2.68444600 | -0.93621900 |
| C | -1.10953400 | -2.17083900 | -3.57744100 |
| H | -0.48416000 | -0.24390500 | -2.88315400 |
| C | -2.01402900 | -3.66032400 | -1.91277800 |
| H | -2.09866000 | -2.90166000 | 0.08900700  |
| C | -1.65910800 | -3.40553500 | -3.23486800 |
| H | -0.83060000 | -1.96665100 | -4.60548200 |
| H | -2.44215300 | -4.61886500 | -1.63992900 |
| H | -1.80855500 | -4.16446700 | -3.99505800 |
| O | 5.90240500  | -0.13027100 | -0.28543400 |
| C | 6.89012800  | 0.83371900  | 0.04945300  |
| H | 6.76864900  | 1.19420600  | 1.07715800  |
| H | 7.84716200  | 0.32236800  | -0.04051500 |
| H | 6.86964200  | 1.68624200  | -0.63875700 |

BS7

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.79369200  | -2.13422400 | -0.45553100 |
| C | 2.08631200  | -0.79631100 | -0.09080900 |
| C | 3.41148200  | -0.42717800 | 0.10980500  |
| C | 4.44162400  | -1.36131200 | -0.05573500 |
| C | 4.14524100  | -2.67226100 | -0.42059600 |
| C | 2.82141200  | -3.06482900 | -0.62055200 |
| C | 0.36422500  | -2.43434700 | -0.62438600 |
| C | -0.51977600 | -1.43172400 | -0.40678000 |
| H | 3.65990200  | 0.58933400  | 0.39906700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.47249000  | -1.06405600 | 0.10264600  |
| H  | 4.94617000  | -3.39235900 | -0.54735800 |
| H  | 2.59212900  | -4.08822400 | -0.90101900 |
| H  | 0.07765400  | -3.44371100 | -0.91460900 |
| Si | 0.44381300  | 0.14032900  | 0.04954000  |
| C  | 0.11913200  | 0.75424600  | 1.80331900  |
| C  | 0.34099800  | 2.09271100  | 2.16245600  |
| C  | -0.29797300 | -0.13453600 | 2.80741800  |
| C  | 0.15458200  | 2.52726200  | 3.47401300  |
| H  | 0.65529200  | 2.80864400  | 1.41030400  |
| C  | -0.48654800 | 0.29579900  | 4.11777600  |
| H  | -0.48389700 | -1.17545200 | 2.56303700  |
| C  | -0.25987400 | 1.62946700  | 4.45433300  |
| H  | 0.33026800  | 3.56706800  | 3.72834200  |
| H  | -0.81292200 | -0.40773200 | 4.87618300  |
| H  | -0.40788200 | 1.96656100  | 5.47454700  |
| C  | 0.32500700  | 1.54565600  | -1.20446400 |
| C  | 1.33169500  | 1.75591500  | -2.16025000 |
| C  | -0.78816200 | 2.40369200  | -1.22096400 |
| C  | 1.23383300  | 2.78532600  | -3.09553000 |
| H  | 2.20194600  | 1.10883400  | -2.17738200 |
| C  | -0.88683300 | 3.43358100  | -2.15265200 |
| H  | -1.58851500 | 2.25051700  | -0.50648700 |
| C  | 0.12493200  | 3.62719900  | -3.09217300 |
| H  | 2.02383200  | 2.92885200  | -3.82489100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.75504200 | 4.08399900  | -2.14856100 |
| H | 0.04768000  | 4.42928900  | -3.81828100 |
| C | -1.97801700 | -1.51092900 | -0.51364300 |
| C | -2.67546000 | -2.67983700 | -0.86886200 |
| N | -2.63473800 | -0.36437900 | -0.23874100 |
| C | -4.05964200 | -2.65389700 | -0.93630100 |
| H | -2.13627700 | -3.59289500 | -1.08863300 |
| C | -3.96599500 | -0.35449600 | -0.30701600 |
| C | -4.73006500 | -1.46609700 | -0.64895500 |
| H | -4.61099400 | -3.54711400 | -1.20900500 |
| H | -4.44641100 | 0.59251300  | -0.07546500 |
| H | -5.81058200 | -1.40128400 | -0.68832100 |

BS8

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.88460500 | -2.00002900 | -0.68677000 |
| C | -2.13511100 | -0.74763400 | -0.07389300 |
| C | -3.43990200 | -0.39772800 | 0.25238900  |
| C | -4.49615600 | -1.27545700 | -0.02000800 |
| C | -4.24344200 | -2.50501500 | -0.62350600 |
| C | -2.94015800 | -2.87236800 | -0.96050500 |
| C | -0.47450700 | -2.27161400 | -0.99605400 |
| C | 0.44960700  | -1.33272100 | -0.66787600 |
| H | -3.65196800 | 0.55764000  | 0.72216500  |
| H | -5.51171500 | -0.99830700 | 0.24007100  |
| H | -5.06432300 | -3.18210000 | -0.83307100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.74784400 | -3.83108300 | -1.43173200 |
| H  | -0.21153800 | -3.20545200 | -1.48871400 |
| Si | -0.47723400 | 0.13118500  | 0.12632300  |
| C  | -0.39836500 | 1.74176200  | -0.85562400 |
| C  | 0.49462600  | 2.77223600  | -0.51859800 |
| C  | -1.21666400 | 1.92411400  | -1.98346000 |
| C  | 0.56900200  | 3.93778300  | -1.27871900 |
| H  | 1.13840400  | 2.66700600  | 0.34793800  |
| C  | -1.14452800 | 3.08782000  | -2.74486300 |
| H  | -1.92238200 | 1.15044500  | -2.26726700 |
| C  | -0.25064000 | 4.09751200  | -2.39353800 |
| H  | 1.26605700  | 4.72050000  | -0.99977400 |
| H  | -1.78668900 | 3.20754200  | -3.61066200 |
| H  | -0.19422600 | 5.00472600  | -2.98512200 |
| C  | 0.03642200  | 0.41366900  | 1.91825800  |
| C  | -0.42684200 | 1.53164300  | 2.63294300  |
| C  | 0.83956400  | -0.51483400 | 2.59988300  |
| C  | -0.10451500 | 1.71309200  | 3.97568000  |
| H  | -1.04224600 | 2.27530000  | 2.13639000  |
| C  | 1.16659300  | -0.33415500 | 3.94227300  |
| H  | 1.22090000  | -1.38458500 | 2.07615500  |
| C  | 0.69401400  | 0.77912200  | 4.63304600  |
| H  | -0.47406500 | 2.58307600  | 4.50762900  |
| H  | 1.79214600  | -1.06182100 | 4.44768300  |
| H  | 0.94851000  | 0.92027900  | 5.67777900  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.87797600 | -1.52188200 | -0.86281700 |
| C | 2.60364300 | -2.69439900 | -0.87744300 |
| S | 2.95540800 | -0.15756100 | -1.10420600 |
| C | 3.99531900 | -2.50639500 | -1.08746000 |
| H | 2.14709000 | -3.66143100 | -0.71159900 |
| C | 4.33850100 | -1.19082100 | -1.22505100 |
| H | 4.71424100 | -3.31449700 | -1.12432900 |
| H | 5.31541500 | -0.76506000 | -1.39450400 |

BS9

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.35390800 | -2.32396500 | 0.00378900  |
| C  | 2.71992000 | -0.95407500 | 0.02168800  |
| C  | 4.06605400 | -0.60996600 | 0.04769900  |
| C  | 5.05092100 | -1.60510200 | 0.05316000  |
| C  | 4.68507200 | -2.94912200 | 0.03508000  |
| C  | 3.33915500 | -3.31462100 | 0.01072500  |
| C  | 0.91027700 | -2.57932100 | -0.02338200 |
| C  | 0.06091100 | -1.51513200 | -0.01768800 |
| H  | 4.36675200 | 0.43309100  | 0.06369900  |
| H  | 6.09952400 | -1.32954500 | 0.07264000  |
| H  | 5.45104500 | -3.71695000 | 0.04039900  |
| H  | 3.05841500 | -4.36304500 | -0.00313100 |
| H  | 0.55207800 | -3.60776800 | -0.05092700 |
| Si | 1.12835100 | 0.06237000  | 0.02105100  |
| C  | 0.88072600 | 1.07979400  | 1.59116500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.44421600  | 2.36058700  | 1.72353300  |
| C | 0.18771300  | 0.55156400  | 2.69257300  |
| C | 1.32110000  | 3.08391800  | 2.90756500  |
| H | 1.98267400  | 2.80393200  | 0.89185300  |
| C | 0.06035300  | 1.27355300  | 3.87737400  |
| H | -0.26219700 | -0.43284500 | 2.62332100  |
| C | 0.62758000  | 2.54100800  | 3.98741800  |
| H | 1.76457300  | 4.07060800  | 2.98687800  |
| H | -0.48291700 | 0.84682800  | 4.71347200  |
| H | 0.52879300  | 3.10388300  | 4.90917500  |
| C | 0.97417500  | 1.14989800  | -1.51508900 |
| C | 1.65097000  | 0.80372900  | -2.69674200 |
| C | 0.15522600  | 2.29068400  | -1.54013000 |
| C | 1.51313200  | 1.56364400  | -3.85562200 |
| H | 2.29721300  | -0.06770900 | -2.71046100 |
| C | 0.01456000  | 3.05334100  | -2.69779300 |
| H | -0.37460300 | 2.59596500  | -0.64373500 |
| C | 0.69362300  | 2.69052700  | -3.85858700 |
| H | 2.04655100  | 1.27752300  | -4.75562200 |
| H | -0.62314400 | 3.93071200  | -2.69260500 |
| H | 0.58632800  | 3.28366500  | -4.76016000 |
| C | -1.37490400 | -1.67186300 | -0.05239100 |
| C | -2.27093400 | -0.66116200 | -0.04536500 |
| H | -1.73642200 | -2.69898500 | -0.08697300 |
| H | -1.89006400 | 0.35637400  | -0.00988400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.72906400 | -0.76364500 | -0.08187900 |
| C | -4.42288900 | -1.98677000 | -0.14583500 |
| C | -4.49094500 | 0.41770000  | -0.05259000 |
| C | -5.81022300 | -2.02019100 | -0.17771800 |
| H | -3.87296500 | -2.91999700 | -0.17300400 |
| C | -5.88080200 | 0.38420700  | -0.08459200 |
| H | -3.97757500 | 1.37246500  | -0.00372600 |
| C | -6.54894200 | -0.83600400 | -0.14715400 |
| H | -6.32174500 | -2.97523200 | -0.22781100 |
| H | -6.44232500 | 1.31161600  | -0.06074500 |
| H | -7.63224100 | -0.86705800 | -0.17264400 |

BS10

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.44930700 | 1.12684100  | 0.04939900  |
| C | -2.05111600 | -0.16073000 | 0.47613700  |
| C | -3.00045900 | -1.02038600 | 1.01774700  |
| C | -4.33505500 | -0.61380000 | 1.13359700  |
| C | -4.71996600 | 0.65579500  | 0.70855300  |
| C | -3.77942800 | 1.53184600  | 0.16470700  |
| C | -1.35800800 | 1.95611200  | -0.50308200 |
| C | -0.09583700 | 1.46144700  | -0.54446400 |
| H | -2.71671100 | -2.01217500 | 1.35591300  |
| H | -5.07127300 | -1.28803500 | 1.55734000  |
| H | -5.75519300 | 0.96534900  | 0.80129600  |
| H | -4.08065200 | 2.52103600  | -0.16586500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.62000500 | 2.95093500  | -0.86603300 |
| Si | -0.19241800 | -0.30026900 | 0.15598100  |
| C  | 0.81264000  | -0.54288400 | 1.73883500  |
| C  | 1.24120600  | -1.81284700 | 2.15880600  |
| C  | 1.08785700  | 0.55025100  | 2.57794300  |
| C  | 1.92051000  | -1.98323300 | 3.36403600  |
| H  | 1.04670000  | -2.68142200 | 1.53880700  |
| C  | 1.76793400  | 0.38438300  | 3.78202000  |
| H  | 0.76299600  | 1.54423300  | 2.28871800  |
| C  | 2.18744200  | -0.88440700 | 4.17720500  |
| H  | 2.24220700  | -2.97389100 | 3.66672500  |
| H  | 1.96974100  | 1.24430400  | 4.41146900  |
| H  | 2.71888100  | -1.01558400 | 5.11339000  |
| C  | 0.20140200  | -1.66185600 | -1.09651800 |
| C  | -0.81088700 | -2.19447100 | -1.91221600 |
| C  | 1.50825400  | -2.14504700 | -1.27948400 |
| C  | -0.53058900 | -3.16746300 | -2.86959900 |
| H  | -1.83217900 | -1.84797800 | -1.79583500 |
| C  | 1.79288200  | -3.11723000 | -2.23586600 |
| H  | 2.31728400  | -1.76203200 | -0.66681300 |
| C  | 0.77254500  | -3.63107100 | -3.03376600 |
| H  | -1.33023500 | -3.56438800 | -3.48558500 |
| H  | 2.81000800  | -3.47381400 | -2.35726100 |
| H  | 0.99208000  | -4.38933000 | -3.77739100 |
| Si | 1.34150600  | 2.46910600  | -1.22723300 |



|   |             |            |             |
|---|-------------|------------|-------------|
| C | 2.02462800  | 3.61875300 | 0.11355800  |
| H | 2.83081300  | 4.24130500 | -0.28809300 |
| H | 1.24866400  | 4.28605800 | 0.49995000  |
| H | 2.43102600  | 3.05366800 | 0.95709100  |
| C | 0.74058800  | 3.52226200 | -2.67969400 |
| H | 1.56083600  | 4.12298100 | -3.08536800 |
| H | 0.35165000  | 2.89650000 | -3.48790900 |
| H | -0.05364100 | 4.21353700 | -2.38261600 |
| C | 2.73677400  | 1.34014500 | -1.81297700 |
| H | 3.15230100  | 0.75553900 | -0.98681800 |
| H | 2.40068200  | 0.63962900 | -2.58172500 |
| H | 3.55274200  | 1.93539100 | -2.23512100 |

BS11

|   |             |            |            |
|---|-------------|------------|------------|
| C | 0.32232700  | 2.58090600 | 0.07479700 |
| C | -0.91173600 | 1.88488300 | 0.07166400 |
| C | -2.10062500 | 2.60430000 | 0.11143200 |
| C | -2.08020200 | 4.00365500 | 0.14833100 |
| C | -0.86446300 | 4.68137700 | 0.14891900 |
| C | 0.33944000  | 3.97476300 | 0.11315200 |
| C | 1.52804000  | 1.72649400 | 0.03228100 |
| C | 1.36056700  | 0.38813000 | 0.00296700 |
| H | -3.05552500 | 2.08761300 | 0.11730800 |
| H | -3.01101800 | 4.55909100 | 0.17887600 |
| H | -0.85068400 | 5.76552100 | 0.17844900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.28445700  | 4.50897300  | 0.11480600  |
| H  | 2.50339100  | 2.20813300  | 0.01926200  |
| Si | -0.50477400 | 0.04470500  | 0.02434100  |
| C  | -1.04145900 | -0.91069000 | 1.56360900  |
| C  | -2.18804300 | -1.72113100 | 1.57313600  |
| C  | -0.31863100 | -0.78545600 | 2.76218400  |
| C  | -2.59512400 | -2.38209700 | 2.73062900  |
| H  | -2.76964400 | -1.84323000 | 0.66549700  |
| C  | -0.72098700 | -1.44555400 | 3.92036300  |
| H  | 0.56861600  | -0.16072800 | 2.79218000  |
| C  | -1.86136300 | -2.24643500 | 3.90649000  |
| H  | -3.48459800 | -3.00262200 | 2.71373900  |
| H  | -0.14609400 | -1.33466600 | 4.83338400  |
| H  | -2.17610500 | -2.76144400 | 4.80751200  |
| C  | -1.12393700 | -0.82207100 | -1.53529800 |
| C  | -1.68325100 | -0.09616400 | -2.59933400 |
| C  | -0.98162000 | -2.21169900 | -1.69430000 |
| C  | -2.08767100 | -0.73131900 | -3.77199400 |
| H  | -1.80348000 | 0.97819100  | -2.51091900 |
| C  | -1.37981500 | -2.84915200 | -2.86685800 |
| H  | -0.56170900 | -2.80818200 | -0.89036700 |
| C  | -1.93566200 | -2.10893400 | -3.90854700 |
| H  | -2.52045900 | -0.15009800 | -4.57899400 |
| H  | -1.25933200 | -3.92244800 | -2.96663500 |
| H  | -2.24883800 | -2.60401200 | -4.82120900 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.45672500 | -0.64311200 | -0.05692200 |
| C | 3.89502700 | -0.11717500 | -0.12131400 |
| H | 2.27390200 | -1.29120900 | -0.92579900 |
| H | 2.35718400 | -1.31074900 | 0.81107000  |
| C | 4.93798400 | -1.23691300 | -0.21191600 |
| H | 4.00239500 | 0.54603300  | -0.98827900 |
| H | 4.10154500 | 0.49721600  | 0.76364000  |
| C | 6.37687000 | -0.71791400 | -0.28001600 |
| H | 4.83103600 | -1.90272600 | 0.65322900  |
| H | 4.72984700 | -1.85227200 | -1.09550500 |
| H | 7.09616300 | -1.53977500 | -0.33271800 |
| H | 6.52848600 | -0.08710700 | -1.16151800 |
| H | 6.62295000 | -0.11752700 | 0.60148900  |

BS12

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.16831500 | -1.89916700 | -0.24075200 |
| C | 0.23346900  | -2.09255300 | -0.27749900 |
| C | 0.73810900  | -3.37560000 | -0.45849000 |
| C | -0.12671600 | -4.46733900 | -0.59341800 |
| C | -1.50393200 | -4.27176200 | -0.54447700 |
| C | -2.03085100 | -2.99172600 | -0.36787900 |
| C | -1.61739200 | -0.48837600 | -0.06396300 |
| C | -0.62647800 | 0.44363100  | 0.02017500  |
| H | 1.81053300  | -3.54033400 | -0.49668700 |
| H | 0.27540900  | -5.46455300 | -0.73526300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.17463700 | -5.11814400 | -0.64490500 |
| H  | -3.10438200 | -2.84942600 | -0.33100500 |
| Si | 1.06835400  | -0.41151500 | -0.05600800 |
| C  | 2.08313700  | -0.37512700 | 1.53853800  |
| C  | 2.00230000  | -1.42471900 | 2.46770400  |
| C  | 2.92990900  | 0.70479100  | 1.84113200  |
| C  | 2.73574900  | -1.39768900 | 3.65326800  |
| H  | 1.36035200  | -2.27479900 | 2.26437000  |
| C  | 3.66742200  | 0.73218200  | 3.02161400  |
| H  | 2.99979700  | 1.53503500  | 1.14863600  |
| C  | 3.57108300  | -0.31946800 | 3.93202000  |
| H  | 2.65538700  | -2.21974900 | 4.35649300  |
| H  | 4.31547400  | 1.57593400  | 3.23396600  |
| H  | 4.14420500  | -0.29745200 | 4.85269600  |
| C  | 2.11398300  | 0.05764900  | -1.55477600 |
| C  | 1.51836700  | 0.58131300  | -2.71344000 |
| C  | 3.49916100  | -0.16810800 | -1.57536400 |
| C  | 2.27462100  | 0.86867500  | -3.84653900 |
| H  | 0.45041000  | 0.77342600  | -2.73021500 |
| C  | 4.26012300  | 0.11705600  | -2.70825900 |
| H  | 3.99483200  | -0.56469100 | -0.69541600 |
| C  | 3.64908600  | 0.63640100  | -3.84663200 |
| H  | 1.79290100  | 1.27626300  | -4.72893300 |
| H  | 5.32963700  | -0.06424900 | -2.69991300 |
| H  | 4.23963400  | 0.86097400  | -4.72822600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.08547100 | -0.23014000 | 0.02098100  |
| C | -3.71281400 | -0.11384600 | 1.26712400  |
| C | -3.86470800 | -0.13216500 | -1.13833900 |
| C | -5.08494600 | 0.11117800  | 1.35132500  |
| H | -3.11799800 | -0.19484600 | 2.16994000  |
| C | -5.23642700 | 0.09722600  | -1.05315200 |
| H | -3.38984200 | -0.22973800 | -2.10836900 |
| C | -5.85025500 | 0.22031600  | 0.19180200  |
| H | -5.55606000 | 0.20104200  | 2.32390400  |
| H | -5.82537100 | 0.17734900  | -1.96017200 |
| H | -6.91791900 | 0.39670300  | 0.25791800  |
| C | -0.70396800 | 1.90247900  | 0.16494900  |
| C | -1.87366800 | 2.68501000  | 0.13934600  |
| N | 0.50967900  | 2.48389800  | 0.30658500  |
| C | -1.77385600 | 4.06336300  | 0.27034200  |
| H | -2.84093700 | 2.22259500  | 0.01633600  |
| C | 0.58892200  | 3.80608400  | 0.43499900  |
| C | -0.51999100 | 4.64767700  | 0.42514900  |
| H | -2.66919500 | 4.67513000  | 0.25013300  |
| H | 1.58981700  | 4.21478500  | 0.54762800  |
| H | -0.40066800 | 5.71919800  | 0.53017100  |

Thpn-DBS1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.75665900 | -0.73331100 | -2.53177600 |
| C | -2.19810800 | -0.59876200 | -1.19192000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.54019300 | -0.80082400 | -0.89344000 |
| C  | -4.44885300 | -1.13914600 | -1.90392200 |
| C  | -4.00853000 | -1.27192800 | -3.21868000 |
| C  | -2.66558300 | -1.06913100 | -3.53873800 |
| C  | -0.32607100 | -0.48482400 | -2.74526900 |
| C  | 0.44236700  | -0.17413900 | -1.66716400 |
| H  | -3.89598300 | -0.70032400 | 0.12755400  |
| H  | -5.49414800 | -1.29923800 | -1.66318800 |
| H  | -4.71359400 | -1.53453300 | -4.00019100 |
| H  | -2.32815100 | -1.17211200 | -4.56548600 |
| H  | 0.07385700  | -0.53960700 | -3.75590700 |
| Si | -0.69615000 | -0.16157300 | -0.13271000 |
| C  | -0.88901700 | 1.50478600  | 0.71619100  |
| C  | -0.14646200 | 1.85540100  | 1.85715300  |
| C  | -1.76283100 | 2.48134800  | 0.20572800  |
| C  | -0.26520000 | 3.10246900  | 2.45620600  |
| H  | 0.53967100  | 1.13722100  | 2.29364300  |
| C  | -1.89205300 | 3.73153800  | 0.79425400  |
| H  | -2.36402000 | 2.25791100  | -0.66970600 |
| C  | -1.14300400 | 4.06499100  | 1.93383600  |
| H  | 0.32614200  | 3.33971400  | 3.33565300  |
| H  | -2.57643400 | 4.46147600  | 0.37220000  |
| C  | -0.20903600 | -1.48714000 | 1.10545900  |
| C  | -0.80753800 | -1.55720900 | 2.37587900  |
| C  | 0.71111300  | -2.49937200 | 0.78335800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51228500 | -2.57493400 | 3.27281800  |
| H | -1.52085300 | -0.79678400 | 2.67858200  |
| C | 1.01808800  | -3.52145700 | 1.67145800  |
| H | 1.20625100  | -2.48764500 | -0.18171100 |
| C | 0.40741200  | -3.57968200 | 2.93346300  |
| H | -0.99048500 | -2.59507100 | 4.24770900  |
| H | 1.74183100  | -4.28148300 | 1.39264000  |
| C | 1.87519700  | 0.02542000  | -1.74004500 |
| C | 2.78869300  | -0.45023500 | -2.65041000 |
| S | 2.72023800  | 0.99975000  | -0.52402000 |
| C | 4.12928200  | -0.04219500 | -2.41930700 |
| H | 2.50144100  | -1.10176900 | -3.46582800 |
| C | 4.26251500  | 0.75175100  | -1.30756000 |
| H | 4.96702000  | -0.33291700 | -3.04088000 |
| N | 5.42692000  | 1.26352300  | -0.74194100 |
| H | 6.20629000  | 1.28807800  | -1.38557400 |
| H | 5.31798500  | 2.15149800  | -0.27150300 |
| N | -1.22668400 | 5.33480500  | 2.49665300  |
| H | -2.07556900 | 5.84472500  | 2.30318300  |
| H | -0.94550200 | 5.40486300  | 3.46311300  |
| N | 0.75190000  | -4.57030000 | 3.84905800  |
| H | 0.06563600  | -4.76014200 | 4.56414800  |
| H | 1.13650100  | -5.41453700 | 3.45197800  |

Thpn-DBS2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.07785500 | -0.61421400 | 3.55603100  |
| C  | 0.02753700  | -1.54800300 | 2.49513000  |
| C  | 0.11592500  | -2.90358600 | 2.78782100  |
| C  | 0.09494600  | -3.34602700 | 4.11628500  |
| C  | -0.01160000 | -2.42347200 | 5.15449600  |
| C  | -0.09651700 | -1.05791000 | 4.88112000  |
| C  | -0.14614800 | 0.79238800  | 3.14495500  |
| C  | -0.12327000 | 1.07741900  | 1.81526700  |
| H  | 0.20071600  | -3.63242000 | 1.98737500  |
| H  | 0.16067900  | -4.40588000 | 4.33698200  |
| H  | -0.02813300 | -2.76793200 | 6.18310700  |
| H  | -0.17713600 | -0.34299000 | 5.69423900  |
| H  | -0.19609500 | 1.56446800  | 3.91032800  |
| Si | 0.00434500  | -0.57903900 | 0.87252900  |
| C  | 1.58273300  | -0.81764300 | -0.11927500 |
| C  | 1.62343100  | -0.68196200 | -1.51610700 |
| C  | 2.80154600  | -1.11811400 | 0.51210700  |
| C  | 2.79739900  | -0.83092200 | -2.24289000 |
| H  | 0.71055400  | -0.46192600 | -2.05993200 |
| C  | 3.98582600  | -1.27033600 | -0.19426600 |
| H  | 2.82920200  | -1.24974100 | 1.58924600  |
| C  | 4.02027100  | -1.11835400 | -1.59845500 |
| H  | 2.75691200  | -0.72605700 | -3.31838700 |
| H  | 4.88659600  | -1.51328400 | 0.35229200  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.50667100 | -0.89465400 | -0.19563500 |
| C | -1.60425100 | -2.04385600 | -0.99817000 |
| C | -2.62527100 | -0.04674200 | -0.18703700 |
| C | -2.73639200 | -2.33510300 | -1.74614400 |
| H | -0.77235000 | -2.74036800 | -1.04735300 |
| C | -3.76639800 | -0.31714100 | -0.93071700 |
| H | -2.61101300 | 0.85573500  | 0.41490600  |
| C | -3.85193400 | -1.46876700 | -1.74235900 |
| H | -2.74833200 | -3.24158500 | -2.33560600 |
| H | -4.59366600 | 0.37702700  | -0.87664700 |
| C | -0.24714100 | 2.41957500  | 1.28641300  |
| C | -0.82495300 | 3.53874800  | 1.83652100  |
| S | 0.38635300  | 2.82179400  | -0.32110700 |
| C | -0.76724000 | 4.70604400  | 1.02869400  |
| H | -1.30919900 | 3.51540000  | 2.80467500  |
| C | -0.14381600 | 4.48200800  | -0.17161700 |
| H | -1.17181300 | 5.66992500  | 1.29776400  |
| N | 0.04924400  | 5.35855300  | -1.23887000 |
| H | 0.85419500  | 5.12460100  | -1.81095600 |
| N | 5.20394000  | -1.24034600 | -2.31133600 |
| N | -4.97516100 | -1.73157700 | -2.51327900 |
| C | -6.18095000 | -0.94615300 | -2.30848900 |
| H | -6.93683700 | -1.26340100 | -3.02627700 |
| H | -6.59782600 | -1.05633300 | -1.29627400 |
| H | -5.99056900 | 0.11654600  | -2.48170300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.12035200 | -3.03290100 | -3.14370100 |
| H | -5.17522000 | -3.85796700 | -2.41771900 |
| H | -6.03362400 | -3.03938500 | -3.73795800 |
| H | -4.28728800 | -3.23524100 | -3.82268700 |
| C | 5.15958000  | -1.31164600 | -3.76221600 |
| H | 4.69596600  | -0.41620300 | -4.18554500 |
| H | 6.17782400  | -1.36438400 | -4.14627000 |
| H | 4.60558000  | -2.18769000 | -4.13140700 |
| C | 6.38775300  | -1.76183400 | -1.64859000 |
| H | 6.26062700  | -2.79572200 | -1.29432900 |
| H | 7.22368300  | -1.74030200 | -2.34713600 |
| H | 6.66236700  | -1.14186700 | -0.79080200 |
| N | -0.07900500 | 6.72761600  | -0.91119000 |
| H | 0.81334400  | 7.13387300  | -0.63607800 |
| H | -0.44188100 | 7.22017200  | -1.71783500 |

Thpn-DBS3

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.60771200 | 0.32270500 | 3.16714800 |
| C | -2.26655100 | 0.40934000 | 1.91506600 |
| C | -3.64141500 | 0.60732400 | 1.87864500 |
| C | -4.37186900 | 0.72515700 | 3.06752200 |
| C | -3.71940300 | 0.64079300 | 4.29527600 |
| C | -2.34002400 | 0.43855600 | 4.35177100 |
| C | -0.15951100 | 0.09932500 | 3.09788400 |
| C | 0.42393000  | 0.01060700 | 1.87160300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.16121400 | 0.67485000  | 0.92784600  |
| H  | -5.44407200 | 0.88354400  | 3.03253700  |
| H  | -4.28692600 | 0.73254100  | 5.21518700  |
| H  | -1.83754500 | 0.37178700  | 5.31175100  |
| H  | 0.40298100  | -0.00165600 | 4.02380400  |
| Si | -0.95689700 | 0.21863000  | 0.57165100  |
| C  | -1.26556300 | -1.28932500 | -0.52023300 |
| C  | -0.71648100 | -1.40375300 | -1.80734700 |
| C  | -2.04172500 | -2.36309800 | -0.05179600 |
| C  | -0.93277000 | -2.53818200 | -2.58529700 |
| H  | -0.12117700 | -0.59401100 | -2.21572900 |
| C  | -2.25469500 | -3.49926000 | -0.82658300 |
| H  | -2.49269600 | -2.30931700 | 0.93376600  |
| C  | -1.69898300 | -3.60288800 | -2.10489100 |
| H  | -0.50536100 | -2.59325800 | -3.58252100 |
| H  | -2.86588100 | -4.31429600 | -0.45779600 |
| C  | -0.70811600 | 1.76511800  | -0.47702600 |
| C  | -1.50051100 | 2.01545900  | -1.61067800 |
| C  | 0.22985900  | 2.74465000  | -0.11614800 |
| C  | -1.36981800 | 3.19038900  | -2.34481600 |
| H  | -2.23139000 | 1.27987200  | -1.93247800 |
| C  | 0.36616300  | 3.91757000  | -0.85418600 |
| H  | 0.87162400  | 2.58594900  | 0.74369100  |
| C  | -0.43448000 | 4.16034900  | -1.97242900 |
| H  | -1.97970300 | 3.36614000  | -3.22298700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.11005100  | 4.65191400  | -0.55861200 |
| C | 1.85076200  | -0.13294100 | 1.67261800  |
| C | 2.89571900  | 0.19463100  | 2.50354000  |
| S | 2.49367600  | -0.81543000 | 0.17140500  |
| C | 4.18509100  | -0.08844700 | 1.98757100  |
| H | 2.73885400  | 0.65422100  | 3.47128700  |
| C | 4.15358200  | -0.62802400 | 0.71687300  |
| H | 5.09755000  | 0.11170700  | 2.52986200  |
| N | 5.21426000  | -0.96210500 | -0.10273100 |
| C | 4.99372000  | -1.91302200 | -1.18241000 |
| H | 5.86549900  | -1.91387500 | -1.83832300 |
| H | 4.82120400  | -2.93834000 | -0.82138300 |
| H | 4.13108800  | -1.61051500 | -1.77943400 |
| C | 6.53251700  | -0.98093900 | 0.51111500  |
| H | 6.63443600  | -1.76383300 | 1.27846400  |
| H | 7.28042000  | -1.15078800 | -0.26409300 |
| H | 6.74327400  | -0.01511500 | 0.97519200  |
| C | -1.89166600 | -4.85141500 | -2.94397900 |
| H | -1.12216300 | -5.58165700 | -2.66455300 |
| H | -1.70396600 | -4.59537200 | -3.99870900 |
| C | -0.30982500 | 5.46131000  | -2.74149100 |
| H | -1.06039800 | 6.16546600  | -2.36179400 |
| H | 0.67175600  | 5.90695100  | -2.51666400 |
| N | -0.57136600 | 5.28164000  | -4.17367800 |
| H | -0.59695100 | 6.18098700  | -4.64220000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.17593800  | 4.74187100  | -4.60005600 |
| N | -3.19332800 | -5.48231700 | -2.70384700 |
| H | -3.93902900 | -4.89798600 | -3.06983900 |
| H | -3.24677000 | -6.37415500 | -3.18395100 |

Thpn-DBS4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.08367400 | -0.42233300 | -2.43000200 |
| C  | -2.49096400 | -0.14175500 | -1.10191900 |
| C  | -3.83662200 | -0.00746800 | -0.80385200 |
| C  | -4.81814000 | -0.15706900 | -1.80509000 |
| C  | -4.40442100 | -0.43495600 | -3.11488100 |
| C  | -3.05315000 | -0.56486000 | -3.42472500 |
| C  | -0.63668300 | -0.52236900 | -2.63144000 |
| C  | 0.18226100  | -0.35914600 | -1.55666400 |
| H  | -4.15764500 | 0.21642900  | 0.21061500  |
| H  | -5.15059800 | -0.54507500 | -3.89611500 |
| H  | -2.75824100 | -0.77983900 | -4.44742900 |
| H  | -0.25455900 | -0.70775100 | -3.63371800 |
| Si | -0.92696500 | -0.02829100 | -0.04236700 |
| C  | -0.74565600 | 1.66593800  | 0.75405200  |
| C  | 0.01597800  | 1.87235300  | 1.91705000  |
| C  | -1.34225800 | 2.80233100  | 0.17920600  |
| C  | 0.17468200  | 3.13309500  | 2.47775400  |
| H  | 0.49468300  | 1.02843000  | 2.40259100  |
| C  | -1.19171300 | 4.06812400  | 0.72807400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.94657700 | 2.69566900  | -0.71589100 |
| C | -0.42823500 | 4.25613900  | 1.89100300  |
| H | 0.77213400  | 3.25543800  | 3.37646300  |
| H | -1.66604600 | 4.92358100  | 0.25620900  |
| C | -0.77016100 | -1.38671100 | 1.24778000  |
| C | -1.41605000 | -1.29489900 | 2.49334900  |
| C | -0.05686700 | -2.56995800 | 0.99147900  |
| C | -1.36053500 | -2.31986500 | 3.42844600  |
| H | -1.97393900 | -0.39848300 | 2.74693400  |
| C | 0.00994100  | -3.60186400 | 1.91859600  |
| H | 0.46564800  | -2.68674200 | 0.04811800  |
| C | -0.64529000 | -3.49620400 | 3.15452000  |
| H | -1.86720300 | -2.21240500 | 4.38309200  |
| H | 0.57956300  | -4.49799900 | 1.69089800  |
| C | 1.62322500  | -0.50099800 | -1.62105500 |
| C | 2.40611800  | -1.19824600 | -2.50876500 |
| S | 2.66333700  | 0.30441900  | -0.43667000 |
| C | 3.80420000  | -1.10093600 | -2.28215900 |
| H | 1.98062000  | -1.79021300 | -3.30949400 |
| C | 4.12278800  | -0.33382300 | -1.18126400 |
| H | 4.54012700  | -1.59057400 | -2.90317400 |
| N | 5.36933000  | -0.08669400 | -0.63121400 |
| C | 5.54433000  | 1.10517600  | 0.18647300  |
| H | 6.51324500  | 1.05327000  | 0.68570900  |
| H | 5.49641200  | 2.03720800  | -0.39760000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.77544700  | 1.14672900  | 0.96019600  |
| C | 6.51764600  | -0.47983700 | -1.43136200 |
| H | 6.60654800  | 0.09788500  | -2.36502000 |
| H | 7.42449700  | -0.33545100 | -0.84275000 |
| H | 6.44871600  | -1.53889300 | -1.68862400 |
| N | -6.17056100 | 0.03376600  | -1.50454500 |
| H | -6.81517000 | -0.41903700 | -2.13634900 |
| H | -6.41707100 | -0.13315900 | -0.53958600 |
| N | -0.22881900 | 5.53035100  | 2.41556000  |
| H | -0.92755200 | 6.21631700  | 2.17180200  |
| H | 0.02157600  | 5.56580400  | 3.39240100  |
| N | -0.53546500 | -4.50359700 | 4.11080300  |
| H | -1.27417100 | -4.53204900 | 4.79779800  |
| H | -0.31221300 | -5.41966000 | 3.75091900  |

Thpn-DBS5

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.27911900 | -1.32615400 | -2.82466900 |
| C | 0.07994500  | -1.86983700 | -1.56644400 |
| C | 0.37657200  | -3.21820100 | -1.44947100 |
| C | 0.31672600  | -4.07145300 | -2.56995900 |
| C | -0.04730200 | -3.52580500 | -3.80841000 |
| C | -0.33874400 | -2.17016900 | -3.93575200 |
| C | -0.53751400 | 0.11711200  | -2.83862500 |
| C | -0.40368600 | 0.81403400  | -1.67023900 |
| H | 0.65780800  | -3.63956600 | -0.48747300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.10190200 | -4.17282600 | -4.67881600 |
| H  | -0.60957800 | -1.77220900 | -4.90910600 |
| H  | -0.78266800 | 0.59459400  | -3.78444400 |
| Si | 0.07908300  | -0.44899200 | -0.32446000 |
| C  | -1.23534400 | -0.66250000 | 1.01279100  |
| C  | -1.32289400 | 0.21337700  | 2.10758500  |
| C  | -2.19463400 | -1.68466800 | 0.92697700  |
| C  | -2.32159500 | 0.07124700  | 3.06661400  |
| H  | -0.60010400 | 1.01455500  | 2.21997400  |
| C  | -3.19660500 | -1.82544600 | 1.88388100  |
| H  | -2.15877100 | -2.38400800 | 0.09842600  |
| C  | -3.27487000 | -0.94592000 | 2.96639400  |
| H  | -2.35762200 | 0.75795600  | 3.90769600  |
| H  | -3.92244600 | -2.62654400 | 1.81038300  |
| C  | 1.77259900  | -0.12077500 | 0.44026200  |
| C  | 2.10703500  | -0.56432000 | 1.72996300  |
| C  | 2.77877000  | 0.51647800  | -0.30415200 |
| C  | 3.38279800  | -0.37680900 | 2.25626200  |
| H  | 1.35882000  | -1.06029500 | 2.33970100  |
| C  | 4.05467600  | 0.70179600  | 0.21915100  |
| H  | 2.56493900  | 0.87123800  | -1.30734300 |
| C  | 4.37350600  | 0.26298700  | 1.50717800  |
| H  | 3.62969700  | -0.73124900 | 3.24999700  |
| H  | 4.81352700  | 1.19399100  | -0.38236100 |
| C  | -0.69498900 | 2.21710500  | -1.50502600 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.62738000 | 3.01069600  | -2.15254000 |
| S | 0.12955600  | 3.17837300  | -0.25335600 |
| C | -1.70336800 | 4.34693100  | -1.64841100 |
| C | -0.83785800 | 4.58779500  | -0.61791400 |
| H | -2.37970300 | 5.09530800  | -2.04457900 |
| N | 0.55203100  | -5.44291800 | -2.42976300 |
| H | 0.83781200  | -5.91428900 | -3.27584300 |
| H | 1.14072600  | -5.69333900 | -1.64833800 |
| N | -0.58178000 | 5.79026500  | 0.03139200  |
| H | -1.27819700 | 6.50123100  | -0.14529900 |
| H | -0.38351700 | 5.70795200  | 1.01924300  |
| N | -2.44686700 | 2.57728900  | -3.19839800 |
| H | -2.56964400 | 1.57139100  | -3.21648000 |
| H | -3.34145400 | 3.04943800  | -3.22431200 |
| C | -4.38336800 | -1.06385200 | 3.99481100  |
| H | -5.25912600 | -0.51259700 | 3.63042900  |
| H | -4.06051100 | -0.55312700 | 4.91583600  |
| C | 5.75394200  | 0.51295700  | 2.08340900  |
| H | 5.73390700  | 1.45475200  | 2.64565800  |
| H | 6.45673400  | 0.66803500  | 1.24980200  |
| N | 6.16057300  | -0.54088600 | 3.01919000  |
| H | 6.32031100  | -1.40975200 | 2.51797100  |
| H | 7.03318400  | -0.29133100 | 3.47222800  |
| N | -4.80209000 | -2.45447600 | 4.19805700  |
| H | -4.06279500 | -2.97903100 | 4.65614300  |

H            -5.61635600   -2.49291900   4.80169200

Ph-BS1

C            1.99324900   -1.53977000   -0.00179500

C            2.45099900   -0.19868100   0.07106000

C            3.81899800   0.04966400   0.12547500

C            4.73581900   -1.00818800   0.10462900

C            4.27886600   -2.32169800   0.02938200

C            2.91144100   -2.59294700   -0.02374600

C            0.53497000   -1.70388700   -0.05144600

C            -0.24898200   -0.59345500   -0.01550900

H            4.19241200   1.06752500   0.19256100

H            5.80023300   -0.80566100   0.14863000

H            4.99039000   -3.14025900   0.01342100

H            2.56196900   -3.61921100   -0.08016500

H            0.13550000   -2.71317300   -0.12800600

Si           0.92522800   0.90472600   0.04721100

C            -1.71690600   -0.59385000   -0.04727500

C            -2.43686900   0.59585300   -0.25966600

C            -2.48284700   -1.76355800   0.12873400

C            -3.82393000   0.62163300   -0.31387700

H            -1.90174700   1.53086400   -0.38273900

C            -3.86584400   -1.75008800   0.07905500

H            -1.98473200   -2.70647700   0.32217700

C            -4.56874000   -0.55438800   -0.15113000

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.33774500 | 1.56314500  | -0.48129700 |
| H | -4.41905200 | -2.67215100 | 0.23003800  |
| C | 0.78483500  | 1.96058400  | 1.62681900  |
| H | 0.97544600  | 1.34032700  | 2.51574600  |
| H | 1.60650000  | 2.68612900  | 1.58533600  |
| C | 0.87499200  | 2.04755400  | -1.48310900 |
| H | 0.85829500  | 1.43847500  | -2.39216100 |
| H | -0.05778400 | 2.61860800  | -1.48676000 |
| N | -0.48661700 | 2.71203300  | 1.65886900  |
| N | 1.99426900  | 3.01003500  | -1.58836500 |
| N | -5.96051900 | -0.53185800 | -0.14498500 |
| H | -6.38605600 | 0.24936800  | -0.62135100 |
| H | -6.41220000 | -1.40716800 | -0.36440300 |
| H | -1.25611000 | 2.08207000  | 1.86298100  |
| H | -0.47454000 | 3.39820500  | 2.40756400  |
| H | 2.00031600  | 3.63917000  | -0.79203400 |
| H | 2.88546800  | 2.52390000  | -1.59472600 |

Ph-BS2

|   |            |             |            |
|---|------------|-------------|------------|
| C | 2.24889600 | -1.93203500 | 0.09799500 |
| C | 2.68535200 | -0.58261700 | 0.13927400 |
| C | 4.04762200 | -0.30930300 | 0.21040700 |
| C | 4.98030000 | -1.35367700 | 0.23531600 |
| C | 4.54508500 | -2.67596300 | 0.19196700 |
| C | 3.18279600 | -2.97091600 | 0.12428500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.79289700  | -2.11832600 | 0.02879600  |
| C  | 0.00481500  | -1.01196300 | 0.01737800  |
| H  | 4.39602400  | 0.71824100  | 0.24927000  |
| H  | 6.04076800  | -1.13342200 | 0.29044600  |
| H  | 5.26922300  | -3.48337800 | 0.21249900  |
| H  | 2.85054700  | -4.00405900 | 0.09350700  |
| H  | 0.40522900  | -3.13423200 | -0.01739200 |
| Si | 1.14801800  | 0.50634300  | 0.09385100  |
| C  | -1.45598700 | -1.00203300 | -0.06041600 |
| C  | -2.19088400 | 0.16852800  | -0.14468900 |
| C  | -2.27824100 | -2.15971300 | -0.05960100 |
| C  | -3.54817000 | 0.32633600  | -0.23813200 |
| C  | -3.65557300 | -2.08674700 | -0.13983700 |
| H  | -1.81397400 | -3.13788500 | 0.01105500  |
| C  | -4.33288900 | -0.84852300 | -0.23110800 |
| H  | -3.99884900 | 1.30813600  | -0.31585900 |
| H  | -4.23892000 | -3.00229900 | -0.12546900 |
| C  | 1.07055200  | 1.65139900  | -1.41936900 |
| H  | 0.73769200  | 1.13394400  | -2.33492200 |
| H  | 0.30997800  | 2.40413800  | -1.18420400 |
| N  | -5.71231400 | -0.81741700 | -0.27773700 |
| N  | 2.36732700  | 2.32864400  | -1.55863400 |
| C  | -6.45467600 | 0.38338100  | -0.60814400 |
| H  | -7.51839300 | 0.14415100  | -0.62351900 |
| H  | -6.30191600 | 1.15453300  | 0.15263700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.17810600 | 0.80630300  | -1.58450700 |
| C | 2.35840600  | 3.42060500  | -2.52788700 |
| H | 1.70579300  | 4.22094500  | -2.16748700 |
| H | 3.36641000  | 3.83260400  | -2.62645800 |
| H | 2.00324100  | 3.12535900  | -3.53071300 |
| H | -6.14942900 | -1.68662700 | -0.53988600 |
| H | 3.06757300  | 1.64645800  | -1.83009100 |
| C | 0.96567400  | 1.57040500  | 1.65734500  |
| H | 1.16628800  | 0.97383000  | 2.56528500  |
| H | 1.76819600  | 2.31660900  | 1.59513500  |
| N | -0.31572100 | 2.28047000  | 1.68800600  |
| H | -1.07645500 | 1.60993200  | 1.72278100  |
| C | -0.43941200 | 3.21594700  | 2.80071300  |
| H | -1.43672600 | 3.66406700  | 2.79467700  |
| H | -0.26946200 | 2.75932700  | 3.79186500  |
| H | 0.28860200  | 4.02395500  | 2.68022500  |

Ph-BS3

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.63194700 | 1.37782200  | -0.20767200 |
| C | 3.10584800 | 0.06355300  | 0.02072100  |
| C | 4.47539500 | -0.16415200 | 0.08189000  |
| C | 5.38013100 | 0.89307500  | -0.08197300 |
| C | 4.90597300 | 2.18254200  | -0.30787000 |
| C | 3.53326600 | 2.43073200  | -0.37297700 |
| C | 1.16578000 | 1.51428100  | -0.26090400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.40706000  | 0.40930000  | -0.05481100 |
| H  | 4.85614700  | -1.16673400 | 0.25492800  |
| H  | 6.44780600  | 0.70829900  | -0.03434500 |
| H  | 5.60680400  | 3.00081700  | -0.43490600 |
| H  | 3.16949900  | 3.43844500  | -0.54966000 |
| H  | 0.74625800  | 2.49424700  | -0.48198000 |
| Si | 1.59773300  | -1.05314900 | 0.23112100  |
| C  | -1.05925900 | 0.38517600  | -0.05496700 |
| C  | -1.76349400 | -0.80759800 | -0.28679600 |
| C  | -1.84284900 | 1.53120900  | 0.17216400  |
| C  | -3.14935100 | -0.86172300 | -0.31145600 |
| H  | -1.20724100 | -1.71872300 | -0.47652300 |
| C  | -3.22713000 | 1.49646000  | 0.15758000  |
| H  | -1.35516500 | 2.47633300  | 0.38424400  |
| C  | -3.92800400 | 0.29187300  | -0.07930200 |
| H  | -3.62488100 | -1.81140500 | -0.51378500 |
| H  | -3.76752200 | 2.41442100  | 0.34340800  |
| N  | -5.31465100 | 0.24481500  | -0.06312000 |
| C  | -6.07237900 | 1.48496500  | -0.06661400 |
| H  | -7.13565200 | 1.25121100  | -0.02497300 |
| H  | -5.83718500 | 2.09298300  | 0.81171300  |
| H  | -5.88819200 | 2.09626100  | -0.96260100 |
| C  | -5.99201700 | -0.96180400 | -0.50554300 |
| H  | -5.79666200 | -1.20100500 | -1.56181100 |
| H  | -5.69064000 | -1.82325700 | 0.09714500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.06630700 | -0.83375700 | -0.37709200 |
| N | 1.25627800  | -1.79842700 | 1.75093100  |
| H | 1.78255800  | -2.63526900 | 1.96296600  |
| N | 1.67912200  | -2.37931700 | -0.87471900 |
| H | 1.01872800  | -3.12963500 | -0.72542500 |
| C | 0.71699400  | -1.14411200 | 2.94030000  |
| H | 0.09126300  | -1.83649800 | 3.51334000  |
| H | 1.49487100  | -0.75351100 | 3.60987200  |
| H | 0.08512300  | -0.30633600 | 2.64148600  |
| C | 2.23713900  | -2.35978700 | -2.22381100 |
| H | 2.70617300  | -3.31948500 | -2.46631200 |
| H | 1.48970300  | -2.14143400 | -2.99811800 |
| H | 3.01069900  | -1.59224300 | -2.28665600 |

Ph-BS4

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.41592400 | 0.11168200  | -0.04272600 |
| C | 2.57871700 | -1.29094800 | -0.10065100 |
| C | 3.84819000 | -1.84326100 | -0.22620800 |
| C | 4.96340600 | -1.00450800 | -0.29852300 |
| C | 4.80930900 | 0.37588500  | -0.20471800 |
| C | 3.54121400 | 0.96152200  | -0.05973100 |
| C | 1.01651900 | 0.57668500  | -0.01153000 |
| C | 0.02551700 | -0.35105900 | 0.03335500  |
| H | 3.97920900 | -2.91945900 | -0.28469000 |
| H | 5.95716800 | -1.42427400 | -0.41403400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.68972500  | 1.00623300  | -0.23618200 |
| H  | 0.83447200  | 1.64584400  | -0.05386900 |
| Si | 0.86095700  | -2.05577800 | 0.00438900  |
| C  | -1.41126700 | -0.05502200 | 0.01255000  |
| C  | -2.35501100 | -1.02708600 | 0.38702500  |
| C  | -1.93226900 | 1.18866300  | -0.38969200 |
| C  | -3.71978800 | -0.77553500 | 0.39152900  |
| H  | -2.00748900 | -2.00574200 | 0.70079200  |
| C  | -3.29069900 | 1.45587600  | -0.39544200 |
| H  | -1.25684400 | 1.96457400  | -0.73217000 |
| C  | -4.23171200 | 0.48355400  | 0.01489300  |
| H  | -4.38849200 | -1.57027400 | 0.69201300  |
| H  | -3.62264300 | 2.42784100  | -0.73369000 |
| N  | -5.59239800 | 0.75836800  | 0.05007800  |
| C  | -6.09181100 | 1.97659100  | -0.56430200 |
| H  | -7.16520100 | 2.04732200  | -0.39061000 |
| H  | -5.62961300 | 2.85962400  | -0.11466100 |
| H  | -5.91480000 | 2.01497800  | -1.64989800 |
| C  | -6.53371600 | -0.33207700 | 0.23954700  |
| H  | -6.49838300 | -1.07560600 | -0.57112400 |
| H  | -6.34590800 | -0.85220700 | 1.18299500  |
| H  | -7.54348300 | 0.07453500  | 0.28693500  |
| N  | 3.35909500  | 2.37052800  | 0.05352300  |
| C  | 4.38824300  | 3.21409000  | -0.53447500 |
| H  | 4.00940800  | 4.23787300  | -0.59818300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.32649900  | 3.24451000  | 0.04710300  |
| H | 4.61787300  | 2.87265800  | -1.54501700 |
| C | 2.97818200  | 2.83137900  | 1.38971400  |
| H | 2.61544500  | 3.86174600  | 1.33100200  |
| H | 2.17915100  | 2.21060300  | 1.79341700  |
| H | 3.82466600  | 2.80428200  | 2.09726400  |
| N | 0.36598100  | -2.96442400 | 1.39217700  |
| H | 0.76979300  | -3.87517600 | 1.56127200  |
| H | 0.17896800  | -2.48088200 | 2.25900800  |
| N | 0.64887800  | -3.13053300 | -1.33044500 |
| H | 1.11773300  | -2.93072800 | -2.20207000 |
| H | -0.24523800 | -3.57355000 | -1.48806200 |

Ph-BS5

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.30713200 | -1.48398400 | -0.05766900 |
| C | 2.78920200 | -0.15342800 | 0.03858300  |
| C | 4.15497800 | 0.08586000  | 0.07489100  |
| C | 5.07988900 | -0.97704300 | 0.01794600  |
| C | 4.59061100 | -2.28665200 | -0.08275000 |
| C | 3.22200700 | -2.53727100 | -0.11967500 |
| C | 0.84836800 | -1.62422000 | -0.08325800 |
| C | 0.07882500 | -0.50428800 | -0.01148600 |
| H | 4.53883800 | 1.10036200  | 0.15454500  |
| H | 5.29248500 | -3.11356800 | -0.13407700 |
| H | 2.86986300 | -3.56174000 | -0.19351400 |
| H | 0.42987300 | -2.62517600 | -0.17223800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 1.27465100  | 0.97110900  | 0.05988800  |
| C  | -1.38880300 | -0.48677900 | -0.00395800 |
| C  | -2.10670100 | 0.69935400  | -0.23354400 |
| C  | -2.16618200 | -1.63736400 | 0.22722100  |
| C  | -3.49443400 | 0.74315200  | -0.24939200 |
| H  | -1.56846400 | 1.62381900  | -0.41258400 |
| C  | -3.55028800 | -1.61331900 | 0.21696100  |
| H  | -1.67524900 | -2.58177100 | 0.43346000  |
| C  | -4.26358700 | -0.41518700 | -0.01614700 |
| H  | -3.97590100 | 1.69061400  | -0.44812900 |
| H  | -4.08167700 | -2.53686500 | 0.40154700  |
| C  | 1.16999200  | 1.99523000  | 1.66340200  |
| H  | 1.34929700  | 1.34822400  | 2.53591500  |
| H  | 2.00624400  | 2.70496900  | 1.63775000  |
| C  | 1.23340300  | 2.15269200  | -1.44100400 |
| H  | 1.16211300  | 1.57006300  | -2.36450100 |
| H  | 0.32807900  | 2.76515900  | -1.39960700 |
| N  | -0.08612300 | 2.77036600  | 1.71678400  |
| N  | 2.39227100  | 3.06705900  | -1.55659700 |
| N  | -5.65154800 | -0.37959800 | 0.00577400  |
| H  | -0.87171700 | 2.14611200  | 1.87174000  |
| H  | -0.07360900 | 3.41395800  | 2.50246400  |
| H  | 2.45320500  | 3.66919200  | -0.74175400 |
| H  | 3.25802900  | 2.53890300  | -1.60551100 |
| C  | -6.39716400 | -1.62699300 | -0.00724900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.46242800 | -1.40382500 | 0.04231900  |
| H | -6.21190300 | -2.22791400 | -0.91023300 |
| H | -6.15198000 | -2.24120800 | 0.86383700  |
| C | -6.33793900 | 0.81800200  | -0.44787300 |
| H | -6.04216600 | 1.68698900  | 0.14650000  |
| H | -6.14501400 | 1.04903700  | -1.50643600 |
| H | -7.41119900 | 0.68355600  | -0.31691200 |
| N | 6.45288300  | -0.72088400 | -0.00213000 |
| H | 6.73267500  | 0.14949200  | 0.42622700  |
| H | 7.03726200  | -1.48906700 | 0.29395400  |

Styryl-DBS1

|   |            |             |            |
|---|------------|-------------|------------|
| C | 2.44838700 | 0.06797400  | 2.69768700 |
| C | 2.89386700 | 0.09209600  | 1.35163300 |
| C | 4.25684400 | 0.15459900  | 1.08760000 |
| C | 5.18264700 | 0.19058500  | 2.13764100 |
| C | 4.73875300 | 0.16553700  | 3.45789600 |
| C | 3.37471100 | 0.10470000  | 3.74386700 |
| C | 0.99359100 | 0.00441600  | 2.86780000 |
| C | 0.20900300 | -0.00967200 | 1.75470100 |
| H | 4.61637200 | 0.17566200  | 0.06315200 |
| H | 6.24484000 | 0.23854600  | 1.92377100 |
| H | 5.45777600 | 0.19390700  | 4.26970100 |
| H | 3.03379500 | 0.08604200  | 4.77445700 |
| H | 0.57678500 | -0.03042500 | 3.87389400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 1.36604600  | 0.04119800  | 0.23714700  |
| C  | 1.11820500  | 1.58300000  | -0.80937300 |
| C  | 1.74641900  | 1.73353000  | -2.05857700 |
| C  | 0.35562200  | 2.67122500  | -0.35149100 |
| C  | 1.62477000  | 2.89570000  | -2.80847300 |
| H  | 2.34442800  | 0.92262000  | -2.46283800 |
| C  | 0.22227700  | 3.83818100  | -1.09204700 |
| H  | -0.15267500 | 2.60575800  | 0.60454400  |
| C  | 0.85861600  | 3.97264700  | -2.33543000 |
| H  | 2.12058300  | 2.97457300  | -3.77149700 |
| H  | -0.38385600 | 4.65467300  | -0.71102600 |
| C  | 1.33684800  | -1.50382900 | -0.83539300 |
| C  | 2.05280200  | -2.65594200 | -0.46538800 |
| C  | 0.56695300  | -1.58952400 | -2.00789500 |
| C  | 2.00521700  | -3.82352900 | -1.21446700 |
| H  | 2.66929600  | -2.63995000 | 0.42758100  |
| C  | 0.50918900  | -2.75058400 | -2.76756000 |
| H  | 0.00263500  | -0.72608600 | -2.34521600 |
| C  | 1.22964100  | -3.89170000 | -2.38238100 |
| H  | 2.57054100  | -4.69467600 | -0.89689400 |
| H  | -0.09944200 | -2.78122500 | -3.66651000 |
| C  | -1.23226600 | -0.07072200 | 1.82249400  |
| C  | -2.06547400 | -0.06001900 | 0.75743000  |
| H  | -1.65720300 | -0.12289400 | 2.82484500  |
| H  | -1.61983700 | 0.00410500  | -0.23230300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.52263300 | -0.11559600 | 0.76219800  |
| C | -4.30133500 | -0.25068700 | 1.92747200  |
| C | -4.21894400 | -0.03197000 | -0.45643500 |
| C | -5.68362300 | -0.29498400 | 1.87729900  |
| H | -3.81667600 | -0.32863900 | 2.89378100  |
| C | -5.60346800 | -0.07538300 | -0.51858600 |
| H | -3.65385100 | 0.07092400  | -1.37723900 |
| C | -6.36580800 | -0.20912100 | 0.65078200  |
| H | -6.25274700 | -0.39653600 | 2.79634300  |
| H | -6.10437600 | -0.00207500 | -1.47895500 |
| N | -7.75807300 | -0.19564200 | 0.60805400  |
| H | -8.16823600 | -0.46507900 | -0.27383000 |
| H | -8.22150400 | -0.62879100 | 1.39300200  |
| N | 0.68279500  | 5.11739800  | -3.10799200 |
| H | 0.42056400  | 5.94881900  | -2.59970100 |
| H | 1.40316700  | 5.29652300  | -3.79164000 |
| N | 1.13322700  | -5.07553500 | -3.10780500 |
| H | 0.85915700  | -4.97586700 | -4.07370000 |
| H | 1.89530200  | -5.72578800 | -2.98760300 |

Styryl-DBS2

|   |            |             |            |
|---|------------|-------------|------------|
| C | 2.62473500 | -0.14662600 | 2.76625300 |
| C | 3.12755400 | -0.15860200 | 1.43657300 |
| C | 4.50298200 | -0.23801500 | 1.22970800 |
| C | 5.38189300 | -0.30622300 | 2.32175300 |

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 4.88052900 | -0.29268900 | 3.62524600  |
| C  | 3.50340500 | -0.21258100 | 3.85420800  |
| C  | 1.16365300 | -0.06552700 | 2.87494800  |
| C  | 0.42811500 | -0.00143900 | 1.72618200  |
| H  | 4.90898600 | -0.24814000 | 0.22031000  |
| H  | 6.45351700 | -0.36949300 | 2.15274400  |
| H  | 5.56419200 | -0.34454100 | 4.46860600  |
| H  | 3.11685500 | -0.20319600 | 4.87079300  |
| H  | 0.70256600 | -0.06327600 | 3.86410800  |
| Si | 1.65069600 | -0.03520600 | 0.26617100  |
| C  | 1.61809100 | 1.55905600  | -0.74250100 |
| C  | 2.33208700 | 1.66711200  | -1.95208000 |
| C  | 0.93182000 | 2.69863900  | -0.28180000 |
| C  | 2.36218800 | 2.86394700  | -2.67030900 |
| H  | 2.86754400 | 0.80558500  | -2.34468100 |
| C  | 0.95806000 | 3.89768900  | -0.99748000 |
| H  | 0.36469300 | 2.64913700  | 0.64405900  |
| C  | 1.67434200 | 3.98253900  | -2.19330400 |
| H  | 2.91932800 | 2.92303300  | -3.60175000 |
| H  | 0.41760900 | 4.76333600  | -0.62327100 |
| C  | 1.49519000 | -1.54260100 | -0.85962500 |
| C  | 2.08248000 | -2.76974400 | -0.49568700 |
| C  | 0.76056000 | -1.49893100 | -2.06010900 |
| C  | 1.93798800 | -3.90666200 | -1.29312800 |
| H  | 2.66611200 | -2.83758200 | 0.41911100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.61313300  | -2.63319600 | -2.86130900 |
| H | 0.30439400  | -0.56624500 | -2.38366300 |
| C | 1.20138700  | -3.84056000 | -2.47811700 |
| H | 2.40270500  | -4.84193300 | -0.99183300 |
| H | 0.04256900  | -2.57334400 | -3.78451200 |
| C | -1.01739700 | 0.06568900  | 1.74027100  |
| C | -1.80733600 | 0.11959400  | 0.64053800  |
| H | -1.48054100 | 0.06636000  | 2.72865400  |
| H | -1.32559400 | 0.11514100  | -0.33660800 |
| C | -3.26928400 | 0.17781900  | 0.59726200  |
| C | -4.08386100 | 0.19049100  | 1.74908100  |
| C | -3.90798500 | 0.22213600  | -0.65821900 |
| C | -5.47060800 | 0.24418100  | 1.64372400  |
| H | -3.62995900 | 0.15727600  | 2.73505300  |
| C | -5.29689300 | 0.27576600  | -0.76351600 |
| H | -3.29964100 | 0.21333500  | -1.55970400 |
| C | -6.08672800 | 0.28704100  | 0.38795300  |
| H | -6.07639900 | 0.25221200  | 2.54609500  |
| H | -5.76192000 | 0.30866100  | -1.74523600 |
| N | 1.70219600  | 5.24301500  | -2.94916500 |
| H | 2.46754400  | 5.80401700  | -2.63370100 |
| H | 1.81307100  | 5.04525800  | -3.92312600 |
| N | 1.05014400  | -5.03544800 | -3.32089100 |
| H | 1.82723800  | -5.10250000 | -3.94669400 |
| H | 1.01739500  | -5.84993800 | -2.74163800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -7.62169900 | 0.34584500  | 0.27838200  |
| H | -7.99304100 | 1.13892100  | 0.89322800  |
| H | -7.90008100 | 0.52335000  | -0.73940700 |
| N | -8.19428600 | -0.93143900 | 0.72736900  |
| H | -8.79218200 | -0.77097500 | 1.51271700  |
| H | -8.72350800 | -1.33935100 | -0.01662900 |

Styryl-DBS3

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.98224500 | 1.70412700  | -0.17473900 |
| C  | 3.21353300 | 0.30789500  | -0.16694900 |
| C  | 4.50752300 | -0.18556400 | -0.28829100 |
| C  | 5.57754600 | 0.70256700  | -0.41819600 |
| C  | 5.35723100 | 2.07764400  | -0.39260000 |
| C  | 4.06532100 | 2.60660800  | -0.25567700 |
| C  | 1.56857500 | 2.09325100  | -0.13627900 |
| C  | 0.62353600 | 1.11366100  | -0.05814200 |
| H  | 4.69257800 | -1.25499000 | -0.29809300 |
| H  | 6.58933400 | 0.32618100  | -0.52645800 |
| H  | 6.20470900 | 2.74776100  | -0.47028700 |
| H  | 1.30682600 | 3.14565700  | -0.20358500 |
| Si | 1.53571700 | -0.55863600 | -0.04153700 |
| C  | 1.11425900 | -1.62797000 | -1.52977400 |
| C  | 1.57405800 | -2.95293900 | -1.63332200 |
| C  | 0.39108700 | -1.12358000 | -2.62404200 |
| C  | 1.33075700 | -3.73087400 | -2.75743900 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.13375000  | -3.39513900 | -0.81471000 |
| C | 0.13749800  | -1.89107100 | -3.75337100 |
| H | 0.01052700  | -0.10836800 | -2.59284500 |
| C | 0.60689200  | -3.21022000 | -3.84146500 |
| H | 1.69670500  | -4.75252300 | -2.80029500 |
| H | -0.43366500 | -1.47118600 | -4.57604900 |
| C | 1.37682600  | -1.55052400 | 1.54991900  |
| C | 2.12743800  | -1.21624600 | 2.69076600  |
| C | 0.47139600  | -2.61700800 | 1.68142300  |
| C | 1.98508900  | -1.89920800 | 3.89077700  |
| H | 2.84718500  | -0.40556900 | 2.64010800  |
| C | 0.31763300  | -3.30970500 | 2.87553000  |
| H | -0.12454400 | -2.92422600 | 0.82797900  |
| C | 1.07369800  | -2.96077900 | 4.00483300  |
| H | 2.58072600  | -1.61190000 | 4.75223700  |
| H | -0.39434700 | -4.12719600 | 2.94071100  |
| C | -0.78897500 | 1.40890700  | -0.02843100 |
| C | -1.78199900 | 0.49386300  | 0.05674300  |
| H | -1.05012100 | 2.46621500  | -0.07616600 |
| H | -1.50075400 | -0.55511000 | 0.11426900  |
| C | -3.21827000 | 0.73828400  | 0.08691800  |
| C | -3.80512800 | 2.01394400  | 0.00059100  |
| C | -4.10457800 | -0.34593800 | 0.19747300  |
| C | -5.17631900 | 2.19632900  | 0.02988900  |
| H | -3.17561300 | 2.89076200  | -0.09913800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.48087400 | -0.18301900 | 0.22773100  |
| H | -3.69844600 | -1.35085400 | 0.25661200  |
| C | -6.06225100 | 1.10085600  | 0.15738400  |
| H | -5.56316100 | 3.20292500  | -0.04884200 |
| H | -6.10356900 | -1.06339400 | 0.30522300  |
| N | 0.30780400  | -4.00365500 | -4.94679900 |
| H | 0.09555500  | -3.50090100 | -5.79578000 |
| H | 0.93536600  | -4.77752100 | -5.10756500 |
| N | 0.88460900  | -3.61228200 | 5.22057000  |
| H | 0.49489800  | -4.54118200 | 5.16260400  |
| H | 1.65452200  | -3.55704600 | 5.87041800  |
| N | 3.81444200  | 4.00882000  | -0.21013800 |
| C | 4.79040400  | 4.86995300  | -0.85998700 |
| H | 4.36095900  | 5.86996400  | -0.96610800 |
| H | 5.73679200  | 4.97415900  | -0.30032500 |
| H | 5.01776200  | 4.48935800  | -1.85694500 |
| C | 3.43426000  | 4.51852500  | 1.10830100  |
| H | 4.29354400  | 4.56966800  | 1.79901300  |
| H | 3.01925000  | 5.52538400  | 1.00488500  |
| H | 2.67490900  | 3.88059300  | 1.55902500  |
| N | -7.43618400 | 1.28356100  | 0.22071200  |
| C | -8.00095000 | 2.58429900  | -0.09704800 |
| H | -7.80021600 | 2.89712800  | -1.13271900 |
| H | -9.08042900 | 2.54681300  | 0.04552900  |
| H | -7.60987100 | 3.35648800  | 0.57136400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -8.31282500 | 0.12829200  | 0.13247200  |
| H | -8.10537700 | -0.58281100 | 0.93700800  |
| H | -9.34552600 | 0.45657900  | 0.24530300  |
| H | -8.22279100 | -0.40608500 | -0.82525500 |

Styryl-DBS4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.70452700 | -1.05692900 | -1.25790600 |
| C  | -2.72058100 | -0.08230000 | -0.23144800 |
| C  | -3.92753300 | 0.44292600  | 0.21526300  |
| C  | -5.12447000 | 0.00324900  | -0.35420500 |
| C  | -5.11541200 | -0.97963400 | -1.34088200 |
| C  | -3.91477600 | -1.54026000 | -1.80170200 |
| C  | -1.36592700 | -1.46005800 | -1.70280500 |
| C  | -0.27993700 | -0.91357300 | -1.08577100 |
| H  | -3.94851000 | 1.20053300  | 0.99191600  |
| H  | -6.07076100 | 0.41582100  | -0.02082900 |
| H  | -6.05803900 | -1.32213100 | -1.74986200 |
| H  | -1.27010500 | -2.15818800 | -2.52973100 |
| Si | -0.92813800 | 0.29610300  | 0.23117800  |
| C  | -0.42938400 | 2.08501500  | -0.09948200 |
| C  | -0.72293300 | 3.10322500  | 0.82412300  |
| C  | 0.17864700  | 2.46553000  | -1.30581800 |
| C  | -0.42213000 | 4.43608400  | 0.55956600  |
| H  | -1.19034200 | 2.85470500  | 1.77213700  |
| C  | 0.47831900  | 3.79912200  | -1.57272900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.42124000  | 1.71303500  | -2.04820500 |
| C | 0.18672600  | 4.80119200  | -0.64460800 |
| H | -0.66380700 | 5.21181100  | 1.27634400  |
| H | 0.94292000  | 4.06361700  | -2.51838400 |
| C | -0.53209900 | -0.18457700 | 2.01352400  |
| C | -1.23522600 | -1.22470600 | 2.64459800  |
| C | 0.50004300  | 0.42848900  | 2.74023600  |
| C | -0.92503200 | -1.63259800 | 3.93786800  |
| H | -2.04431000 | -1.72153000 | 2.11873600  |
| C | 0.81523600  | 0.01829900  | 4.03361700  |
| H | 1.06809000  | 1.23903100  | 2.29538800  |
| C | 0.10586500  | -1.01356100 | 4.65149900  |
| H | -1.46927400 | -2.44316100 | 4.40788800  |
| H | 1.62525400  | 0.50642200  | 4.56820200  |
| C | 1.07306200  | -1.25149300 | -1.45848100 |
| C | 2.19094700  | -0.75550800 | -0.88072600 |
| H | 1.17261800  | -1.97159600 | -2.27053800 |
| H | 2.06646100  | -0.04062000 | -0.07071800 |
| C | 3.57826700  | -1.06545000 | -1.20562700 |
| C | 3.96824600  | -1.98145500 | -2.20141700 |
| C | 4.61100400  | -0.42630300 | -0.49704200 |
| C | 5.30101000  | -2.23940000 | -2.47084400 |
| H | 3.21440100  | -2.50501300 | -2.77782400 |
| C | 5.94954400  | -0.67616400 | -0.75922300 |
| H | 4.35121700  | 0.28680300  | 0.27873300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 6.32255100  | -1.58949700 | -1.75581700 |
| H | 5.56516000  | -2.95691700 | -3.24174900 |
| H | 6.71736100  | -0.16478700 | -0.18694400 |
| N | -3.87976500 | -2.55774000 | -2.79800800 |
| C | -5.00576800 | -2.61157000 | -3.71809100 |
| H | -4.73981900 | -3.25505400 | -4.56112700 |
| H | -5.92898700 | -3.01856300 | -3.26940900 |
| H | -5.21894700 | -1.61400800 | -4.10513300 |
| C | -3.52193100 | -3.88785000 | -2.30142000 |
| H | -4.34624200 | -4.35728500 | -1.73778100 |
| H | -3.27172500 | -4.53736500 | -3.14522400 |
| H | -2.65406100 | -3.82972100 | -1.64562300 |
| C | 0.55745100  | 6.24416900  | -0.92924800 |
| H | 0.65679600  | 6.36954700  | -2.01892100 |
| H | 1.55074500  | 6.44086200  | -0.50706000 |
| C | 0.42684200  | -1.42543000 | 6.07503000  |
| H | -0.25324900 | -0.89781900 | 6.75525000  |
| H | 1.44129500  | -1.07330100 | 6.31957500  |
| N | -0.37363000 | 7.18724000  | -0.30155200 |
| H | -0.03676700 | 8.13807400  | -0.40758100 |
| H | -1.28094800 | 7.13727700  | -0.75528000 |
| N | 0.22302900  | -2.86193700 | 6.28864200  |
| H | 0.91051600  | -3.39431700 | 5.76374200  |
| H | 0.34657800  | -3.09407700 | 7.26834500  |
| N | 7.66154400  | -1.89390700 | -1.98882700 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 7.87036000 | -2.26942500 | -2.90196400 |
| H | 8.32403400 | -1.18759000 | -1.70483100 |

Styryl-DBS5

|    |            |             |             |
|----|------------|-------------|-------------|
| C  | 2.78665100 | -0.10708200 | -2.59111300 |
| C  | 3.23174300 | -0.09669900 | -1.24470000 |
| C  | 4.58672300 | -0.14301300 | -0.96378200 |
| C  | 5.53986200 | -0.20409500 | -2.00130300 |
| C  | 5.08919700 | -0.21021000 | -3.32870500 |
| C  | 3.72908300 | -0.16280900 | -3.62071200 |
| C  | 1.33520600 | -0.05848800 | -2.76461000 |
| C  | 0.54353400 | -0.02080300 | -1.65516000 |
| H  | 4.93766600 | -0.13137300 | 0.06532500  |
| H  | 5.81414600 | -0.24965800 | -4.13622500 |
| H  | 0.91958400 | -0.05278600 | -3.77213600 |
| Si | 1.69520400 | -0.02546600 | -0.13801100 |
| C  | 1.46121400 | -1.54184900 | 0.95028900  |
| C  | 2.09625200 | -1.65904600 | 2.19941600  |
| C  | 0.69600200 | -2.64170500 | 0.52616600  |
| C  | 1.97969300 | -2.80119400 | 2.98076300  |
| H  | 2.69406400 | -0.83627800 | 2.57953900  |
| C  | 0.56751700 | -3.78879800 | 1.29836200  |
| H  | 0.18092100 | -2.59982900 | -0.42756700 |
| C  | 1.21100000 | -3.89016200 | 2.54097100  |
| H  | 2.47956600 | -2.85391200 | 3.94359300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.04175100 | -4.61474800 | 0.94341600  |
| C | 1.66743700  | 1.54350300  | 0.90054700  |
| C | 2.38462400  | 2.68652400  | 0.50565300  |
| C | 0.89495300  | 1.65671500  | 2.06898700  |
| C | 2.33536600  | 3.87133600  | 1.22736500  |
| H | 3.00290500  | 2.64995700  | -0.38542800 |
| C | 0.83534800  | 2.83535400  | 2.80119900  |
| H | 0.32907300  | 0.80168500  | 2.42468700  |
| C | 1.55659600  | 3.96703000  | 2.39104000  |
| H | 2.90129100  | 4.73490500  | 0.89058700  |
| H | 0.22382500  | 2.88727200  | 3.69725400  |
| C | -0.89737600 | 0.02640200  | -1.72918300 |
| C | -1.73957200 | 0.04162700  | -0.67059700 |
| H | -1.31696900 | 0.04587300  | -2.73518700 |
| H | -1.30186000 | 0.01819300  | 0.32465100  |
| C | -3.19664500 | 0.08252300  | -0.68863000 |
| C | -3.97371900 | 0.12854400  | -1.86033000 |
| C | -3.90530800 | 0.06673400  | 0.52418600  |
| C | -5.35693800 | 0.16179800  | -1.82509700 |
| H | -3.48765700 | 0.13577600  | -2.82937200 |
| C | -5.29026800 | 0.09863600  | 0.57918100  |
| H | -3.34884800 | 0.02129000  | 1.45519700  |
| C | -6.06275700 | 0.16055600  | -0.59961100 |
| H | -5.89495300 | 0.18944500  | -2.76262200 |
| H | -5.76924700 | 0.07456800  | 1.54814300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -7.44908200 | 0.23047200  | -0.56038400 |
| H | 3.40496800  | -0.17148300 | -4.65705100 |
| N | 6.90622000  | -0.19264000 | -1.70804000 |
| H | 7.14694900  | -0.54462900 | -0.79273400 |
| H | 7.50068800  | -0.58110500 | -2.42584900 |
| C | -8.13789400 | -0.00295500 | 0.69707500  |
| H | -9.20829100 | 0.13433300  | 0.54654300  |
| H | -7.97232500 | -1.01537200 | 1.09578700  |
| H | -7.81962900 | 0.71574600  | 1.45752300  |
| C | -8.20931800 | 0.05572100  | -1.78611500 |
| H | -9.26866900 | 0.18898400  | -1.56855600 |
| H | -7.93185300 | 0.80740200  | -2.53036000 |
| H | -8.07255400 | -0.93801200 | -2.23908900 |
| N | 1.03871700  | -5.01414100 | 3.34566000  |
| H | 0.77488900  | -5.85853200 | 2.85997700  |
| H | 1.76466800  | -5.17563800 | 4.02785400  |
| N | 1.45763900  | 5.16839400  | 3.08774200  |
| H | 1.18158400  | 5.09092700  | 4.05513900  |
| H | 2.22128900  | 5.81437500  | 2.95493900  |