

**A QUANTUM-MECHANICAL BASED QUANTITATIVE STRUCTURE-  
PROPERTY RELATIONSHIPS FOR ELECTRONIC PROPERTIES OF TWO  
LARGE CLASSES OF ORGANIC SEMI-CONDUCTOR MATERIALS:  
POLYCYCLIC AROMATIC HYDROCARBONS AND THIENOACENES**

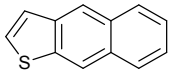
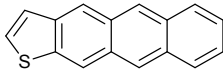
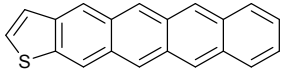
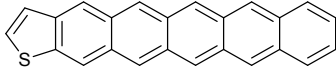
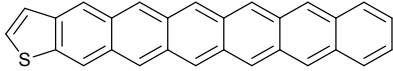
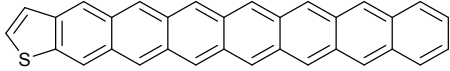
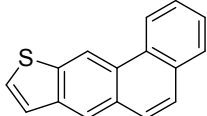
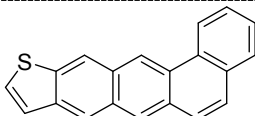
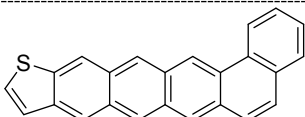
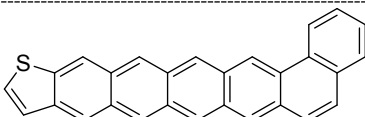
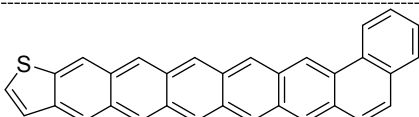
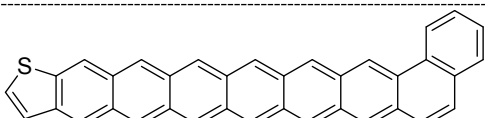
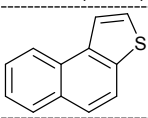
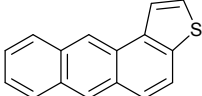
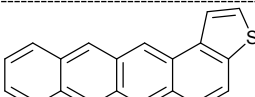
*Lam H. Nguyen<sup>a</sup>, Tuan H. Nguyen<sup>a</sup>, and Thanh N. Truong<sup>b\*</sup>*

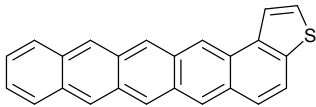
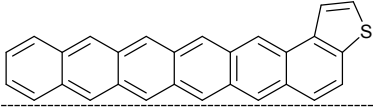
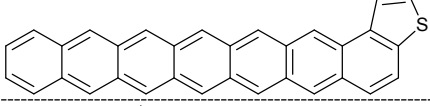
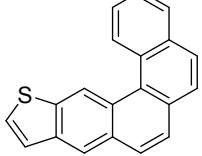
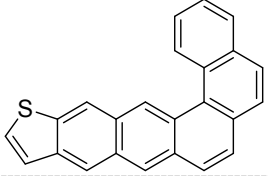
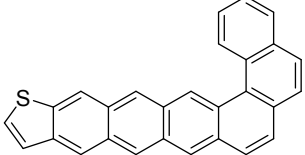
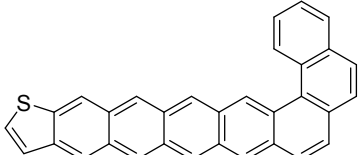
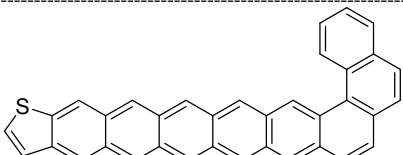
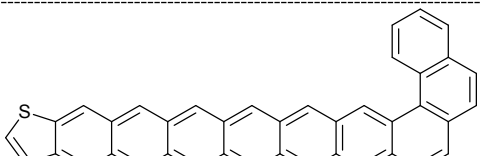
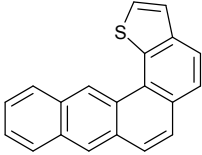
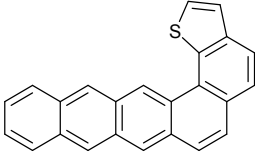
<sup>a</sup>Institute for Computational Science and Technology, Ho Chi Minh City, Viet Nam

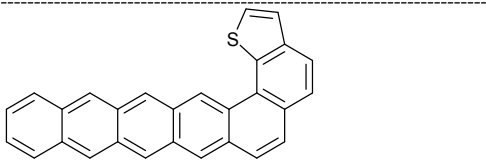
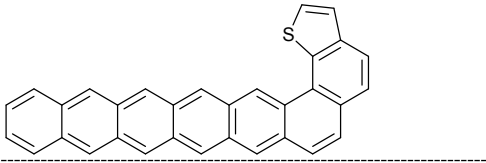
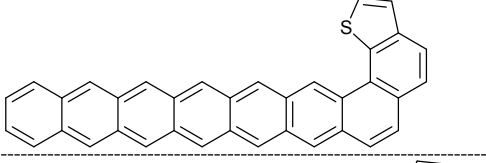
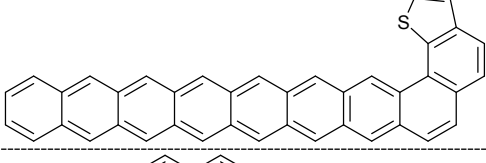
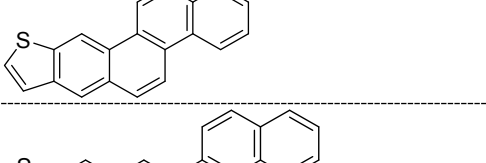
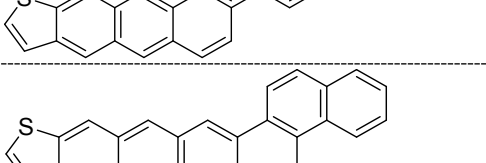
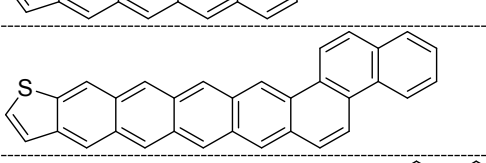
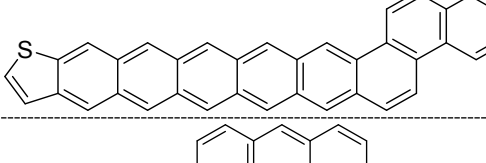
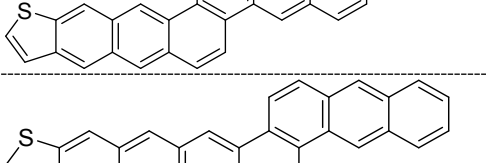
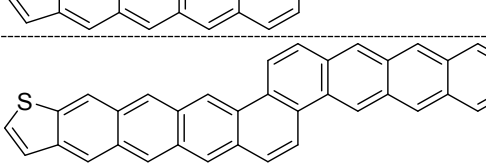


<sup>b</sup>Department of Chemistry, University of Utah, Salt Lake City, UT, USA

**KEYWORDS** quantitative structure-property relationships, polycyclic aromatic hydrocarbons, thienoacenes, degree of  $\pi$ -orbital overlap, electronic properties

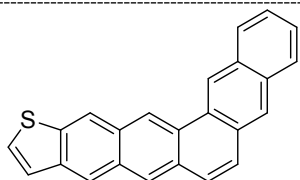
**Table S1:** Thienoacene molecules used for determining DPO parameters

| No  | Structures  | Band gap (eV) |
|-----|---|---------------|
| A1  |    | 3.970         |
| A2  |    | 3.086         |
| A3  |    | 2.450         |
| A4  |    | 1.984         |
| A5  |    | 1.633         |
| A6  |    | 1.364         |
| B1  |    | 4.126         |
| B2  |   | 3.264         |
| B3  |  | 2.607         |
| B4  |  | 2.116         |
| B5  |  | 1.743         |
| B6  |  | 1.456         |
| B1* |  | 4.481         |
| B2* |  | 3.538         |
| B3* |  | 2.795         |

|            |   |       |
|------------|---|-------|
| <b>B4*</b> |    | 2.244 |
| <b>B5*</b> |    | 1.832 |
| <b>B6*</b> |    | 1.518 |
| <b>C1</b>  |    | 3.716 |
| <b>C2</b>  |    | 3.048 |
| <b>C3</b>  |   | 2.485 |
| <b>C4</b>  |  | 2.041 |
| <b>C5</b>  |  | 1.694 |
| <b>C6</b>  |  | 1.309 |
| <b>C1*</b> |  | 3.551 |
| <b>C2*</b> |  | 2.846 |

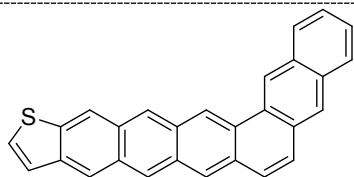
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|------------|---|-------|
| <b>C3*</b> |    | 2.298 |
| <b>C4*</b> |    | 1.880 |
| <b>C5*</b> |    | 1.559 |
| <b>C6*</b> |    | 1.309 |
| <b>D1</b>  |    | 3.805 |
| <b>D2</b>  |   | 3.095 |
| <b>D3</b>  |  | 2.502 |
| <b>D4</b>  |  | 2.044 |
| <b>D5</b>  |  | 1.691 |
| <b>D6</b>  |  | 2.877 |
| <b>D7</b>  |  | 2.402 |
| <b>D8</b>  |  | 2.253 |

**D9**



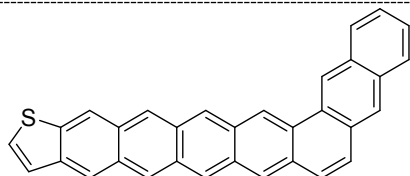
3.337

**D10**



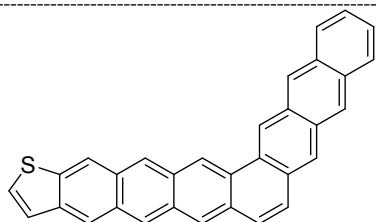
2.678

**D11**



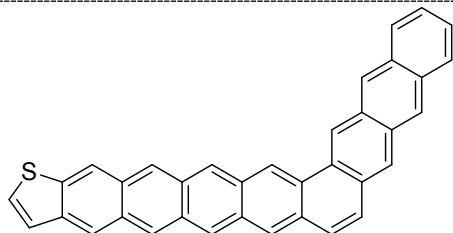
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**D12**



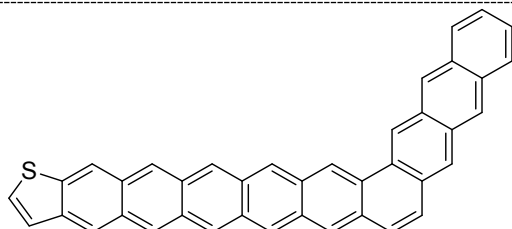
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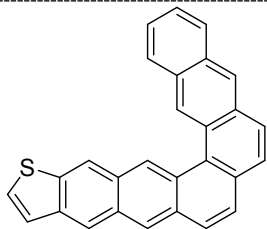
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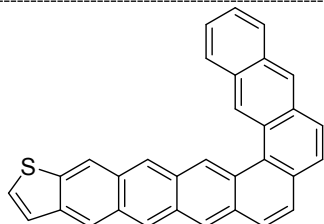
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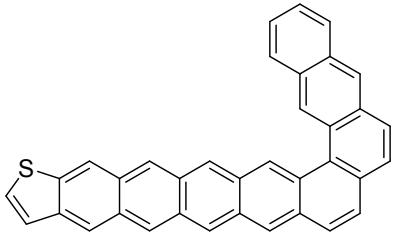
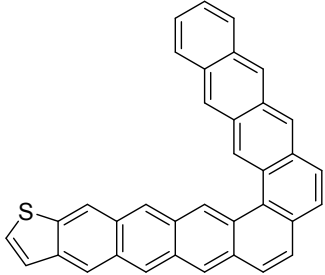
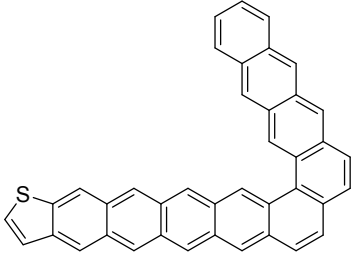
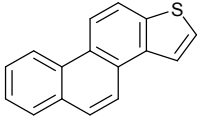
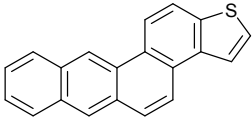
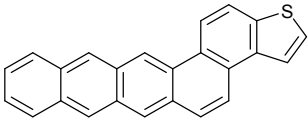
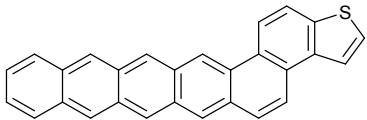
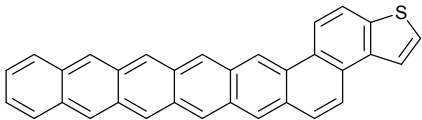
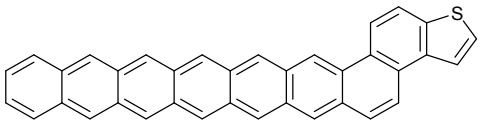
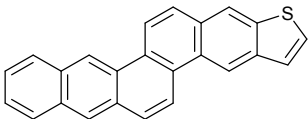


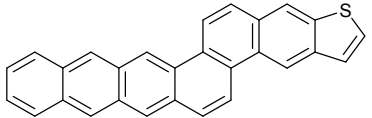
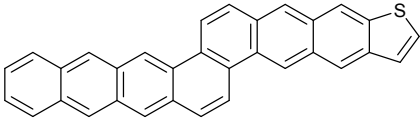
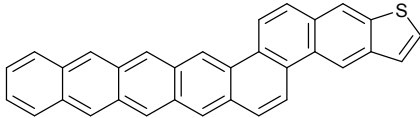
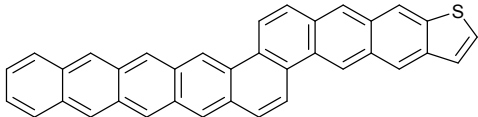
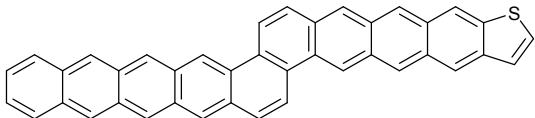
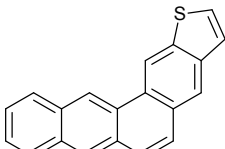
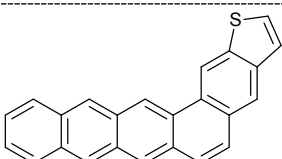
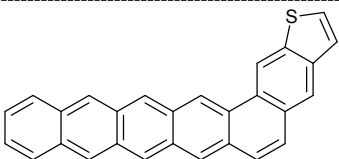
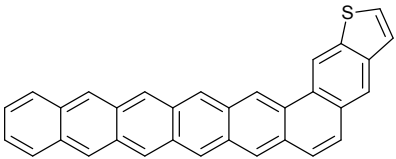
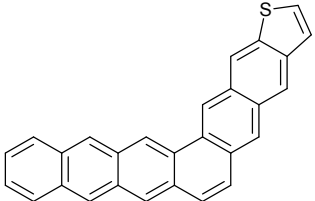
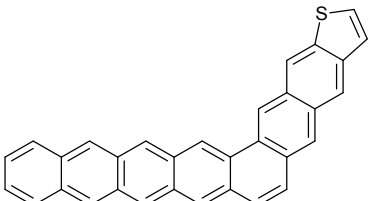
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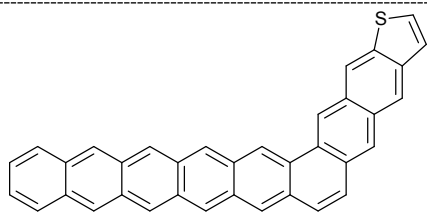


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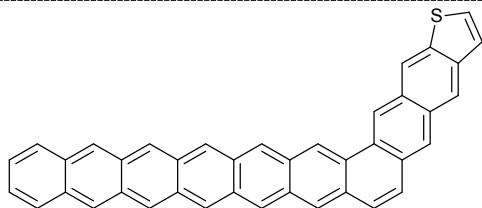
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| <b>D17</b> |    | 1.965 |
| <b>D18</b> |    | 2.191 |
| <b>D19</b> |    | 1.884 |
| <b>D1*</b> |   | 4.324 |
| <b>D2*</b> |  | 3.585 |
| <b>D3*</b> |  | 2.85  |
| <b>D4*</b> |  | 2.293 |
| <b>D5*</b> |  | 1.872 |
| <b>D6*</b> |  | 1.551 |
| <b>D7*</b> |  | 3.31  |

|             |   |       |
|-------------|---|-------|
| <b>D8*</b>  |    | 2.722 |
| <b>D9*</b>  |    | 2.539 |
| <b>D10*</b> |    | 2.217 |
| <b>D11*</b> |    | 2.136 |
| <b>D12*</b> |    | 2.014 |
| <b>D13*</b> |    | 3.681 |
| <b>D14*</b> |   | 2.934 |
| <b>D15*</b> |  | 2.351 |
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| <b>D18*</b> |  | 2.406 |

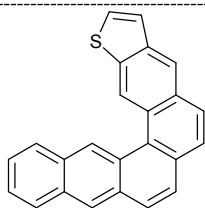
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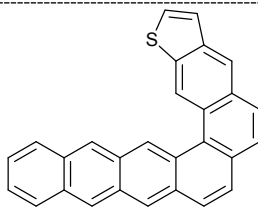
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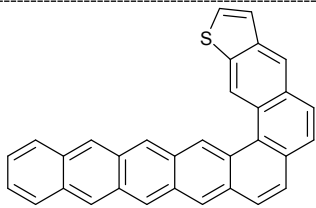
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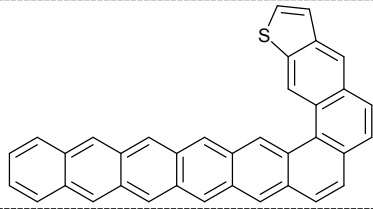
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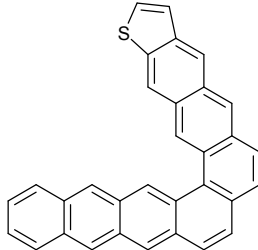
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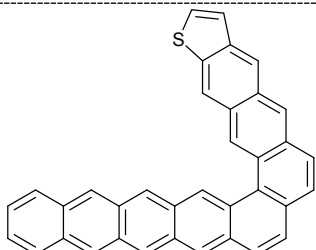
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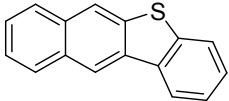
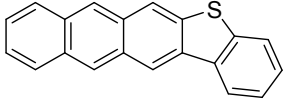
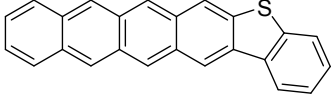
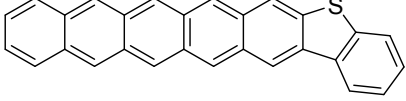
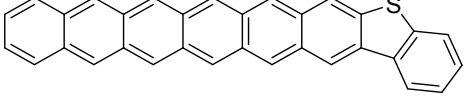
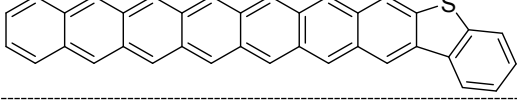
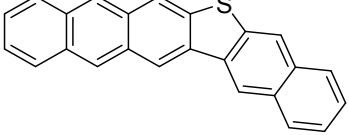
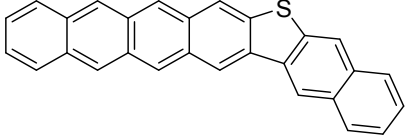
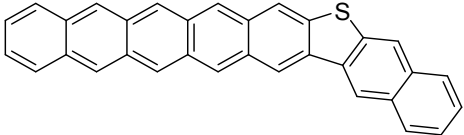
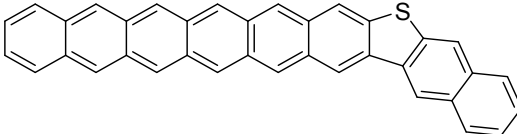
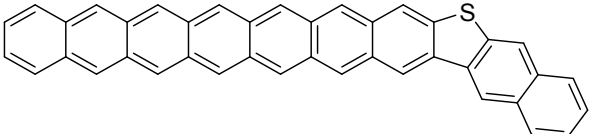
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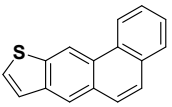
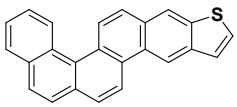
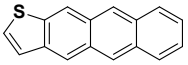
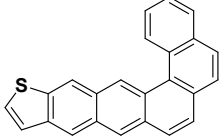
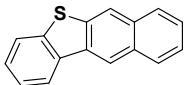
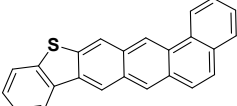
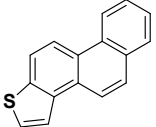
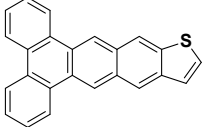
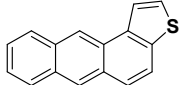
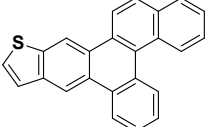
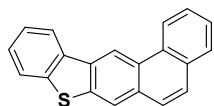
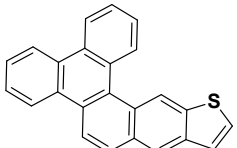
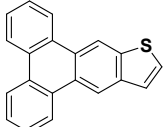
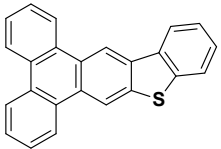
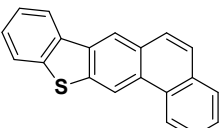
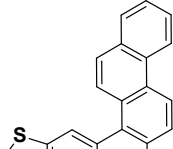
**D26\***2.091

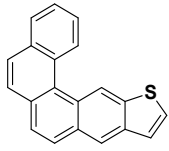
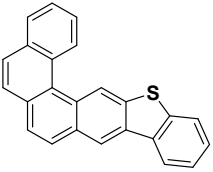
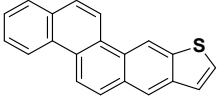
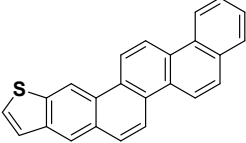
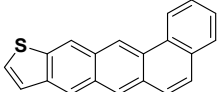
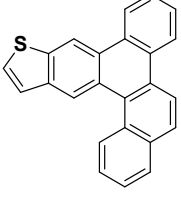
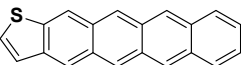
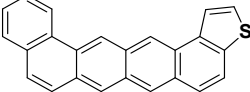
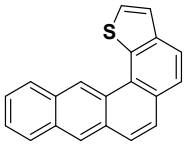
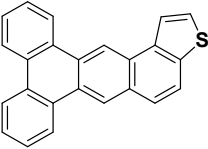
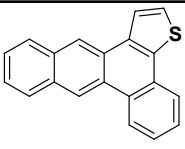
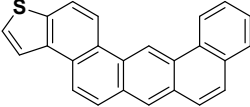
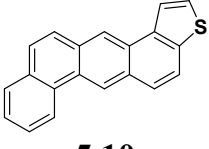
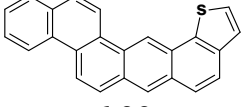
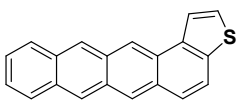
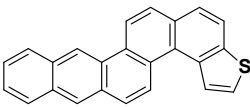
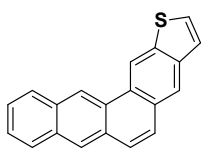
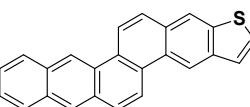
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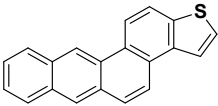
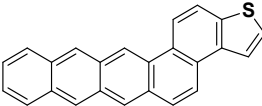
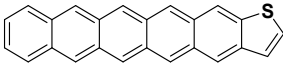
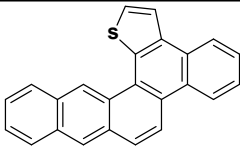
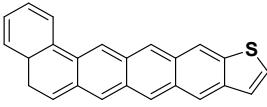
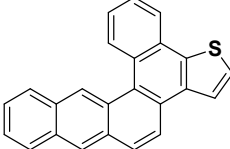
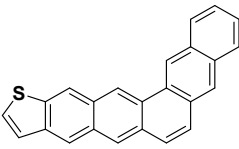
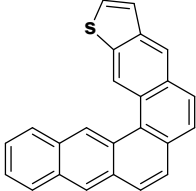
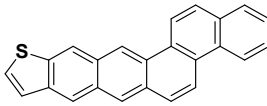
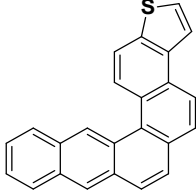
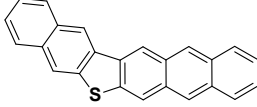
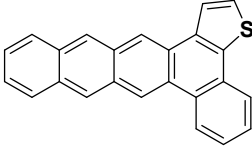
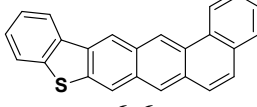
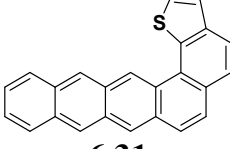
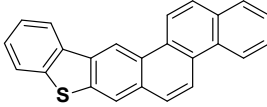
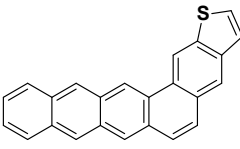


|            |   |       |
|------------|---|-------|
| <b>E1</b>  |    | 3.913 |
| <b>E2</b>  |    | 3.109 |
| <b>E3</b>  |    | 2.488 |
| <b>E4</b>  |    | 2.022 |
| <b>E5</b>  |    | 1.668 |
| <b>E6</b>  |    | 1.393 |
| <b>E7</b>  |    | 3.079 |
| <b>E8</b>  |   | 2.493 |
| <b>E9</b>  |  | 2.034 |
| <b>E10</b> |  | 1.680 |
| <b>E11</b> |  | 1.405 |

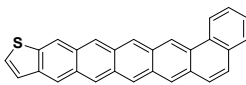
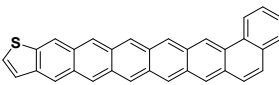
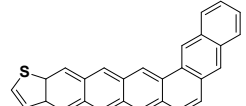
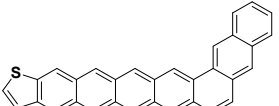
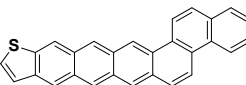
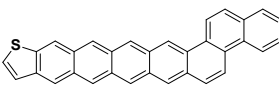
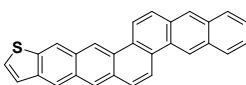
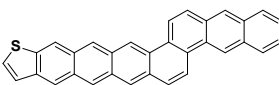
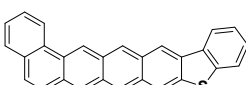
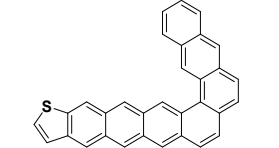
**Table S1a:** Calculated Egap, IP and EA (in eV) properties for 4 to 6 fused-ring-structures of 1T-subclass thienoacene.

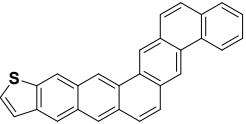
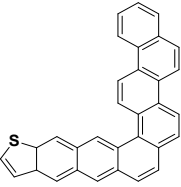
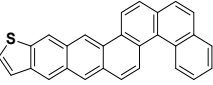
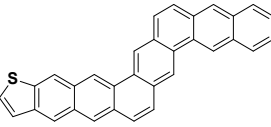
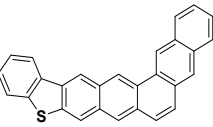
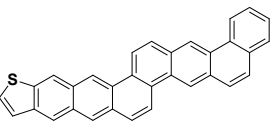
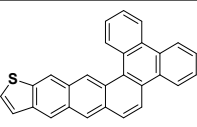
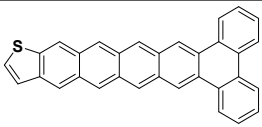
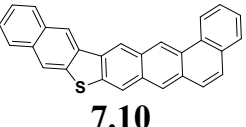
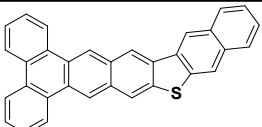
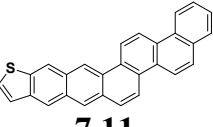
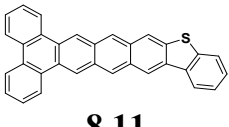
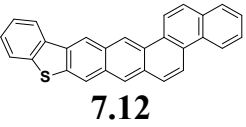
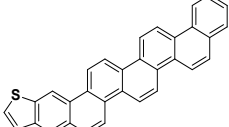
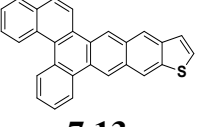
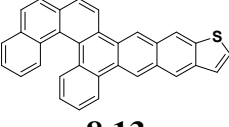
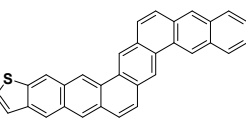
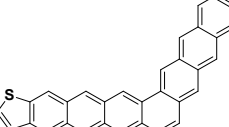
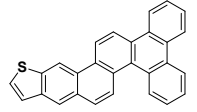
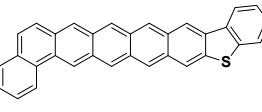
| Structure   | Parameters |       | Structure   | Parameters |       |
|---|------------|-------|---|------------|-------|
| <br><b>4.1</b>   | Egap       | 4.126 | <br><b>6.8</b>    | Egap       | 3.789 |
|   | IP         | 5.713 |   | IP         | 5.563 |
|   | EA         | 1.587 |   | EA         | 1.774 |
|   | DPO        | 1.20  |   | DPO        | 1.45  |
| <br><b>4.2</b>   | Egap       | 3.086 | <br><b>6.9</b>    | Egap       | 3.048 |
|   | IP         | 5.239 |   | IP         | 5.236 |
|   | EA         | 2.152 |   | EA         | 2.187 |
|   | DPO        | 2.35  |   | DPO        | 2.43  |
| <br><b>4.3</b>   | Egap       | 3.913 | <br><b>6.10</b>   | Egap       | 3.276 |
|   | IP         | 5.692 |   | IP         | 5.396 |
|   | EA         | 1.779 |   | EA         | 2.120 |
|   | DPO        | 1.45  |   | DPO        | 2.10  |
| <br><b>4.4</b>   | Egap       | 4.324 | <br><b>6.11</b>   | Egap       | 3.361 |
|   | IP         | 5.846 |   | IP         | 5.405 |
|   | EA         | 1.522 |   | EA         | 2.043 |
|   | DPO        | 0.90  |   | DPO        | 1.85  |
| <br><b>4.5</b> | Egap       | 3.538 | <br><b>6.12</b>  | Egap       | 3.787 |
|   | IP         | 5.500 |   | IP         | 5.593 |
|   | EA         | 1.962 |   | EA         | 1.806 |
|   | DPO        | 1.95  |   | DPO        | 1.28  |
| <br><b>5.1</b> | Egap       | 4.020 | <br><b>6.13</b> | Egap       | 3.620 |
|   | IP         | 5.769 |   | IP         | 5.478 |
|   | EA         | 1.749 |   | EA         | 1.858 |
|   | DPO        | 1.20  |   | DPO        | 1.87  |
| <br><b>5.2</b> | Egap       | 4.217 | <br><b>6.14</b> | Egap       | 4.107 |
|   | IP         | 5.800 |   | IP         | 5.828 |
|   | EA         | 1.584 |   | EA         | 1.721 |
|   | DPO        | 0.95  |   | DPO        | 0.95  |
| <br><b>5.3</b> | Egap       | 4.011 | <br><b>6.15</b> | Egap       | 3.802 |
|   | IP         | 5.727 |   | IP         | 5.582 |
|   | EA         | 1.715 |   | EA         | 1.780 |
|   | DPO        | 1.20  |   | DPO        | 1.45  |
|   | Egap       | 3.716 |   | Egap       | 3.704 |
|   | IP         | 5.545 |   | IP         | 5.604 |
|   | EA         | 1.829 |   | EA         | 1.900 |

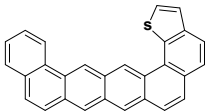
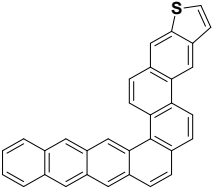
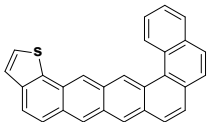
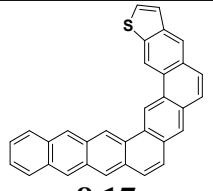
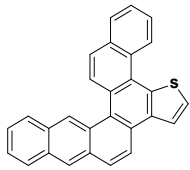
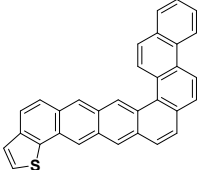
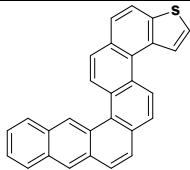
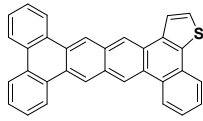
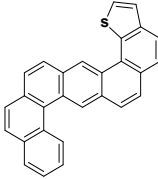
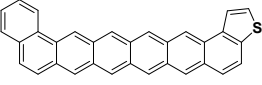
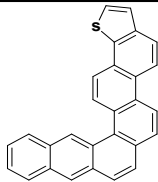
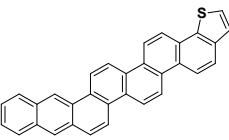
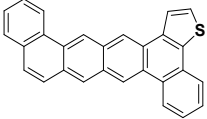
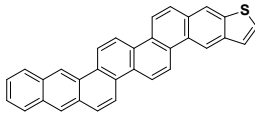
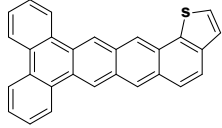
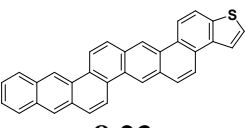
|  |      |       |   |      |       |
|--|------|-------|---|------|-------|
| <br><b>5.4</b>    | DPO  | 1.53  | <br><b>6.16</b>   | DPO  | 1.53  |
| <br><b>5.5</b>    | Egap | 3.805 | <br><b>6.17</b>   | Egap | 3.860 |
|  | IP   | 5.575 |   | IP   | 5.615 |
|  | EA   | 1.770 |   | EA   | 1.755 |
|  | DPO  | 1.53  |   | DPO  | 1.45  |
| <br><b>5.6</b>    | Egap | 3.264 | <br><b>6.18</b>   | Egap | 3.847 |
|  | IP   | 5.335 |   | IP   | 5.593 |
|  | EA   | 2.071 |   | EA   | 1.746 |
|  | DPO  | 2.10  |   | DPO  | 1.28  |
| <br><b>5.7</b>    | Egap | 2.450 | <br><b>6.19</b>   | Egap | 2.959 |
|  | IP   | 4.963 |   | IP   | 5.250 |
|  | EA   | 2.512 |   | EA   | 2.291 |
|  | DPO  | 3.20  |   | DPO  | 2.60  |
| <br><b>5.8</b>  | Egap | 3.551 | <br><b>6.20</b> | Egap | 3.804 |
|  | IP   | 5.540 |   | IP   | 5.667 |
|  | EA   | 1.988 |   | EA   | 1.863 |
|  | DPO  | 1.70  |   | DPO  | 1.45  |
| <br><b>5.9</b>  | Egap | 3.706 | <br><b>6.21</b> | Egap | 3.743 |
|  | IP   | 5.598 |   | IP   | 5.619 |
|  | EA   | 1.892 |   | EA   | 1.876 |
|  | DPO  | 1.70  |   | DPO  | 1.60  |
| <br><b>5.10</b> | Egap | 3.685 | <br><b>6.22</b> | Egap | 3.451 |
|  | IP   | 5.567 |   | IP   | 5.482 |
|  | EA   | 1.882 |   | EA   | 2.031 |
|  | DPO  | 1.70  |   | DPO  | 2.03  |
| <br><b>5.11</b> | Egap | 2.795 | <br><b>6.23</b> | Egap | 3.417 |
|  | IP   | 5.149 |   | IP   | 5.456 |
|  | EA   | 2.354 |   | EA   | 2.039 |
|  | DPO  | 2.85  |   | DPO  | 2.00  |
| <br><b>5.12</b> | Egap | 3.681 | <br><b>6.24</b> | Egap | 3.310 |
|  | IP   | 5.574 |   | IP   | 5.383 |
|  | EA   | 1.893 |   | EA   | 2.073 |
|  | DPO  | 1.66  |   | DPO  | 1.99  |

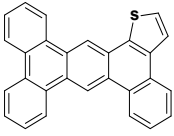
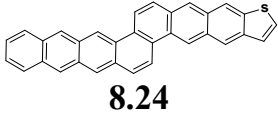
|   |      |       |   |      |       |
|---|------|-------|---|------|-------|
| <b>5.12</b>   |      |       |   |      |       |
| <br><b>5.13</b>  | Egap | 3.585 | <br><b>6.25</b>   | Egap | 2.850 |
|   | IP   | 5.536 |   | IP   | 5.205 |
|   | EA   | 1.951 |   | EA   | 2.355 |
|   | DPO  | 1.85  |   | DPO  | 2.75  |
| <br><b>6.1</b>   | Egap | 1.984 | <br><b>6.26</b>   | Egap | 3.328 |
|   | IP   | 4.757 |   | IP   | 5.434 |
|   | EA   | 2.773 |   | EA   | 2.106 |
|   | DPO  | 4.00  |   | DPO  | 2.03  |
| <br><b>6.2</b>   | Egap | 2.607 | <br><b>6.27</b>   | Egap | 3.367 |
|   | IP   | 5.047 |   | IP   | 5.424 |
|   | EA   | 2.439 |   | EA   | 2.057 |
|   | DPO  | 2.95  |   | DPO  | 2.18  |
| <br><b>6.3</b>   | Egap | 3.337 | <br><b>6.28</b>   | Egap | 3.209 |
|   | IP   | 5.382 |   | IP   | 5.322 |
|   | EA   | 2.045 |   | EA   | 2.113 |
|   | DPO  | 2.02  |   | DPO  | 2.08  |
| <br><b>6.4</b> | Egap | 3.095 | <br><b>6.29</b> | Egap | 3.421 |
|   | IP   | 5.265 |   | IP   | 5.451 |
|   | EA   | 2.170 |   | EA   | 2.029 |
|   | DPO  | 2.43  |   | DPO  | 2.00  |
| <br><b>6.5</b> | Egap | 3.079 | <br><b>6.30</b> | Egap | 2.948 |
|   | IP   | 5.363 |   | IP   | 5.257 |
|   | EA   | 2.284 |   | EA   | 2.308 |
|   | DPO  | 2.35  |   | DPO  | 2.60  |
| <br><b>6.6</b> | Egap | 3.275 | <br><b>6.31</b> | Egap | 2.846 |
|   | IP   | 5.403 |   | IP   | 5.209 |
|   | EA   | 2.127 |   | EA   | 2.363 |
|   | DPO  | 2.10  |   | DPO  | 2.60  |
| <br><b>6.7</b> | Egap | 3.774 | <br><b>6.32</b> | Egap | 2.934 |
|   | IP   | 5.632 |   | IP   | 5.240 |
|   | EA   | 1.857 |   | EA   | 2.306 |
|   | DPO  | 1.53  |   | DPO  | 2.56  |

**Table S1b:** Calculated Egap, IP and EA (in eV) properties for 7 to 8 fused-ring-structures of 1T-subclass thienoacene.

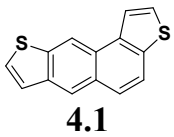
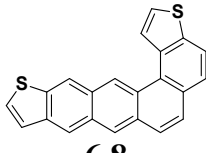
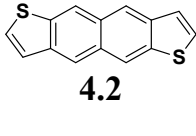
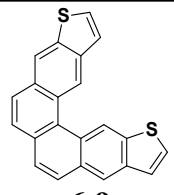
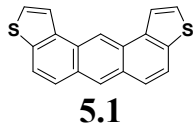
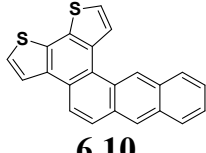
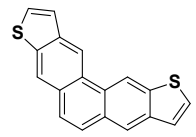
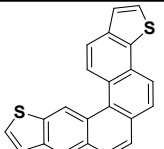
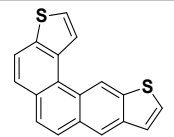
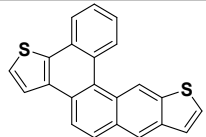
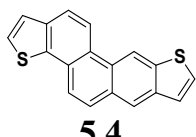
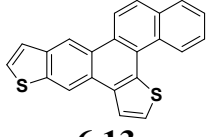
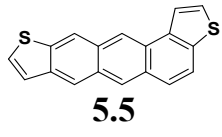
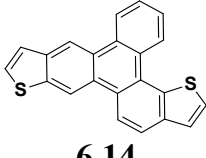
| Structure   | Parameters |       | Structure  | Parameters |       |
|---|------------|-------|--|------------|-------|
|  <p><b>7.1</b></p>  | Egap       | 2.116 |  <p><b>8.1</b></p>  | Egap       | 1.743 |
|   | IP         | 4.828 |  | IP         | 4.660 |
|   | EA         | 2.712 |  | EA         | 2.916 |
|   | DPO        | 3.75  |  | DPO        | 4.50  |
|  <p><b>7.2</b></p> | Egap       | 2.678 |  <p><b>8.2</b></p> | Egap       | 2.173 |
|   | IP         | 5.079 |  | IP         | 4.862 |
|   | EA         | 2.401 |  | EA         | 2.689 |
|   | DPO        | 2.87  |  | DPO        | 3.67  |
|  <p><b>7.3</b></p> | Egap       | 2.502 |  <p><b>8.3</b></p> | Egap       | 2.044 |
|   | IP         | 5.006 |  | IP         | 4.802 |
|   | EA         | 2.504 |  | EA         | 2.758 |
|   | DPO        | 3.28  |  | DPO        | 4.08  |
|  <p><b>7.4</b></p> | Egap       | 2.877 |  <p><b>8.4</b></p> | Egap       | 2.402 |
|   | IP         | 5.170 |  | IP         | 4.967 |
|   | EA         | 2.292 |  | EA         | 2.565 |
|   | DPO        | 2.75  |  | DPO        | 3.60  |
|  <p><b>7.5</b></p> | Egap       | 2.643 |  <p><b>8.5</b></p> | Egap       | 2.355 |
|   | IP         | 5.106 |  | IP         | 4.935 |
|   | EA         | 2.463 |  | EA         | 2.580 |
|   | DPO        | 2.95  |  | DPO        | 3.39  |
|   | Egap       | 3.250 |  | Egap       | 3.058 |
|   | IP         | 5.335 |  | IP         | 5.245 |
|   | EA         | 2.085 |  | EA         | 2.187 |

|  |      |       |   |      |       |
|--|------|-------|---|------|-------|
| <br><b>7.6</b>    | DPO  | 2.13  | <br><b>8.6</b>    | DPO  | 2.46  |
| <br><b>7.7</b>    | Egap | 3.099 | <br><b>8.7</b>    | Egap | 3.096 |
|  | IP   | 5.254 |   | IP   | 5.280 |
|  | EA   | 2.155 |   | EA   | 2.184 |
|  | DPO  | 2.35  |   | DPO  | 2.23  |
| <br><b>7.8</b>    | Egap | 3.348 | <br><b>8.8</b>    | Egap | 2.944 |
|  | IP   | 5.447 |   | IP   | 5.205 |
|  | EA   | 2.100 |   | EA   | 2.261 |
|  | DPO  | 2.02  |   | DPO  | 2.67  |
| <br><b>7.9</b>    | Egap | 2.977 | <br><b>8.9</b>    | Egap | 2.176 |
|  | IP   | 5.182 |   | IP   | 4.857 |
|  | EA   | 2.205 |   | EA   | 2.681 |
|  | DPO  | 2.77  |   | DPO  | 3.50  |
| <br><b>7.10</b>  | Egap | 3.231 | <br><b>8.10</b>  | Egap | 3.314 |
|  | IP   | 5.446 |   | IP   | 5.502 |
|  | EA   | 2.215 |   | EA   | 2.188 |
|  | DPO  | 2.10  |   | DPO  | 1.85  |
| <br><b>7.11</b> | Egap | 3.132 | <br><b>8.11</b> | Egap | 2.722 |
|  | IP   | 5.284 |   | IP   | 5.159 |
|  | EA   | 2.152 |   | EA   | 2.437 |
|  | DPO  | 2.35  |   | DPO  | 2.70  |
| <br><b>7.12</b> | Egap | 3.114 | <br><b>8.12</b> | Egap | 3.762 |
|  | IP   | 5.326 |   | IP   | 5.577 |
|  | EA   | 2.212 |   | EA   | 1.815 |
|  | DPO  | 2.43  |   | DPO  | 1.53  |
| <br><b>7.13</b> | Egap | 3.247 | <br><b>8.13</b> | Egap | 3.231 |
|  | IP   | 5.328 |   | IP   | 5.322 |
|  | EA   | 2.081 |   | EA   | 2.091 |
|  | DPO  | 2.18  |   | DPO  | 2.10  |
| <br><b>7.14</b> | Egap | 3.096 | <br><b>8.14</b> | Egap | 2.699 |
|  | IP   | 5.280 |   | IP   | 5.101 |
|  | EA   | 2.185 |   | EA   | 2.402 |
|  | DPO  | 2.23  |   | DPO  | 2.84  |
| <br><b>7.15</b> | Egap | 3.847 | <br><b>8.15</b> | Egap | 2.155 |
|  | IP   | 5.610 |   | IP   | 4.876 |
|  | EA   | 1.762 |   | EA   | 2.721 |

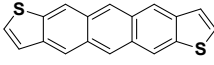
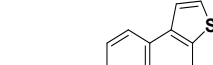
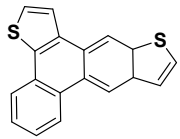
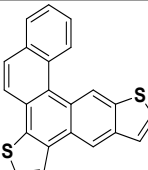
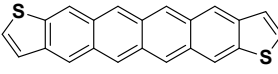
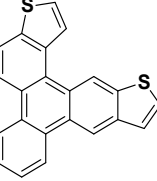
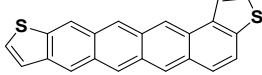
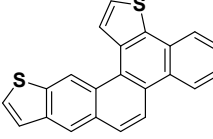
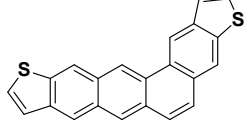
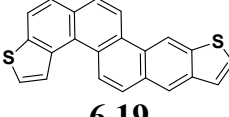
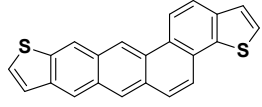
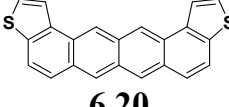
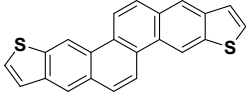
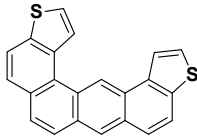
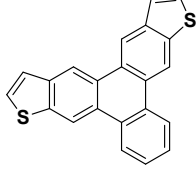
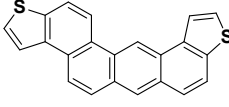
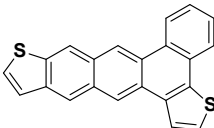
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|--|------|-------|---|------|-------|
| <b>7.15</b>  | DPO  | 1.37  | <b>8.15</b>   | DPO  | 3.75  |
| <br><b>7.16</b>   | Egap | 3.008 | <br><b>8.16</b>   | Egap | 2.807 |
|  | IP   | 5.297 |   | IP   | 5.174 |
|  | EA   | 2.289 |   | EA   | 2.367 |
|  | DPO  | 2.35  |   | DPO  | 2.89  |
| <br><b>7.17</b>   | Egap | 2.772 | <br><b>8.17</b>   | Egap | 2.890 |
|  | IP   | 5.171 |   | IP   | 5.218 |
|  | EA   | 2.399 |   | EA   | 2.328 |
|  | DPO  | 2.93  |   | DPO  | 2.57  |
| <br><b>7.18</b>   | Egap | 3.428 | <br><b>8.18</b>   | Egap | 2.820 |
|  | IP   | 5.468 |   | IP   | 5.196 |
|  | EA   | 2.039 |   | EA   | 2.375 |
|  | DPO  | 2.10  |   | DPO  | 2.85  |
| <br><b>7.19</b>  | Egap | 3.410 | <br><b>8.19</b>  | Egap | 3.204 |
|  | IP   | 5.474 |   | IP   | 5.408 |
|  | EA   | 2.064 |   | EA   | 2.204 |
|  | DPO  | 1.97  |   | DPO  | 2.10  |
| <br><b>7.20</b> | Egap | 3.442 | <br><b>8.20</b> | Egap | 1.954 |
|  | IP   | 5.476 |   | IP   | 4.783 |
|  | EA   | 2.034 |   | EA   | 2.829 |
|  | DPO  | 1.78  |   | DPO  | 4.25  |
| <br><b>7.21</b> | Egap | 3.424 | <br><b>8.21</b> | Egap | 3.447 |
|  | IP   | 5.465 |   | IP   | 5.494 |
|  | EA   | 2.041 |   | EA   | 2.047 |
|  | DPO  | 1.95  |   | DPO  | 2.06  |
| <br><b>7.22</b> | Egap | 3.108 | <br><b>8.22</b> | Egap | 3.385 |
|  | IP   | 5.340 |   | IP   | 5.432 |
|  | EA   | 2.232 |   | EA   | 2.047 |
|  | DPO  | 2.35  |   | DPO  | 1.99  |
| <br><b>7.23</b> | Egap | 3.024 | <br><b>8.23</b> | Egap | 3.171 |
|  | IP   | 5.324 |   | IP   | 5.348 |
|  | EA   | 2.300 |   | EA   | 2.177 |
|  | DPO  | 2.35  |   | DPO  | 2.29  |
|  | Egap | 3.859 |   | Egap | 2.539 |

|   |     |       |  |     |       |
|---|-----|-------|--|-----|-------|
| <br>7.24 | IP  | 5.717 | <br>8.24 | IP  | 5.045 |
|   | EA  | 1.858 |  | EA  | 2.506 |
|   | DPO | 1.20  |  | DPO | 3.03  |

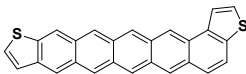
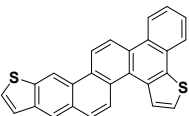
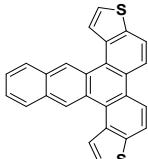
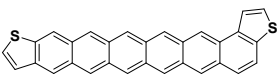
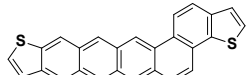
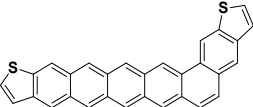
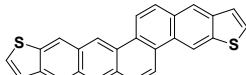
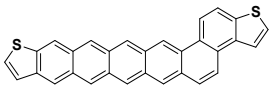
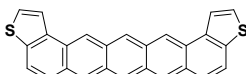
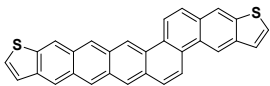
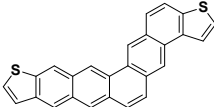
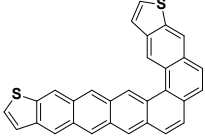
**Table S2a:** Calculated Egap, IP and EA (in eV) properties for 4 to 6 fused-ring-structures of 2T-subclass thienoacene.

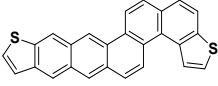
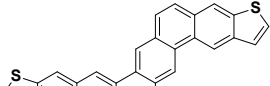
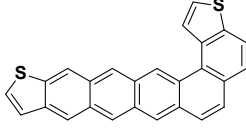
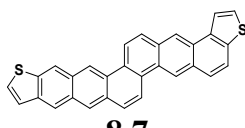
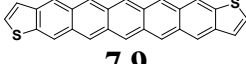
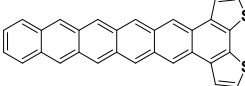
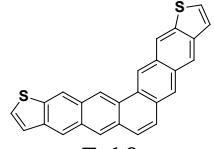
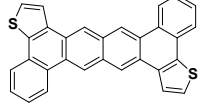
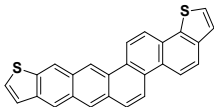
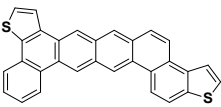
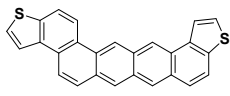
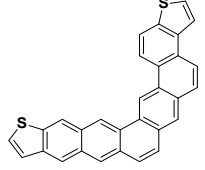
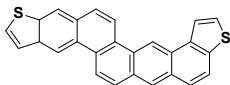
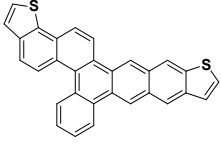
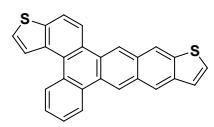
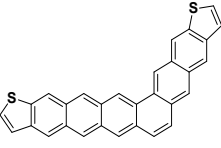
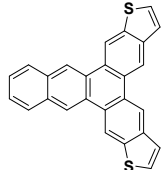
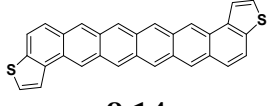
| Structure  | Parameters |       | Structure  | Parameters |       |
|--|------------|-------|--|------------|-------|
| <br>4.1   | Egap       | 3.959 | <br>6.8    | Egap       | 3.161 |
|  | IP         | 5.597 |  | IP         | 5.293 |
|  | EA         | 1.638 |  | EA         | 2.132 |
|  | DPO        | 1.45  |  | DPO        | 2.10  |
| <br>4.2   | Egap       | 3.450 | <br>6.9    | Egap       | 3.466 |
|  | IP         | 5.322 |  | IP         | 5.397 |
|  | EA         | 1.872 |  | EA         | 1.931 |
|  | DPO        | 2.35  |  | DPO        | 1.58  |
| <br>5.1  | Egap       | 3.554 | <br>6.10  | Egap       | 3.504 |
|  | IP         | 5.493 |  | IP         | 5.493 |
|  | EA         | 1.938 |  | EA         | 1.989 |
|  | DPO        | 1.95  |  | DPO        | 1.85  |
| <br>5.2 | Egap       | 4.035 | <br>6.11 | Egap       | 3.678 |
|  | IP         | 5.636 |  | IP         | 5.530 |
|  | EA         | 1.601 |  | EA         | 1.853 |
|  | DPO        | 1.16  |  | DPO        | 1.50  |
| <br>5.3 | Egap       | 3.908 | <br>6.12 | Egap       | 3.677 |
|  | IP         | 5.627 |  | IP         | 5.517 |
|  | EA         | 1.719 |  | EA         | 1.840 |
|  | DPO        | 1.20  |  | DPO        | 1.68  |
| <br>5.4 | Egap       | 3.940 | <br>6.13 | Egap       | 3.663 |
|  | IP         | 5.634 |  | IP         | 5.518 |
|  | EA         | 1.694 |  | EA         | 1.854 |
|  | DPO        | 1.35  |  | DPO        | 1.53  |
| <br>5.5 | Egap       | 3.132 | <br>6.14 | Egap       | 3.961 |
|  | IP         | 5.252 |  | IP         | 5.667 |
|  | EA         | 2.120 |  | EA         | 1.706 |
|  | DPO        | 2.35  |  | DPO        | 1.10  |
|  | Egap       | 2.745 |  | Egap       | 3.813 |

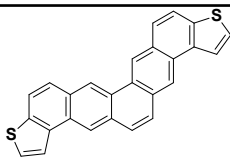
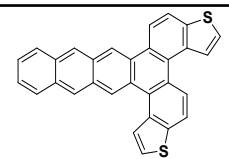
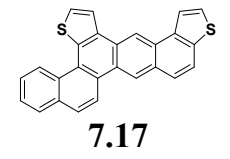
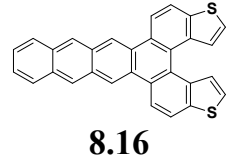


|   |      |       |   |      |       |
|---|------|-------|---|------|-------|
| <br><b>5.6</b>   | IP   | 5.035 | <br><b>6.15</b>   | IP   | 5.577 |
|   | EA   | 2.290 |   | EA   | 1.764 |
|   | DPO  | 3.20  |   | DPO  | 1.50  |
| <br><b>5.7</b>   | Egap | 4.044 | <br><b>6.16</b>   | Egap | 3.643 |
|   | IP   | 5.661 |   | IP   | 5.503 |
|   | EA   | 1.617 |   | EA   | 1.860 |
|   | DPO  | 1.20  |   | DPO  | 1.53  |
| <br><b>6.1</b>   | Egap | 2.216 | <br><b>6.17</b>   | Egap | 3.966 |
|   | IP   | 4.817 |   | IP   | 5.662 |
|   | EA   | 2.601 |   | EA   | 1.696 |
|   | DPO  | 4.00  |   | DPO  | 0.95  |
| <br><b>6.2</b>   | Egap | 2.508 | <br><b>6.18</b>   | Egap | 3.704 |
|   | IP   | 4.987 |   | IP   | 5.526 |
|   | EA   | 2.479 |   | EA   | 1.822 |
|   | DPO  | 3.20  |   | DPO  | 1.53  |
| <br><b>6.3</b>  | Egap | 3.279 | <br><b>6.19</b>  | Egap | 3.719 |
|   | IP   | 5.334 |   | IP   | 5.546 |
|   | EA   | 2.055 |   | EA   | 1.827 |
|   | DPO  | 2.06  |   | DPO  | 1.50  |
| <br><b>6.4</b> | Egap | 3.171 | <br><b>6.20</b> | Egap | 2.844 |
|   | IP   | 5.305 |   | IP   | 5.178 |
|   | EA   | 2.134 |   | EA   | 2.334 |
|   | DPO  | 2.25  |   | DPO  | 2.85  |
| <br><b>6.5</b> | Egap | 3.549 | <br><b>6.21</b> | Egap | 3.563 |
|   | IP   | 5.430 |   | IP   | 5.517 |
|   | EA   | 1.881 |   | EA   | 1.955 |
|   | DPO  | 1.49  |   | DPO  | 1.70  |
| <br><b>6.6</b> | Egap | 4.112 | <br><b>6.22</b> | Egap | 3.596 |
|   | IP   | 5.741 |   | IP   | 5.526 |
|   | EA   | 1.629 |   | EA   | 1.930 |
|   | DPO  | 0.91  |   | DPO  | 1.85  |
| <br><b>6.7</b> | Egap | 3.281 |   | Egap |       |
|   | IP   | 5.350 |   | IP   |       |
|   | EA   | 2.069 |   | EA   |       |
|   | DPO  | 2.10  |   | DPO  |       |

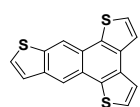
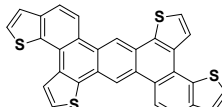
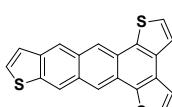
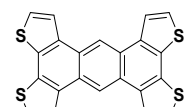
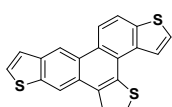
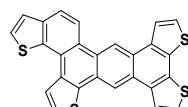
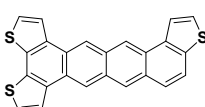
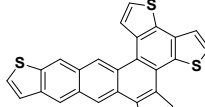
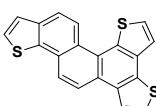
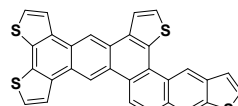
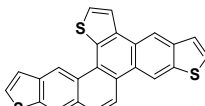
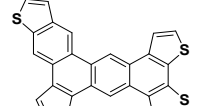
**Table S2b:** Calculated Egap, IP and EA (in eV) properties for 7 to 8 fused-ring-structures of 2T-subclass thienoacene.

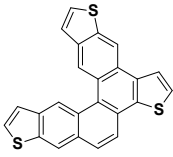
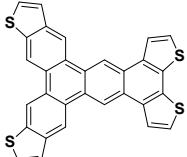
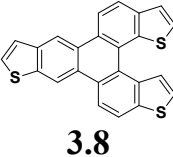
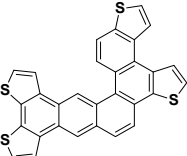
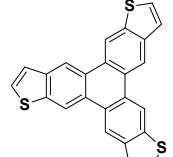
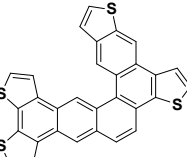
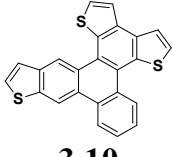
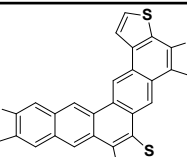
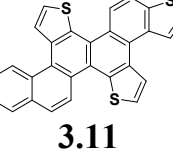
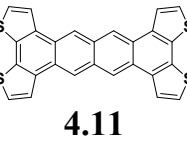
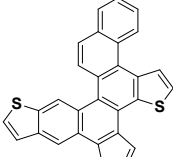
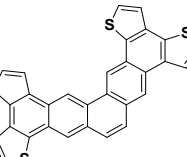
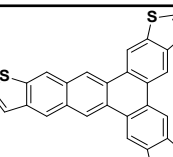
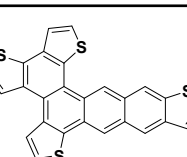
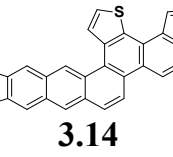
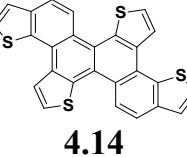
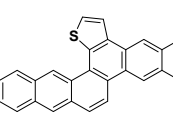
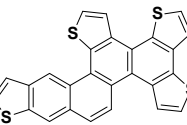
| Structure   | Parameters |       | Structure  | Parameters |       |
|---|------------|-------|--|------------|-------|
|  <p><b>7.1</b></p>   | Egap       | 2.040 |  <p><b>7.18</b></p>  | Egap       | 3.800 |
|   | IP         | 4.773 |  | IP         | 5.584 |
|   | EA         | 2.733 |  | EA         | 1.784 |
|   | DPO        | 4.00  |  | DPO        | 1.41  |
|  <p><b>7.2</b></p>  | Egap       | 3.533 |  <p><b>8.1</b></p>  | Egap       | 1.683 |
|   | IP         | 5.527 |  | IP         | 4.616 |
|   | EA         | 1.994 |  | EA         | 2.933 |
|   | DPO        | 1.45  |  | DPO        | 4.75  |
|  <p><b>7.3</b></p> | Egap       | 2.555 |  <p><b>8.2</b></p> | Egap       | 2.133 |
|   | IP         | 5.026 |  | IP         | 4.820 |
|   | EA         | 2.472 |  | EA         | 2.688 |
|   | DPO        | 3.10  |  | DPO        | 3.71  |
|  <p><b>7.4</b></p> | Egap       | 2.994 |  <p><b>8.3</b></p> | Egap       | 2.082 |
|   | IP         | 5.199 |  | IP         | 4.806 |
|   | EA         | 2.205 |  | EA         | 2.723 |
|   | DPO        | 2.39  |  | DPO        | 3.90  |
|  <p><b>7.5</b></p> | Egap       | 2.300 |  <p><b>8.4</b></p> | Egap       | 2.465 |
|   | IP         | 4.922 |  | IP         | 4.973 |
|   | EA         | 2.622 |  | EA         | 2.508 |
|   | DPO        | 3.70  |  | DPO        | 3.24  |
|  <p><b>7.6</b></p> | Egap       | 3.309 |  <p><b>8.5</b></p> | Egap       | 2.430 |
|   | IP         | 5.354 |  | IP         | 4.954 |
|   | EA         | 2.044 |  | EA         | 2.523 |
|   | DPO        | 2.04  |  | DPO        | 3.33  |
|   | Egap       | 3.066 |  | Egap       | 3.195 |
|   | IP         | 5.248 |  | IP         | 5.302 |

|  |      |       |   |      |       |
|--|------|-------|---|------|-------|
| <br><b>7.7</b>    | EA   | 2.182 | <br><b>8.6</b>    | EA   | 2.108 |
|  | DPO  | 2.40  |   | DPO  | 2.06  |
| <br><b>7.8</b>    | Egap | 2.554 | <br><b>8.7</b>    | Egap | 2.902 |
|  | IP   | 5.018 |   | IP   | 5.180 |
|  | EA   | 2.465 |   | EA   | 2.278 |
|  | DPO  | 2.95  |   | DPO  | 2.71  |
| <br><b>7.9</b>    | Egap | 1.815 | <br><b>8.8</b>    | Egap | 1.868 |
|  | IP   | 4.649 |   | IP   | 4.727 |
|  | EA   | 2.834 |   | EA   | 2.859 |
|  | DPO  | 4.75  |   | DPO  | 4.50  |
| <br><b>7.10</b>   | Egap | 3.269 | <br><b>8.9</b>    | Egap | 3.132 |
|  | IP   | 5.357 |   | IP   | 5.344 |
|  | EA   | 2.088 |   | EA   | 2.212 |
|  | DPO  | 2.06  |   | DPO  | 2.35  |
| <br><b>7.11</b>   | Egap | 3.089 | <br><b>8.10</b>   | Egap | 3.042 |
|  | IP   | 5.269 |   | IP   | 5.300 |
|  | EA   | 2.180 |   | EA   | 2.258 |
|  | DPO  | 2.40  |   | DPO  | 2.50  |
| <br><b>7.12</b> | Egap | 2.898 | <br><b>8.11</b> | Egap | 3.256 |
|  | IP   | 5.210 |   | IP   | 5.352 |
|  | EA   | 2.311 |   | EA   | 2.095 |
|  | DPO  | 2.75  |   | DPO  | 2.12  |
| <br><b>7.13</b> | Egap | 3.331 | <br><b>8.12</b> | Egap | 3.213 |
|  | IP   | 5.378 |   | IP   | 5.327 |
|  | EA   | 2.048 |   | EA   | 2.114 |
|  | DPO  | 1.99  |   | DPO  | 2.15  |
| <br><b>7.14</b> | Egap | 3.325 | <br><b>8.13</b> | Egap | 2.681 |
|  | IP   | 5.359 |   | IP   | 5.078 |
|  | EA   | 2.034 |   | EA   | 2.397 |
|  | DPO  | 2.00  |   | DPO  | 2.91  |
| <br><b>7.15</b> | Egap | 3.780 | <br><b>8.14</b> | Egap | 1.883 |
|  | IP   | 5.681 |   | IP   | 4.732 |
|  | EA   | 1.901 |   | EA   | 2.849 |
|  | DPO  | 1.38  |   | DPO  | 4.50  |
|  | Egap | 3.575 |   | Egap | 2.947 |
|  | IP   | 5.522 |   | IP   | 5.250 |

|  |      |       |   |      |       |
|--|------|-------|---|------|-------|
| <br><b>7.16</b> | EA   | 1.947 | <br><b>8.15</b> | EA   | 2.303 |
|  | DPO  | 1.64  |   | DPO  | 2.50  |
| <br><b>7.17</b> | Egap | 3.408 | <br><b>8.16</b> | Egap | 2.968 |
|  | IP   | 5.447 |   | IP   | 5.255 |
|  | EA   | 2.039 |   | EA   | 2.286 |
|  | DPO  | 2.03  |   | DPO  | 2.65  |

**Table S3:** Calculated Egap, IP and EA (in eV) properties for 3 to 4-thiophene-ring thienoacenes.

| Structure   | Parameters |       | Structure  | Parameters |       |
|---|------------|-------|--|------------|-------|
| <br><b>3.1</b>   | Egap       | 3.856 | <br><b>4.1</b>   | Egap       | 3.478 |
|   | IP         | 5.625 |  | IP         | 5.532 |
|   | EA         | 1.769 |  | EA         | 2.055 |
|   | DPO        | 1.45  |  | DPO        | 1.75  |
| <br><b>3.2</b>  | Egap       | 3.089 | <br><b>4.2</b>  | Egap       | 3.489 |
|   | IP         | 5.280 |  | IP         | 5.454 |
|   | EA         | 2.191 |  | EA         | 1.965 |
|   | DPO        | 2.35  |  | DPO        | 1.95  |
| <br><b>3.3</b> | Egap       | 3.089 | <br><b>4.3</b> | Egap       | 3.496 |
|   | IP         | 5.280 |  | IP         | 5.503 |
|   | EA         | 2.191 |  | EA         | 2.008 |
|   | DPO        | 1.35  |  | DPO        | 1.85  |
| <br><b>3.4</b> | Egap       | 2.866 | <br><b>4.4</b> | Egap       | 3.065 |
|   | IP         | 5.19  |  | IP         | 5.267 |
|   | EA         | 2.325 |  | EA         | 2.202 |
|   | DPO        | 2.85  |  | DPO        | 2.25  |
| <br><b>3.5</b> | Egap       | 4.033 | <br><b>4.5</b> | Egap       | 3.233 |
|   | IP         | 5.755 |  | IP         | 5.354 |
|   | EA         | 1.722 |  | EA         | 2.121 |
|   | DPO        | 0.90  |  | DPO        | 1.99  |
| <br><b>3.6</b> | Egap       | 3.401 | <br><b>4.6</b> | Egap       | 3.571 |
|   | IP         | 5.389 |  | IP         | 5.522 |
|   | EA         | 1.988 |  | EA         | 1.951 |
|   | DPO        | 1.49  |  | DPO        | 1.66  |
|   | Egap       | 3.468 |  | Egap       | 3.749 |
|   | IP         | 5.391 |  | IP         | 5.607 |

|  |      |       |   |      |       |
|--|------|-------|---|------|-------|
| <br><b>3.7</b>    | EA   | 1.922 | <br><b>4.7</b>    | EA   | 1.857 |
|  | DPO  | 1.58  |   | DPO  | 1.38  |
| <br><b>3.8</b>    | Egap | 3.961 | <br><b>4.8</b>    | Egap | 3.347 |
|  | IP   | 5.625 |   | IP   | 5.402 |
|  | EA   | 1.664 |   | EA   | 2.055 |
|  | DPO  | 1.25  |   | DPO  | 2.15  |
| <br><b>3.9</b>    | Egap | 4.157 | <br><b>4.9</b>    | Egap | 3.213 |
|  | IP   | 5.758 |   | IP   | 5.333 |
|  | EA   | 1.601 |   | EA   | 2.120 |
|  | DPO  | 0.88  |   | DPO  | 2.23  |
| <br><b>3.10</b>   | Egap | 3.752 | <br><b>4.10</b>   | Egap | 3.289 |
|  | IP   | 5.548 |   | IP   | 5.368 |
|  | EA   | 1.796 |   | EA   | 2.079 |
|  | DPO  | 1.10  |   | DPO  | 2.04  |
| <br><b>3.11</b> | Egap | 3.677 | <br><b>4.11</b> | Egap | 2.891 |
|  | IP   | 5.543 |   | IP   | 5.203 |
|  | EA   | 1.866 |   | EA   | 2.312 |
|  | DPO  | 0.98  |   | DPO  | 2.85  |
| <br><b>3.12</b> | Egap | 3.576 | <br><b>4.12</b> | Egap | 3.573 |
|  | IP   | 5.493 |   | IP   | 5.532 |
|  | EA   | 1.917 |   | EA   | 1.958 |
|  | DPO  | 1.60  |   | DPO  | 1.64  |
| <br><b>3.13</b> | Egap | 3.326 | <br><b>4.13</b> | Egap | 3.076 |
|  | IP   | 5.393 |   | IP   | 5.265 |
|  | EA   | 2.067 |   | EA   | 2.189 |
|  | DPO  | 1.78  |   | DPO  | 2.25  |
| <br><b>3.14</b> | Egap | 3.058 | <br><b>4.14</b> | Egap | 3.648 |
|  | IP   | 5.236 |   | IP   | 5.576 |
|  | EA   | 2.178 |   | EA   | 1.927 |
|  | DPO  | 2.40  |   | DPO  | 0.80  |
| <br>            | Egap | 2.825 | <br>            | Egap | 3.461 |
|  | IP   | 5.160 |   | IP   | 5.462 |
|  | EA   | 2.335 |   | EA   | 2.001 |

|             |     |      |             |     |      |
|-------------|-----|------|-------------|-----|------|
| <b>3.15</b> | DPO | 2.71 | <b>4.15</b> | DPO | 1.46 |
|-------------|-----|------|-------------|-----|------|