

## Supporting Information

### Reactivity of Phenoxathiin-Based Thiacalixarenes Towards C-Nucleophiles

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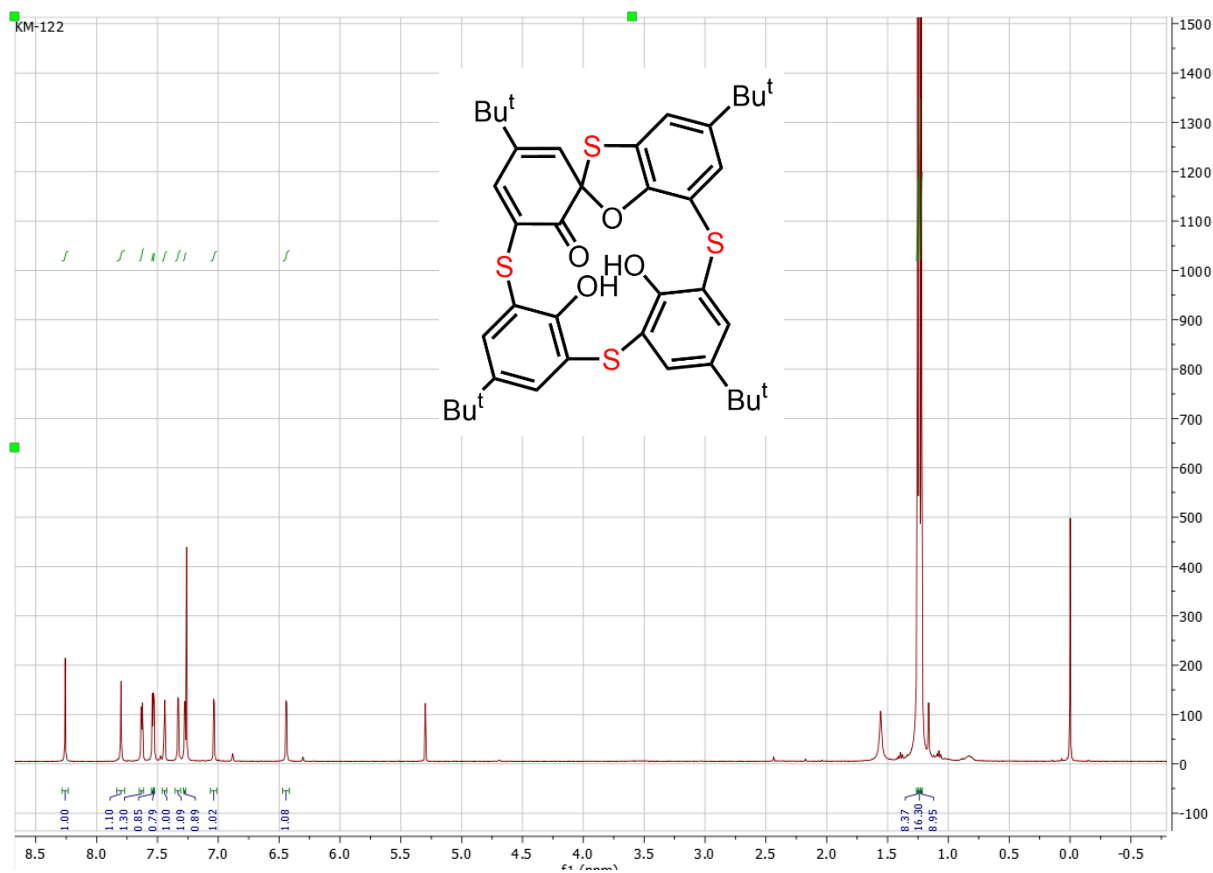
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<sup>c)</sup> Laboratory of NMR Spectroscopy, UCTP, 166 28 Prague 6, Czech Republic.

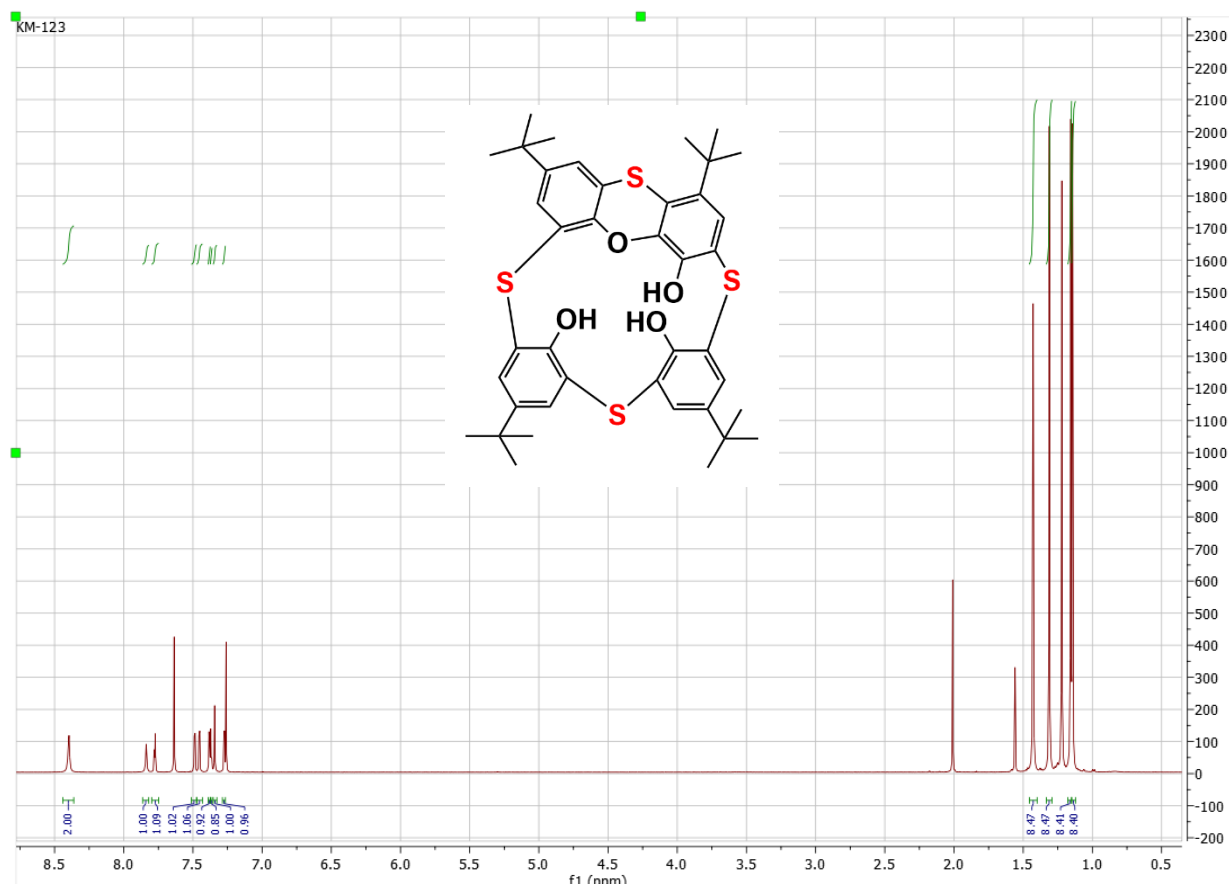
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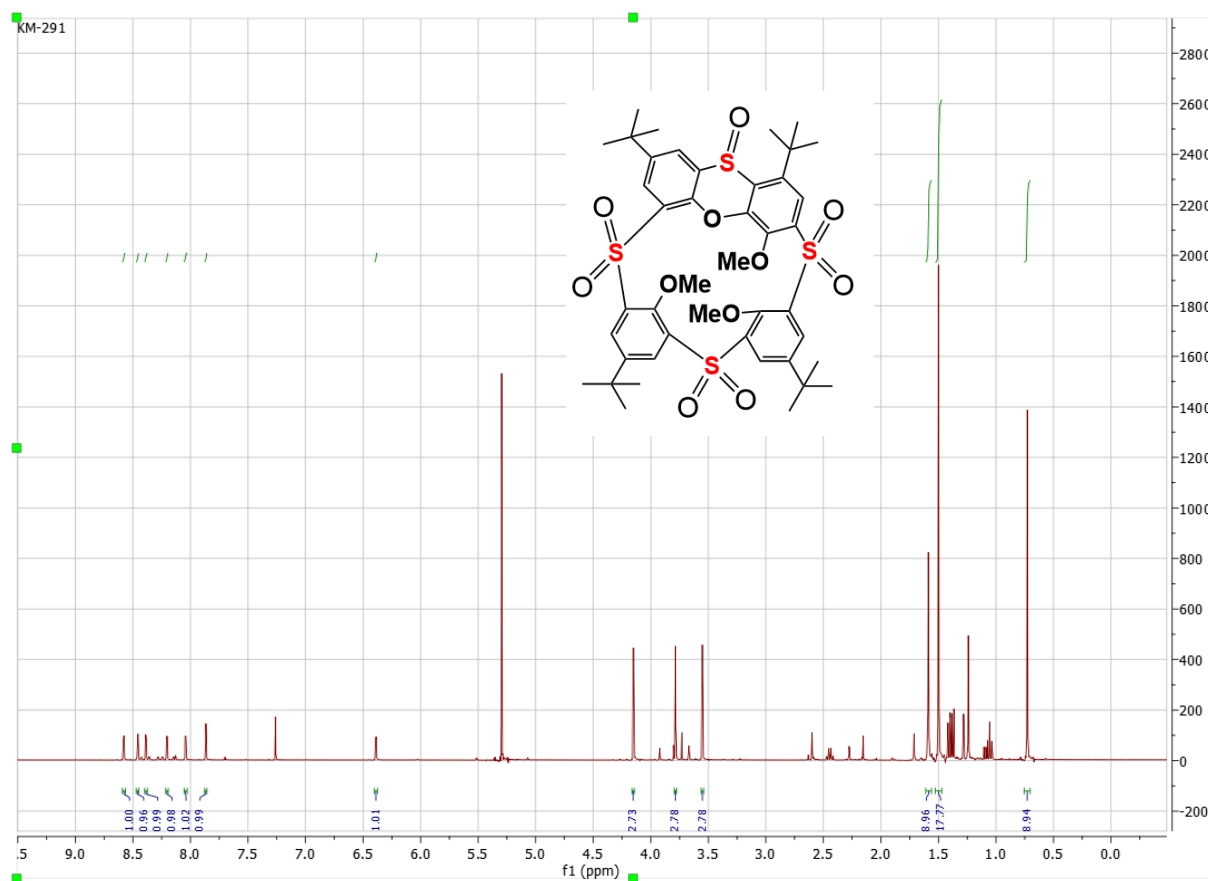
# 1. Spectral characterization of compounds



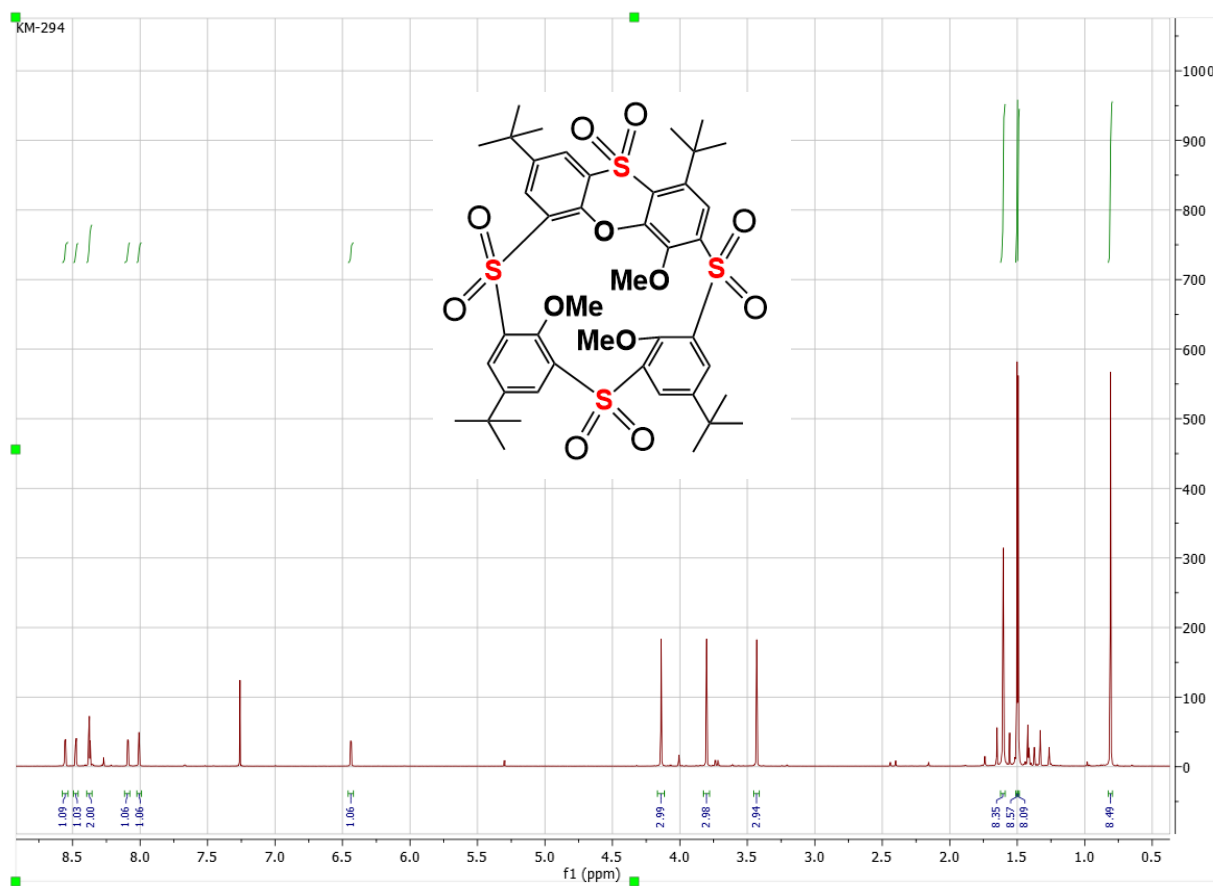
**Figure S1:**  $^1\text{H}$  NMR of compound **2** ( $\text{CDCl}_3$ , 400 MHz).



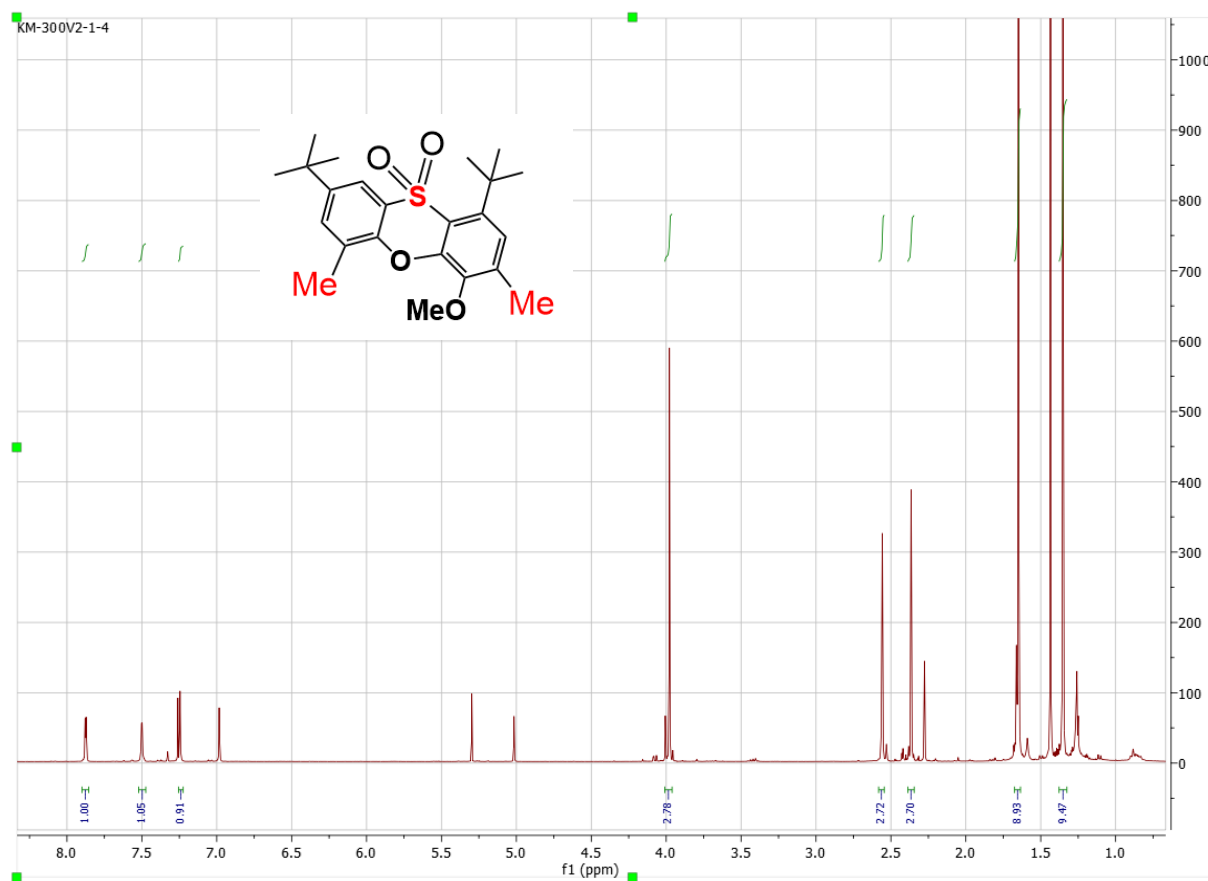
**Figure S2:**  $^1\text{H}$  NMR of compound **4** (CDCl<sub>3</sub>, 400 MHz).



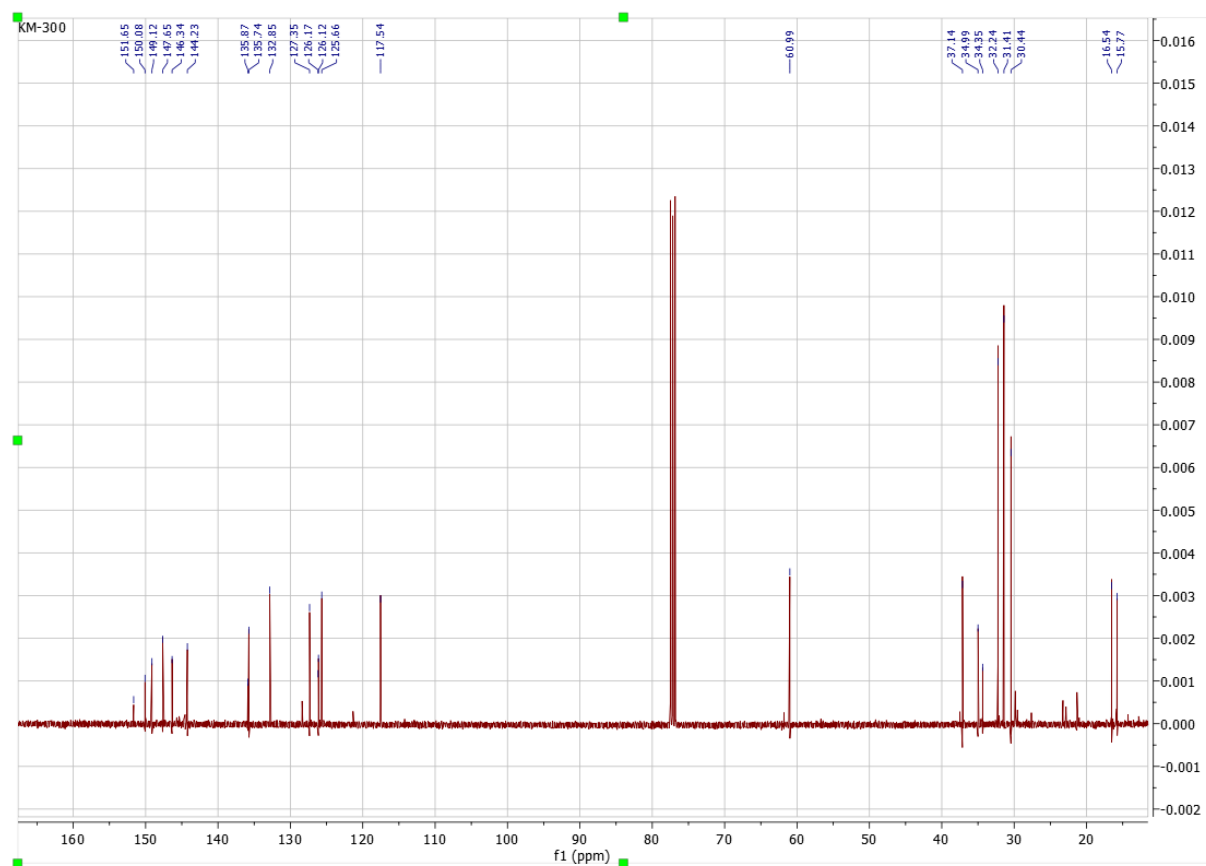
**Figure S3:**  $^1\text{H}$  NMR of compound 9' (CDCl<sub>3</sub>, 400 MHz).



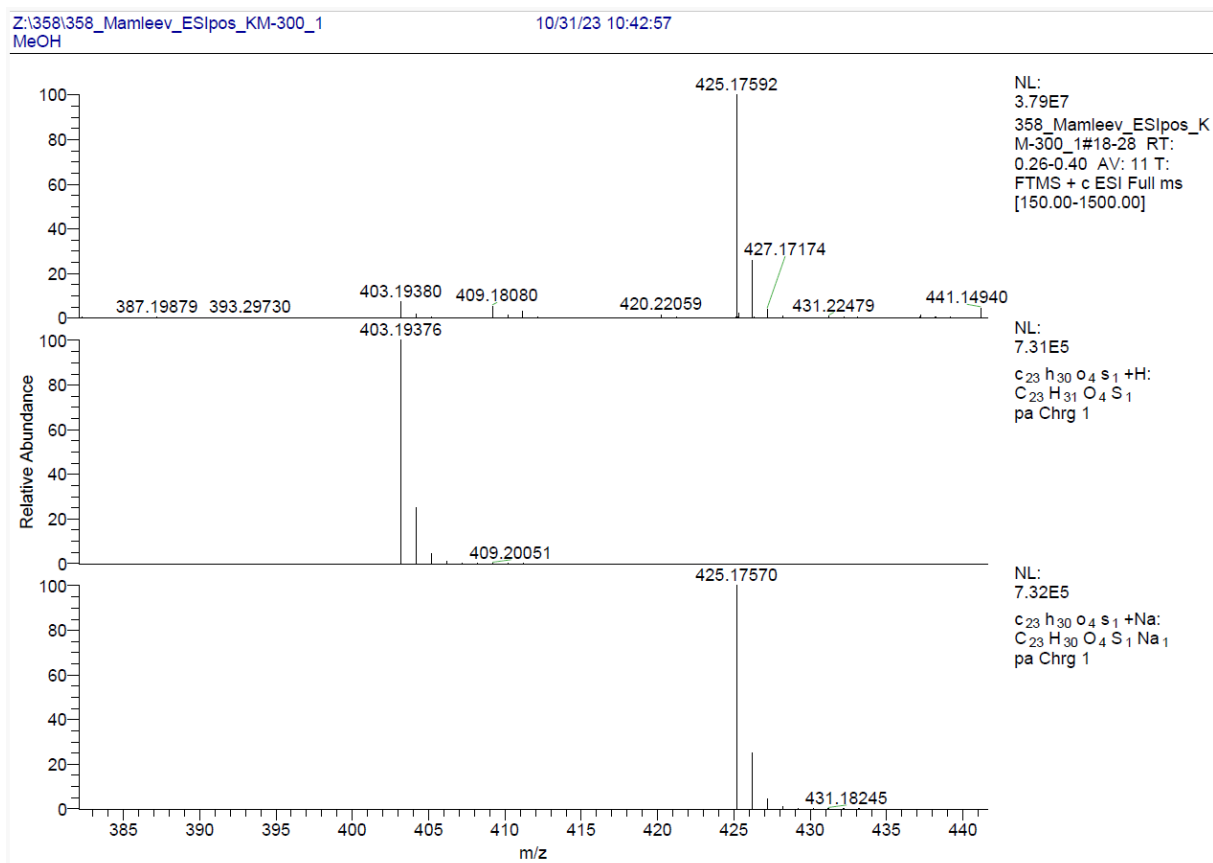
**Figure S4:** <sup>1</sup>H NMR of compound **9** (CDCl<sub>3</sub>, 400 MHz).



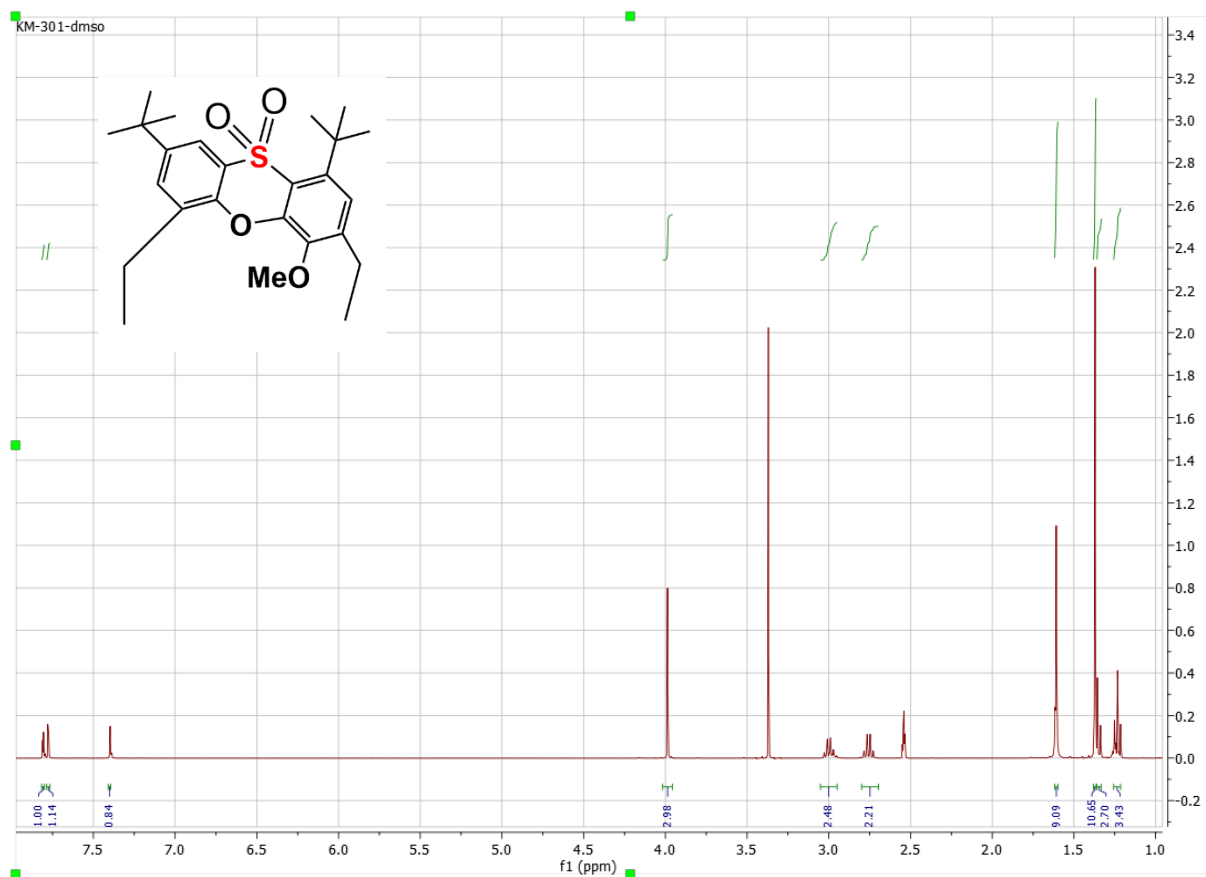
**Figure S5:** <sup>1</sup>H NMR of compound **10a** (CDCl<sub>3</sub>, 400 MHz).



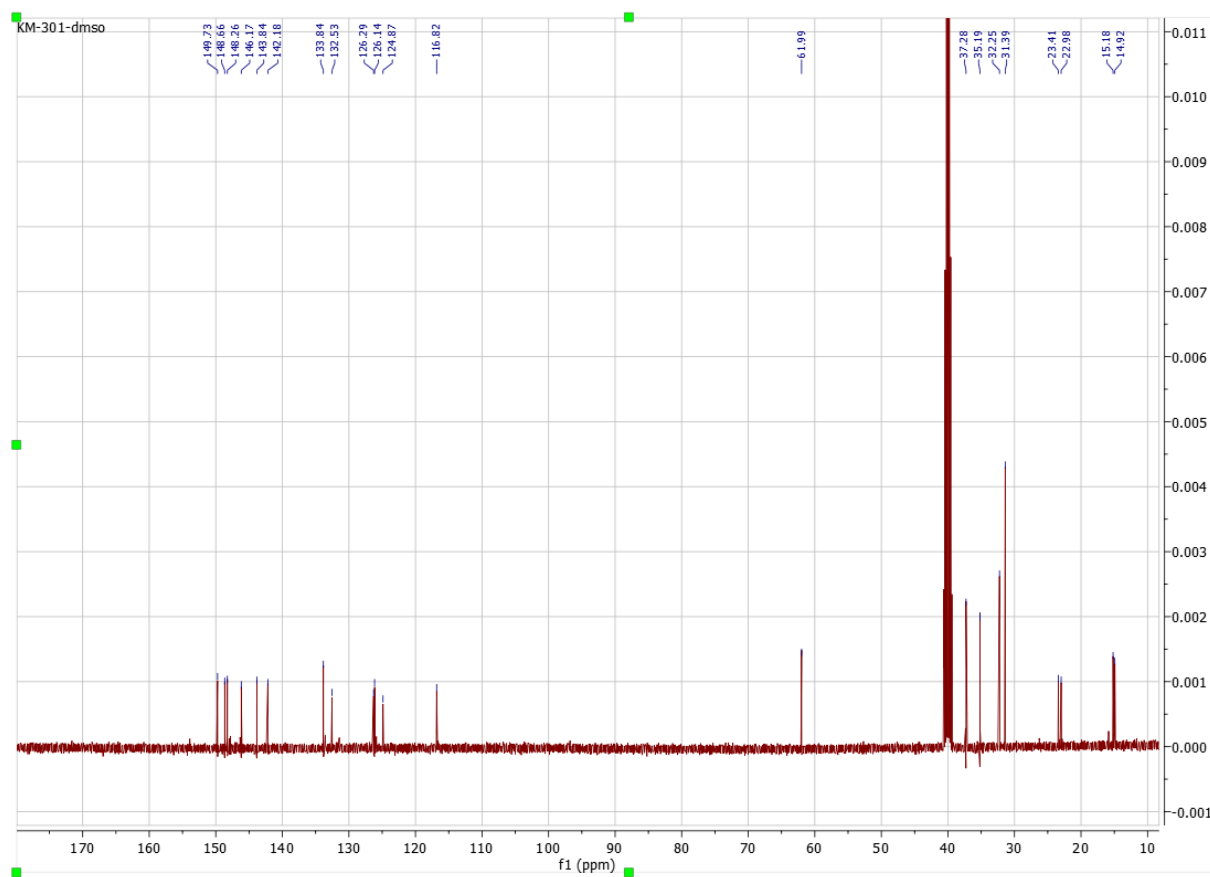
**Figure S6:**  $^{13}\text{C}$  NMR of compound **10a** ( $\text{CDCl}_3$ , 100 MHz)



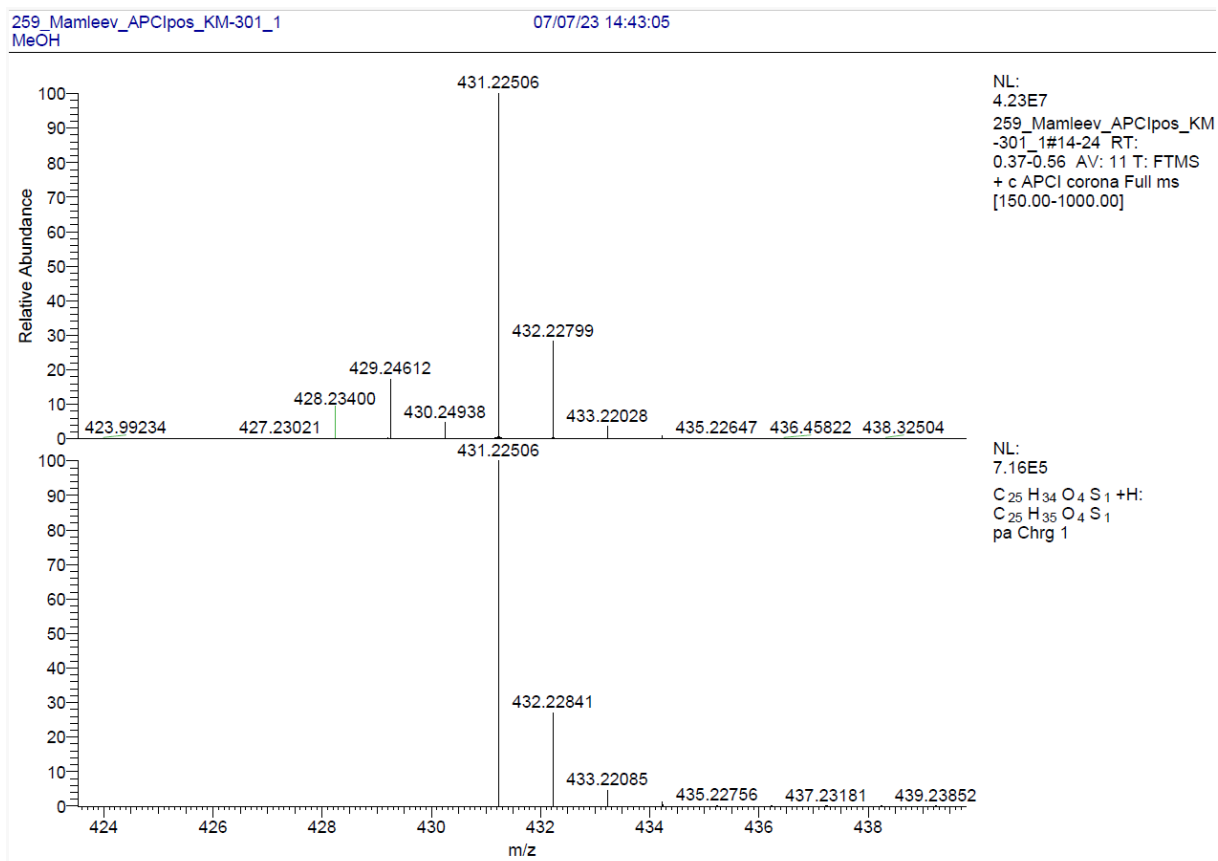
**Figure S7:** HRMS of compound **10a** (ESI<sup>+</sup>).



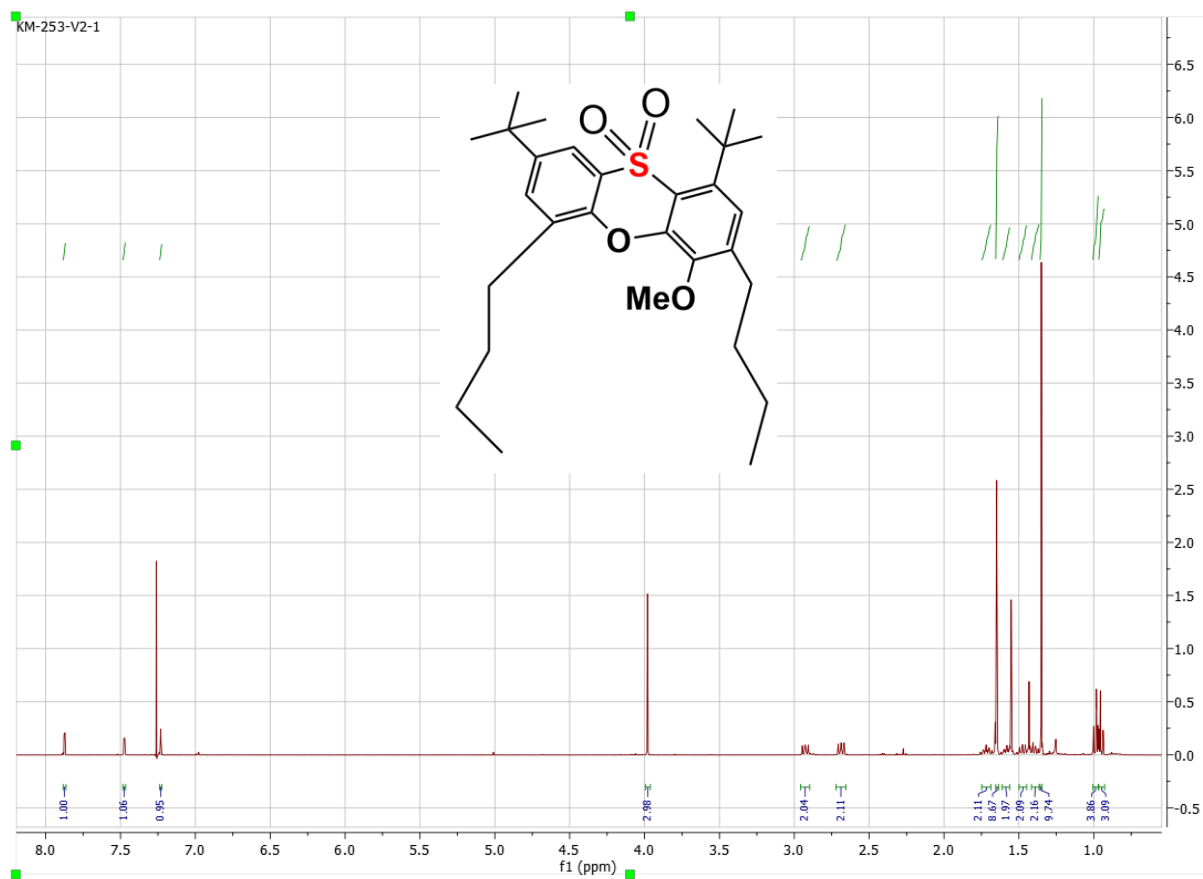
**Figure S8:** <sup>1</sup>H NMR of compound **10b** (DMSO-d<sub>6</sub>, 400 MHz).



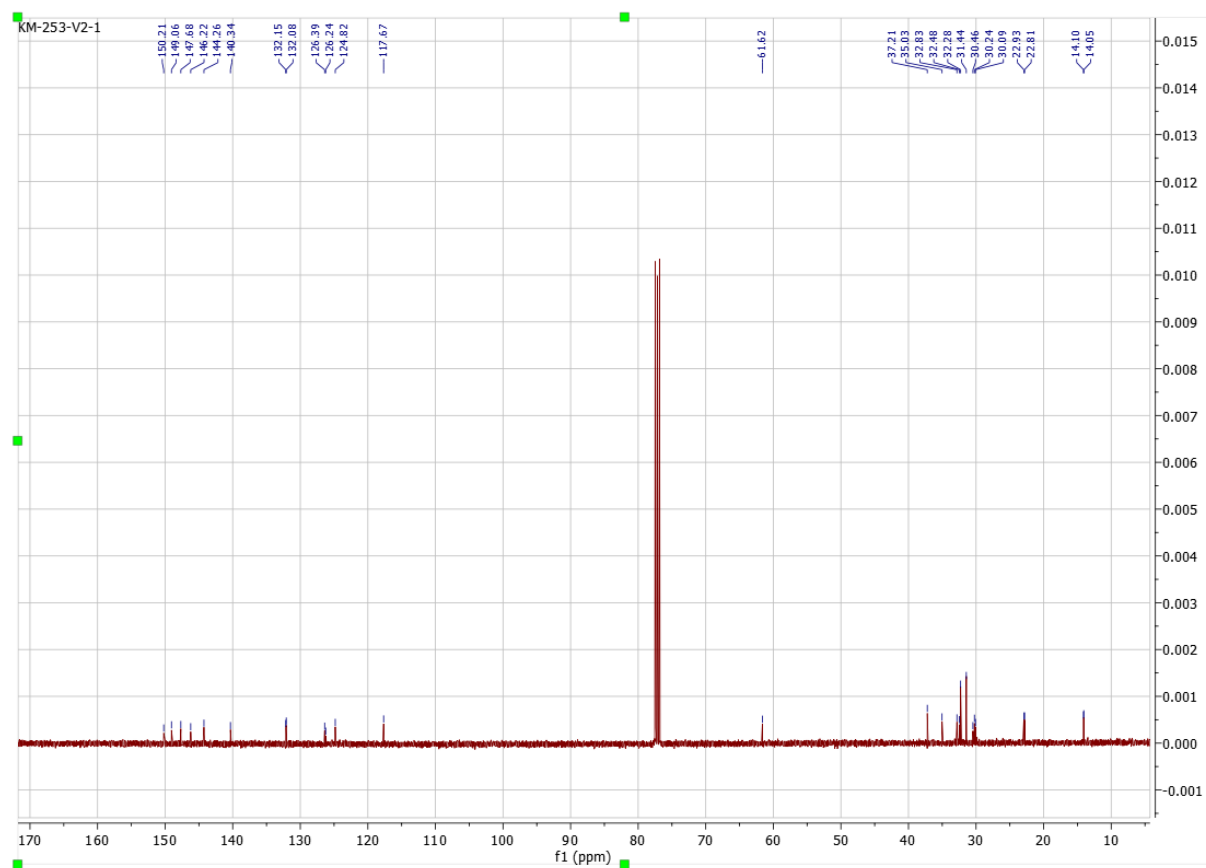
**Figure S9:**  $^{13}\text{C}$  NMR of compound **10b** (DMSO- $\text{d}_6$ , 100 MHz)



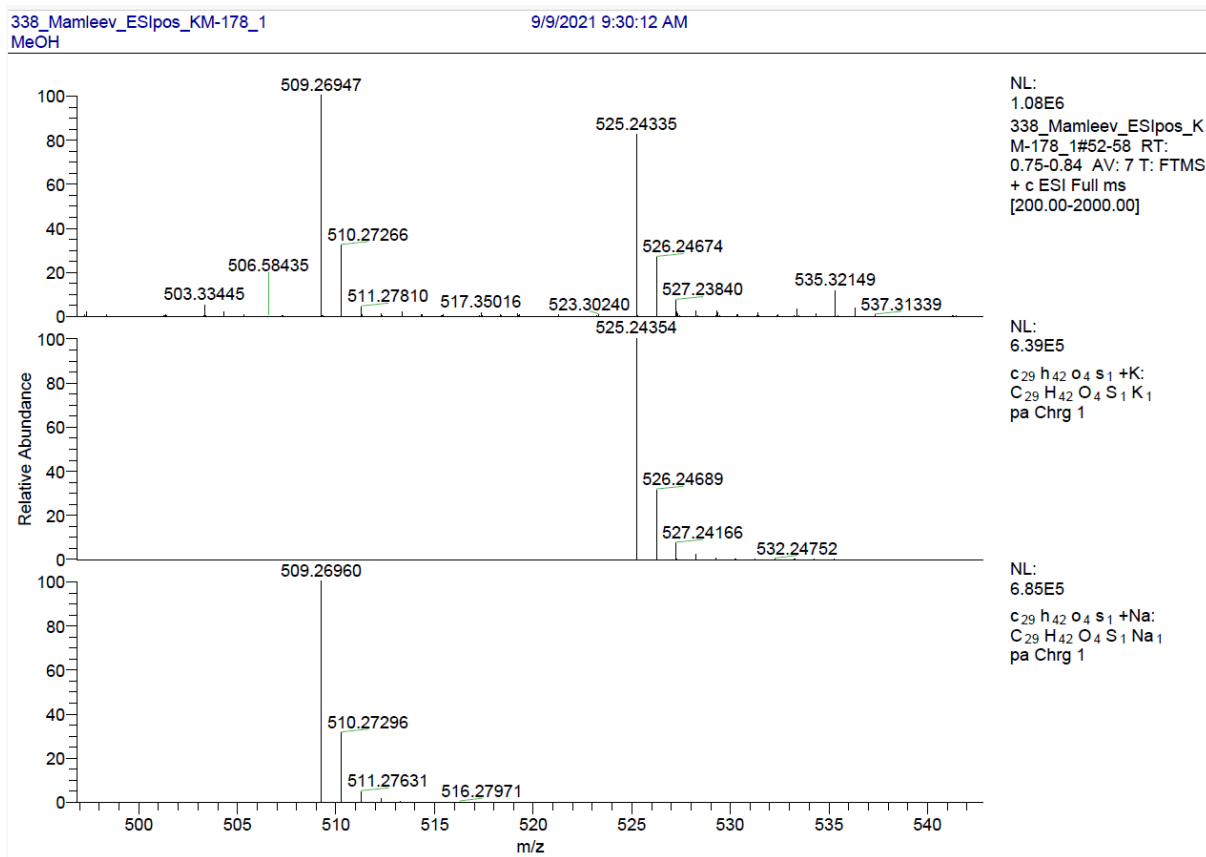
**Figure S10:** HRMS of compound **10b** (ESI<sup>+</sup>).



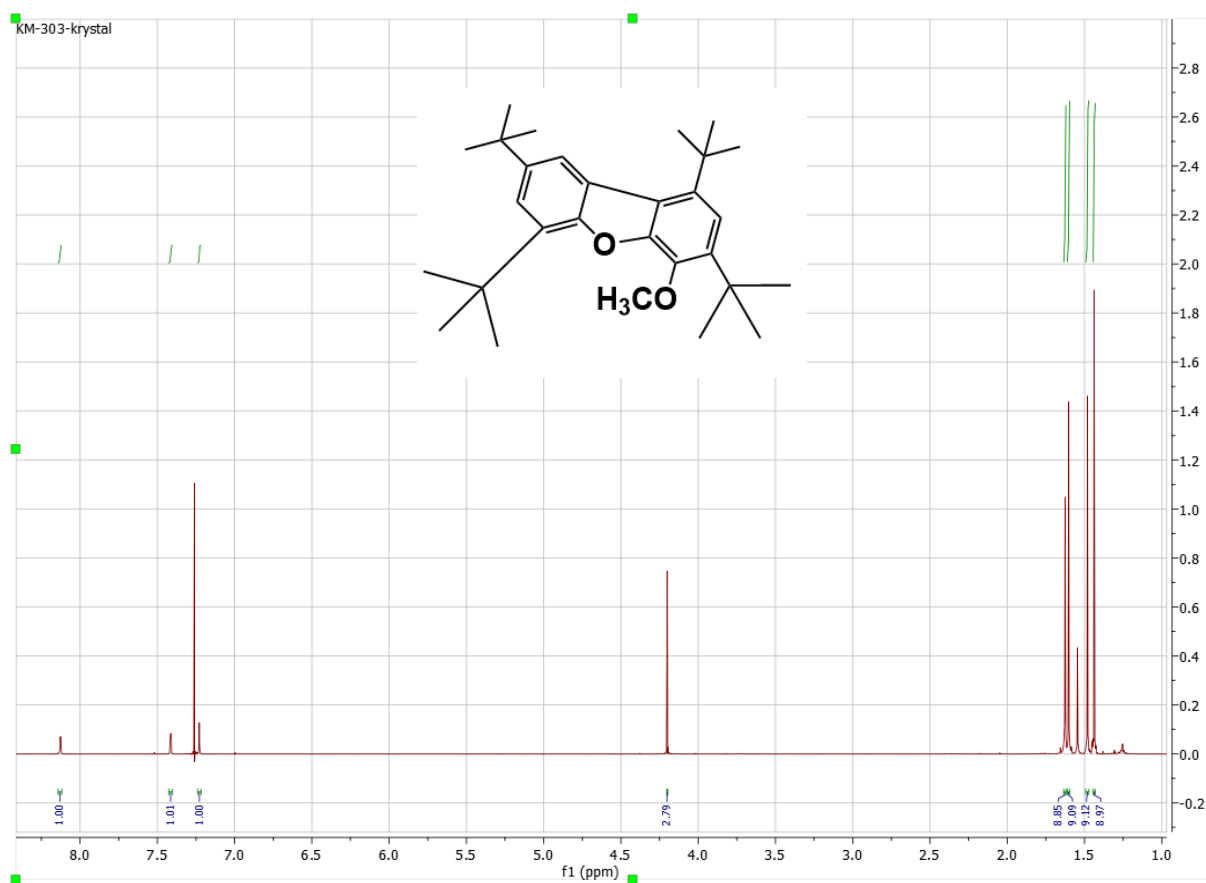
**Figure S11:** <sup>1</sup>H NMR of compound **10c** (CDCl<sub>3</sub>, 400 MHz).



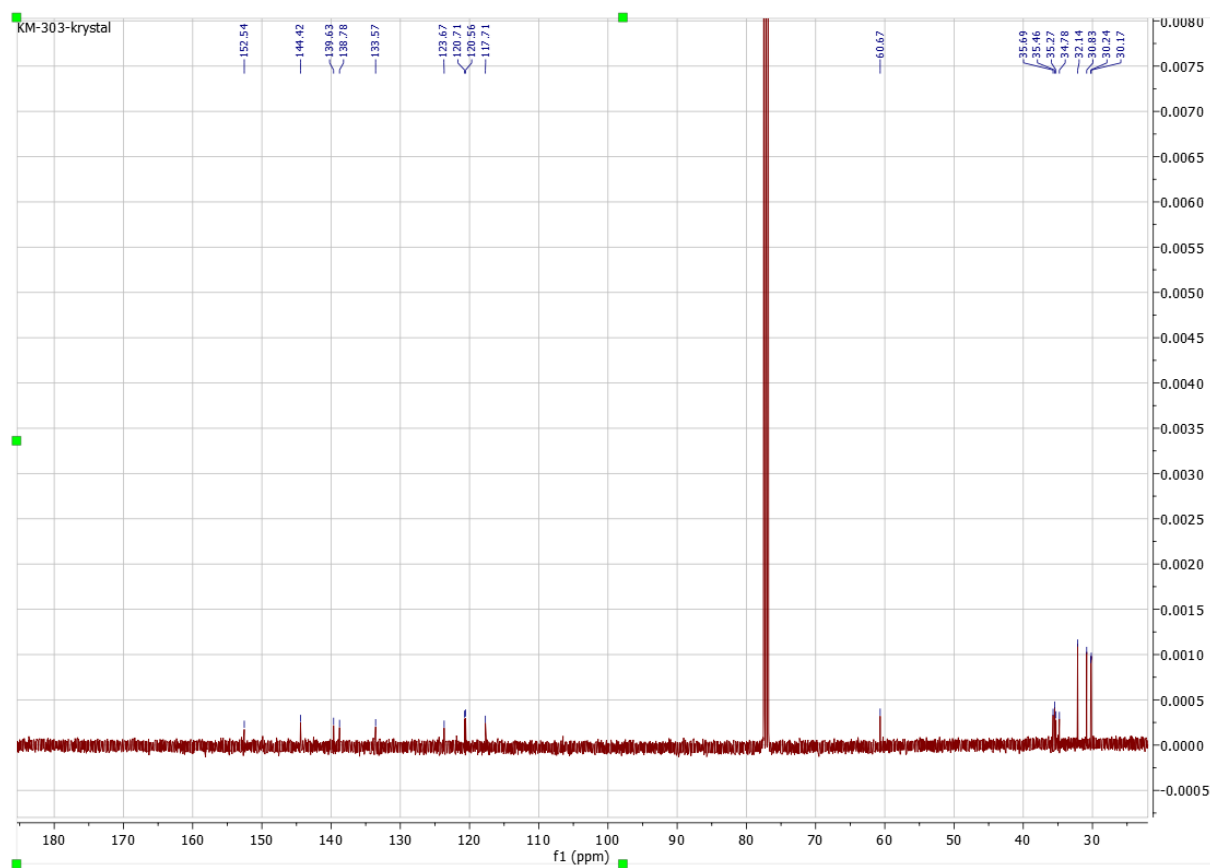
**Figure S12:**  $^{13}\text{C}$  NMR of compound **10c** ( $\text{CDCl}_3$ , 100 MHz)



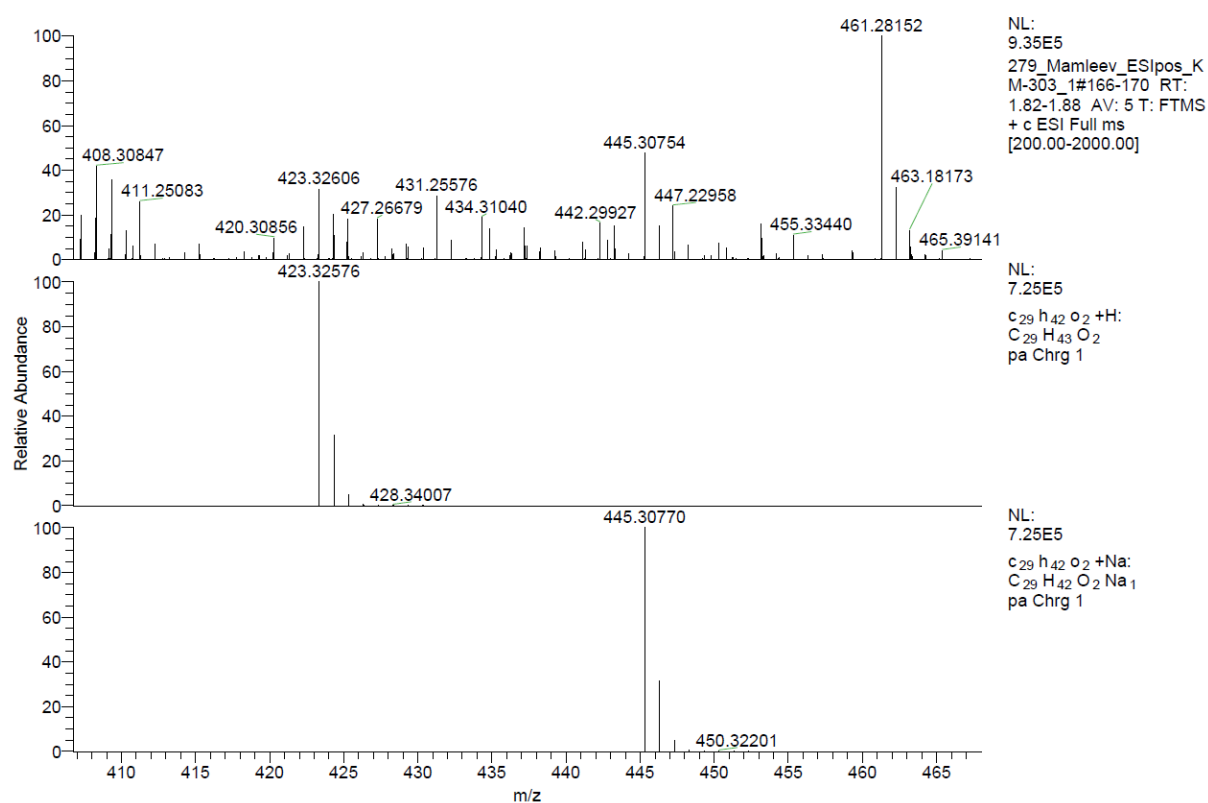
**Figure S13:** HRMS of compound **10c** (ESI<sup>+</sup>).



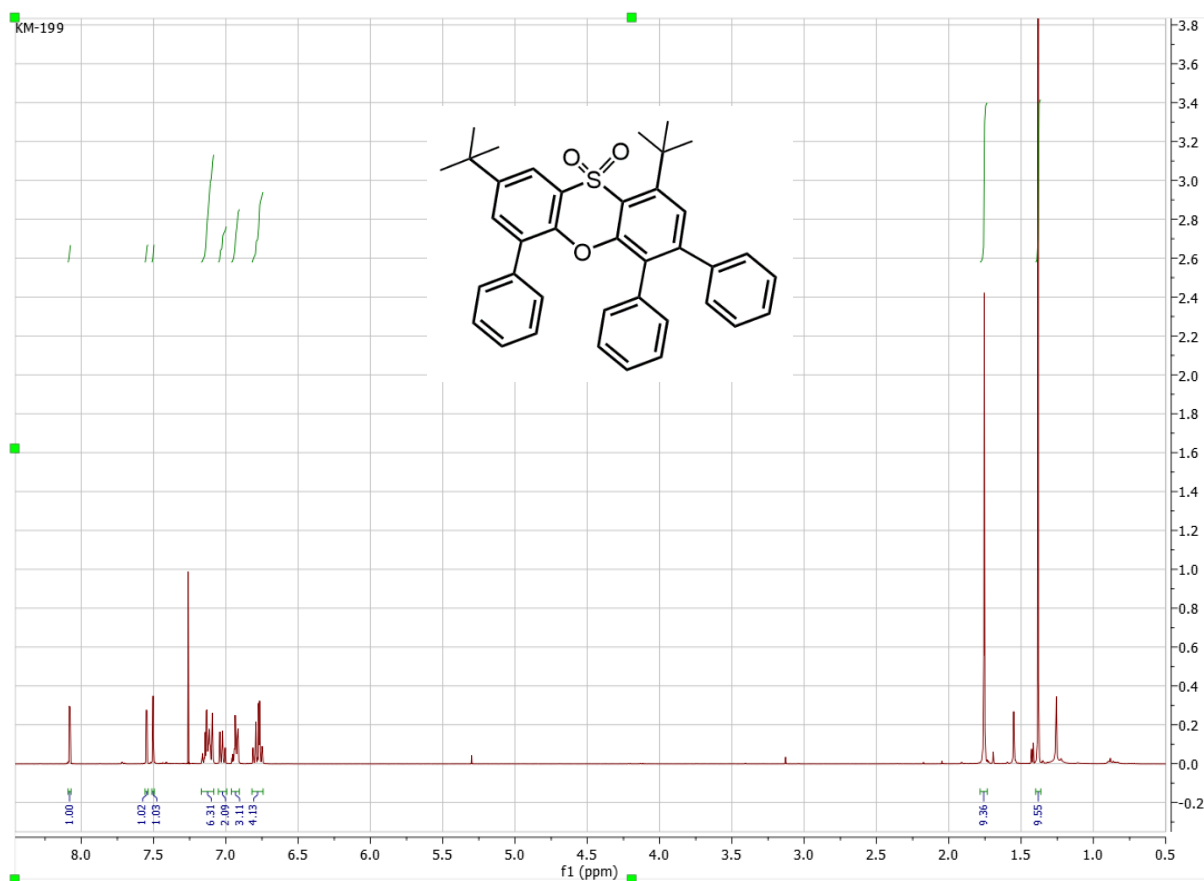
**Figure S14:**  $^1\text{H}$  NMR of compound **11** ( $\text{CDCl}_3$ , 400 MHz).



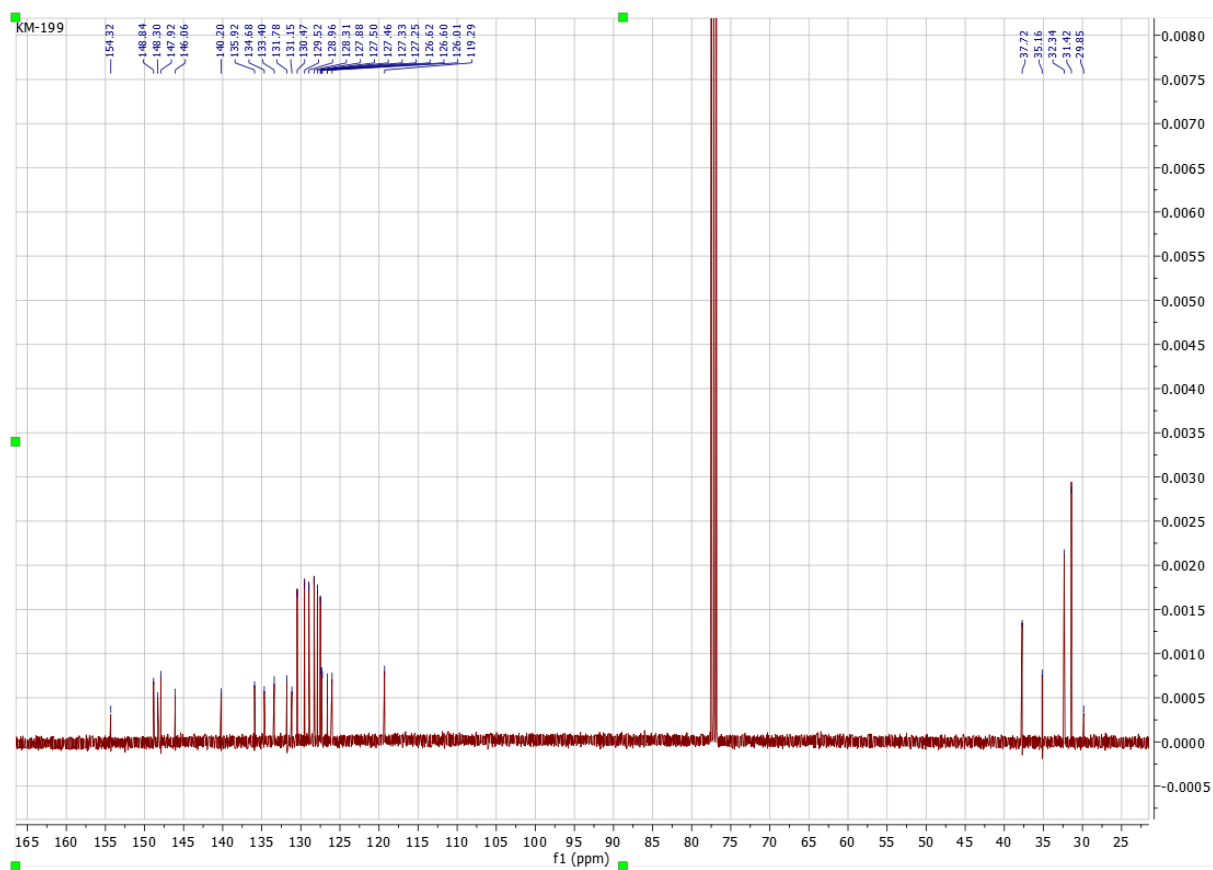
**Figure S15:** <sup>13</sup>C NMR of compound **11** (CDCl<sub>3</sub>, 100 MHz)



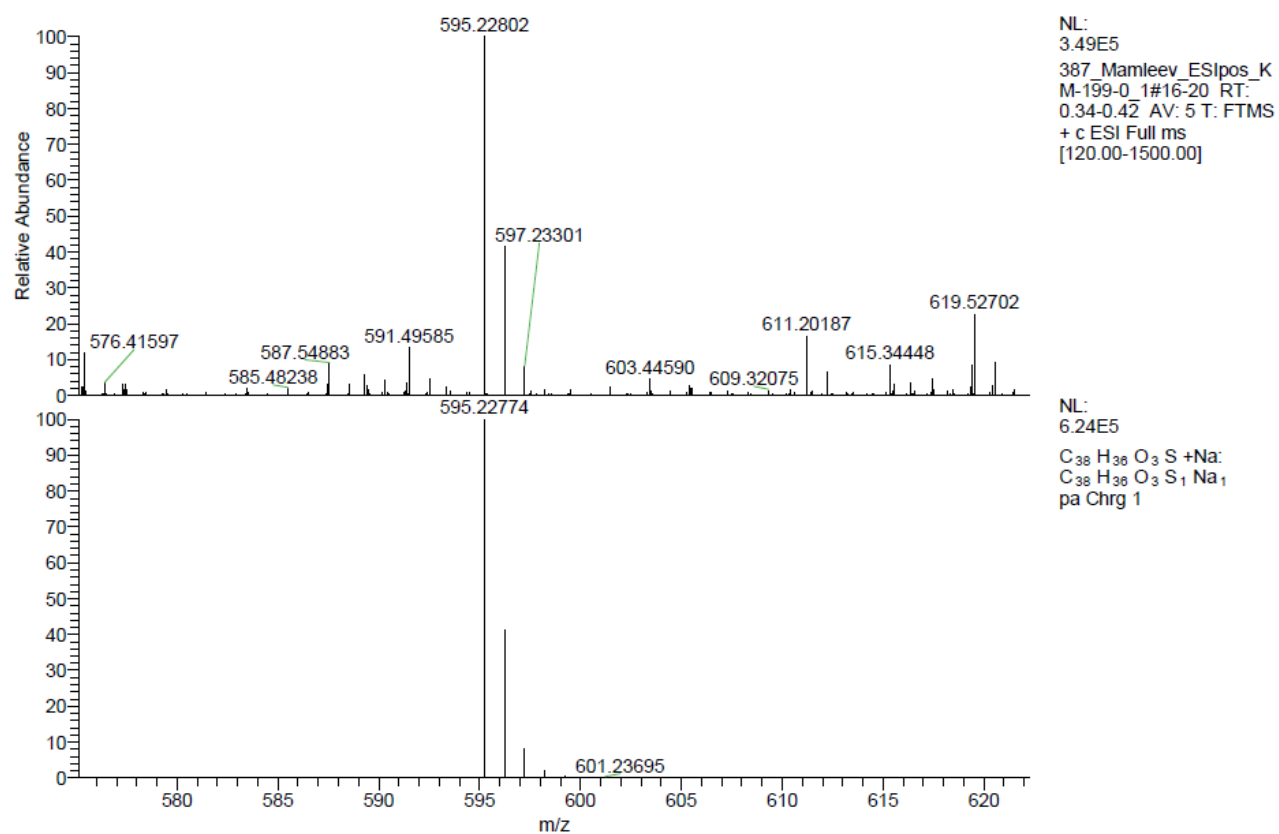
**Figure S16:** HRMS of compound **11** (ESI<sup>+</sup>).



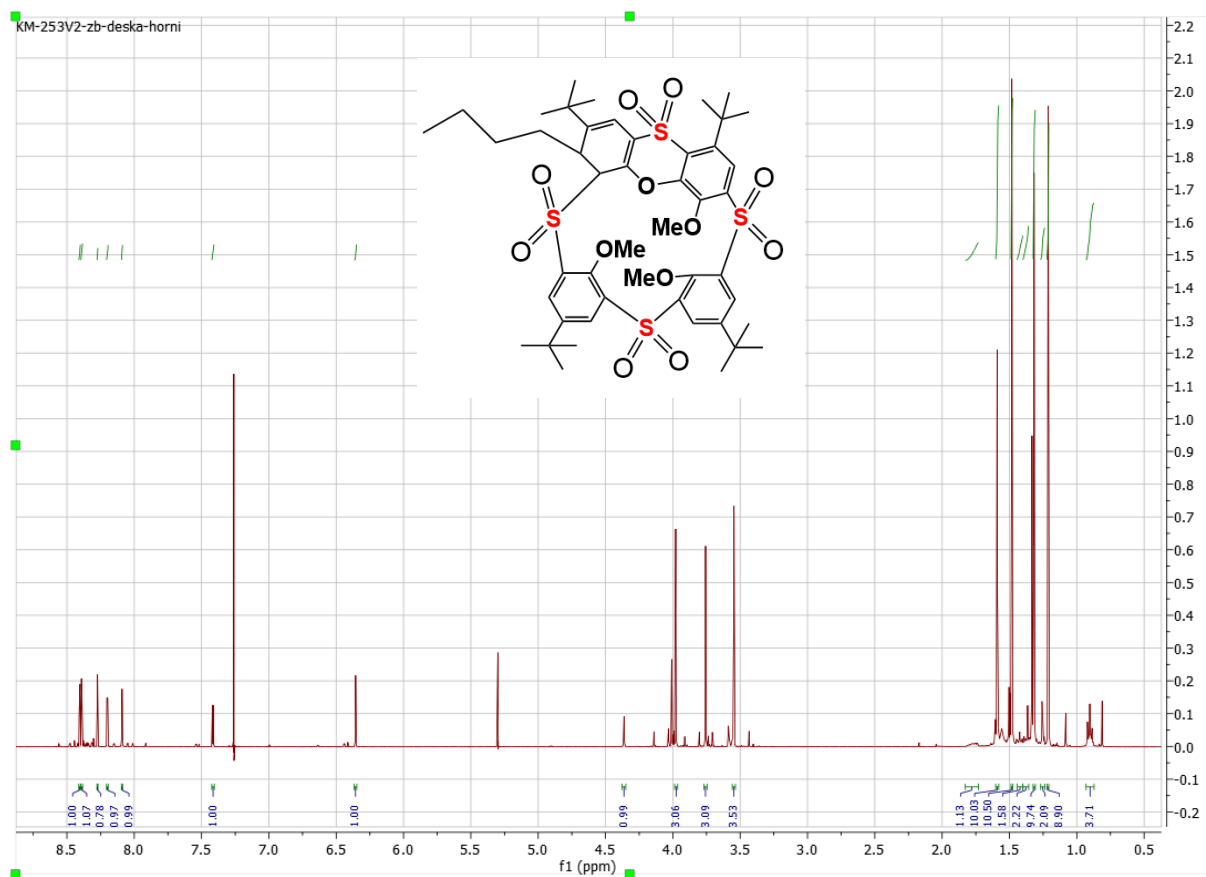
**Figure S17:** <sup>1</sup>H NMR of compound **12** (CDCl<sub>3</sub>, 400 MHz).



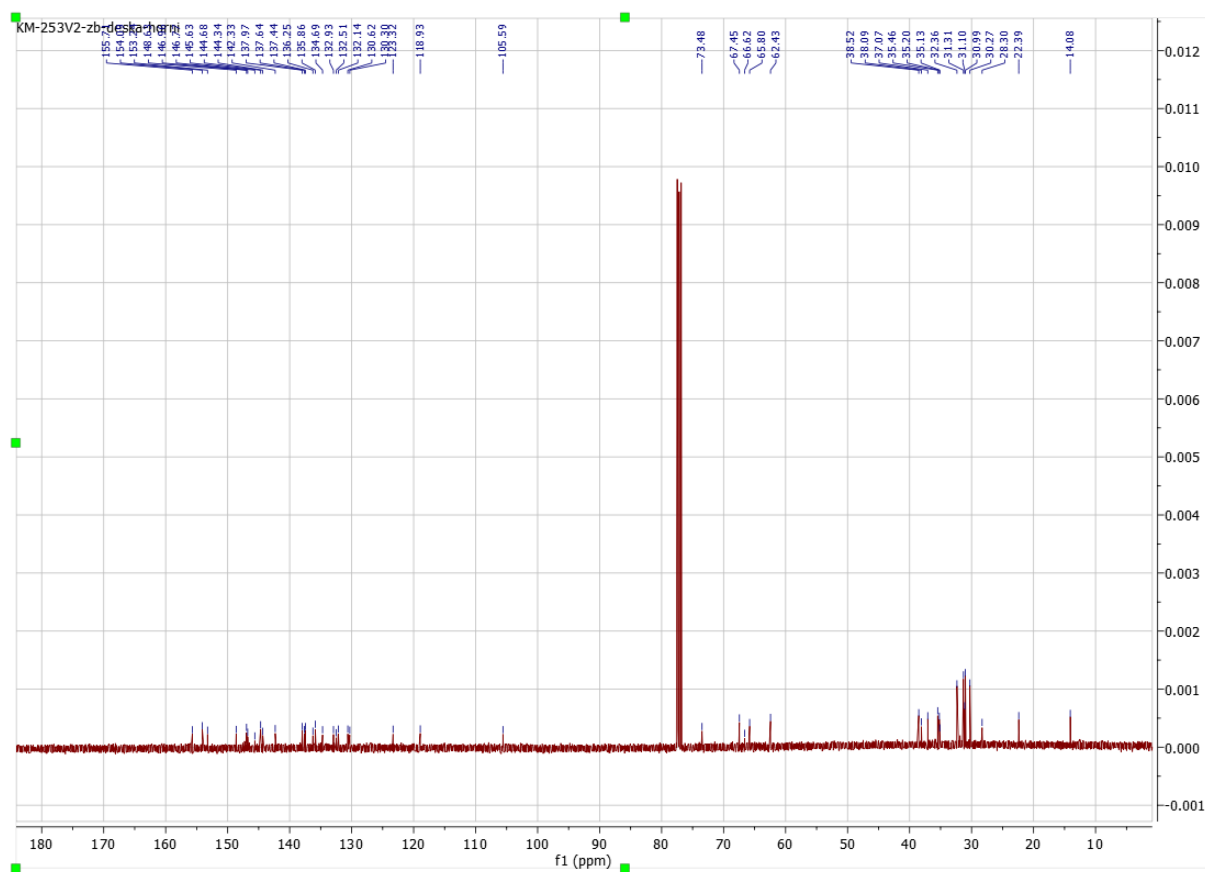
**Figure S18:**  $^{13}\text{C}$  NMR of compound **12** ( $\text{CDCl}_3$ , 100 MHz)



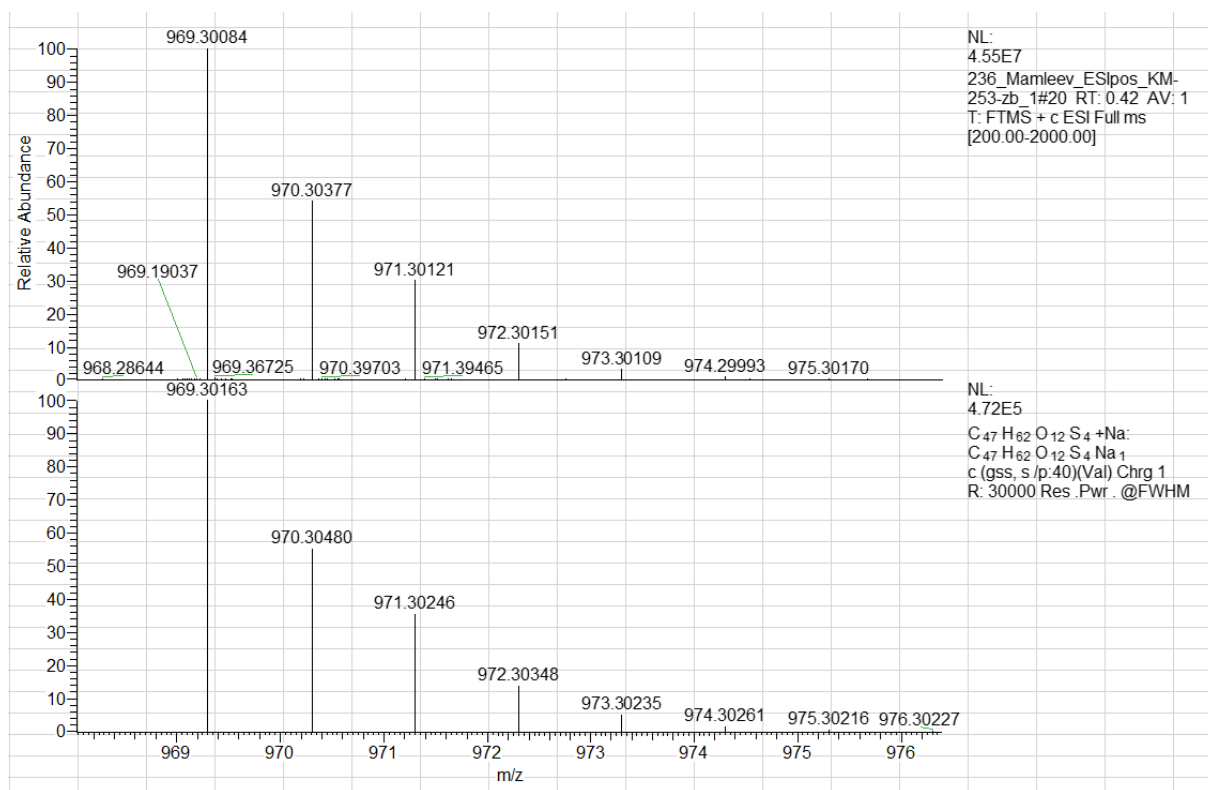
**Figure S19:** HRMS of compound **12** (ESI<sup>+</sup>).



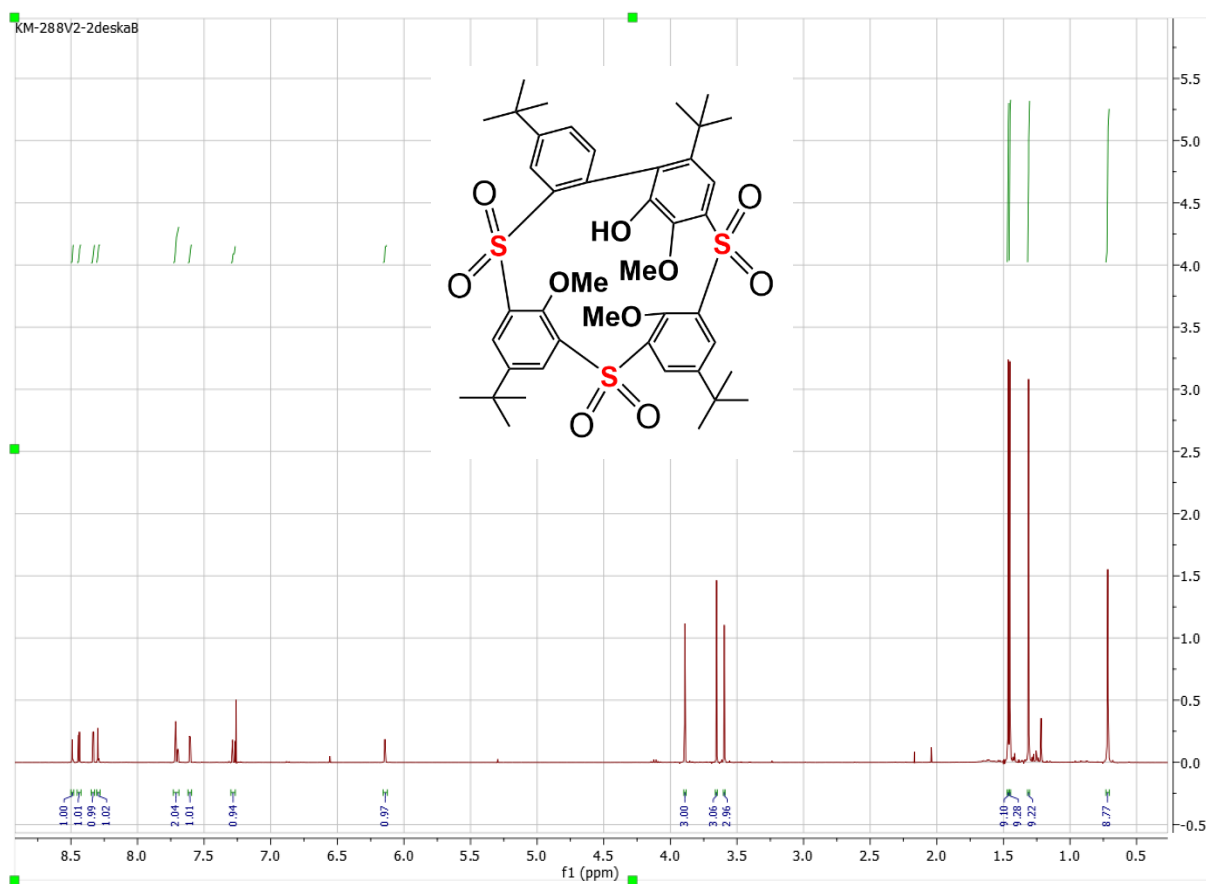
**Figure S20:**  $^1\text{H}$  NMR of compound **13** (CDCl<sub>3</sub>, 400 MHz).



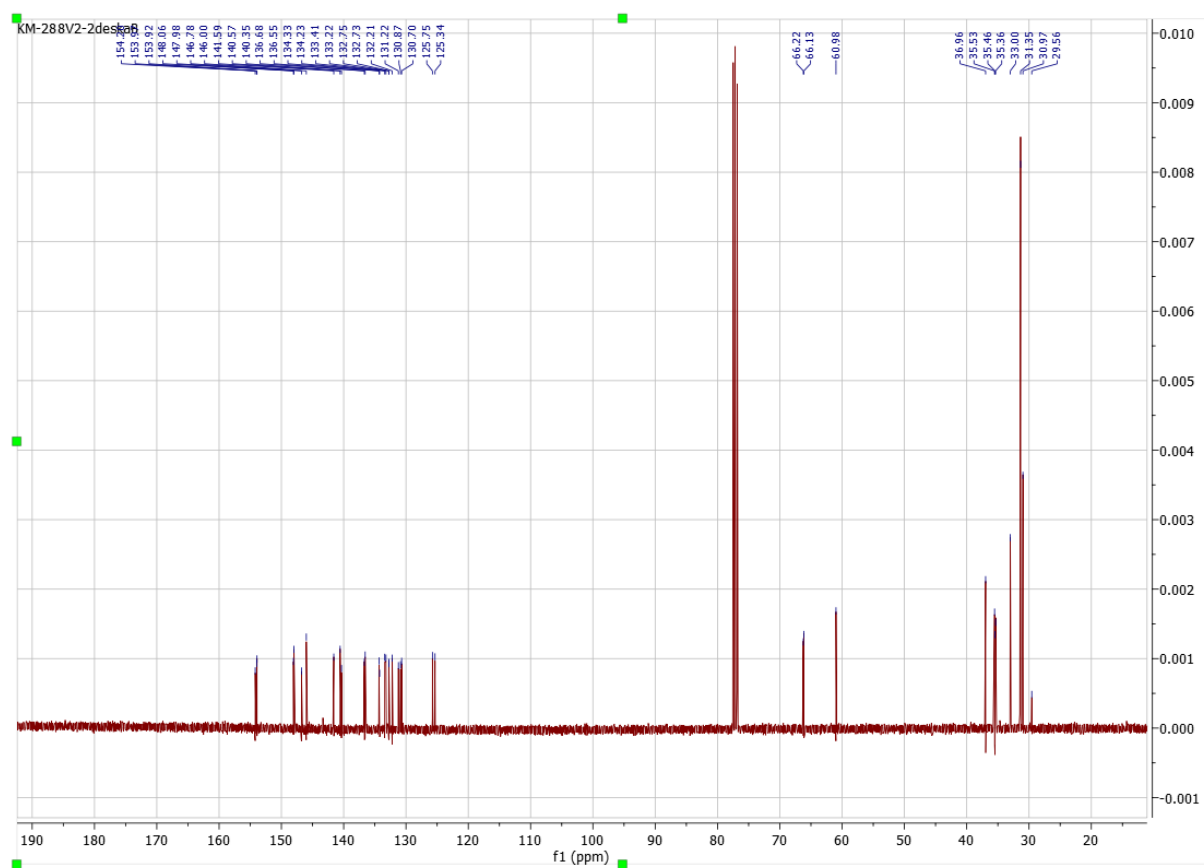
**Figure S21:**  $^{13}\text{C}$  NMR of compound **13** ( $\text{CDCl}_3$ , 100 MHz)



**Figure S22:** HRMS of compound **13** (ESI<sup>+</sup>).



**Figure S23:** <sup>1</sup>H NMR of compound **14** (CDCl<sub>3</sub>, 400 MHz).



**Figure S24:**  $^{13}\text{C}$  NMR of compound **14** ( $\text{CDCl}_3$ , 100 MHz)

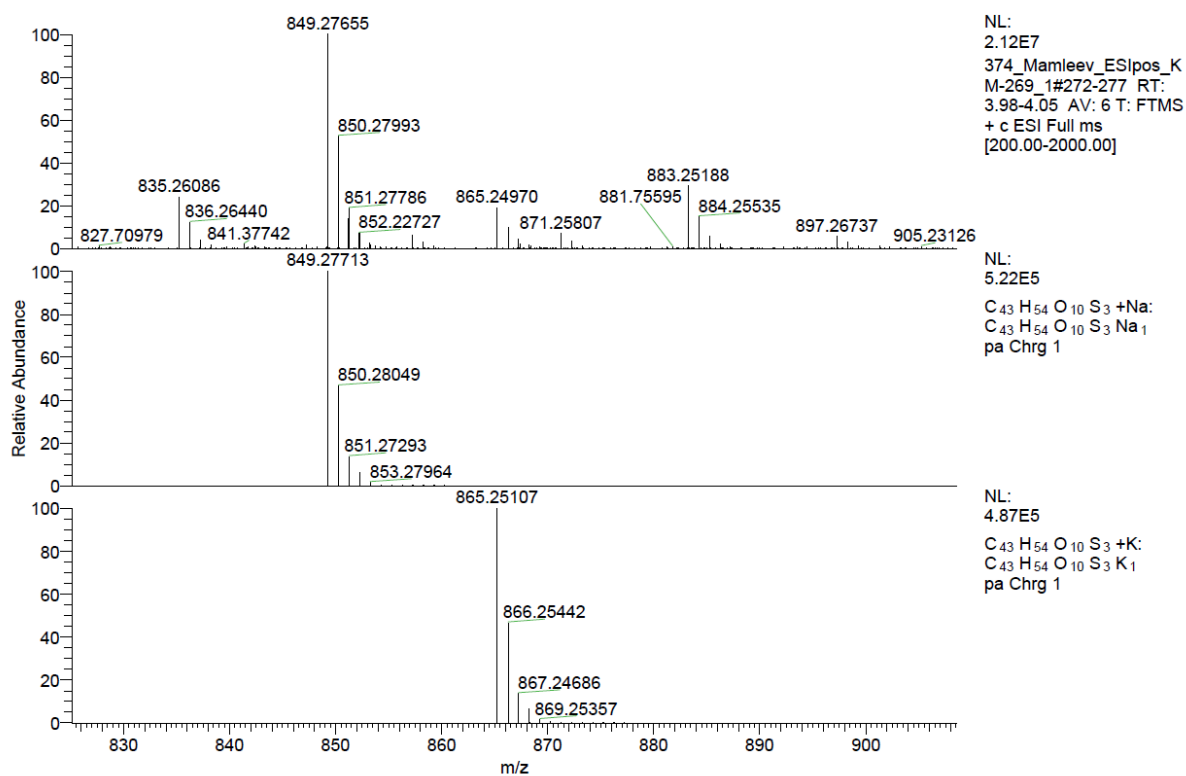
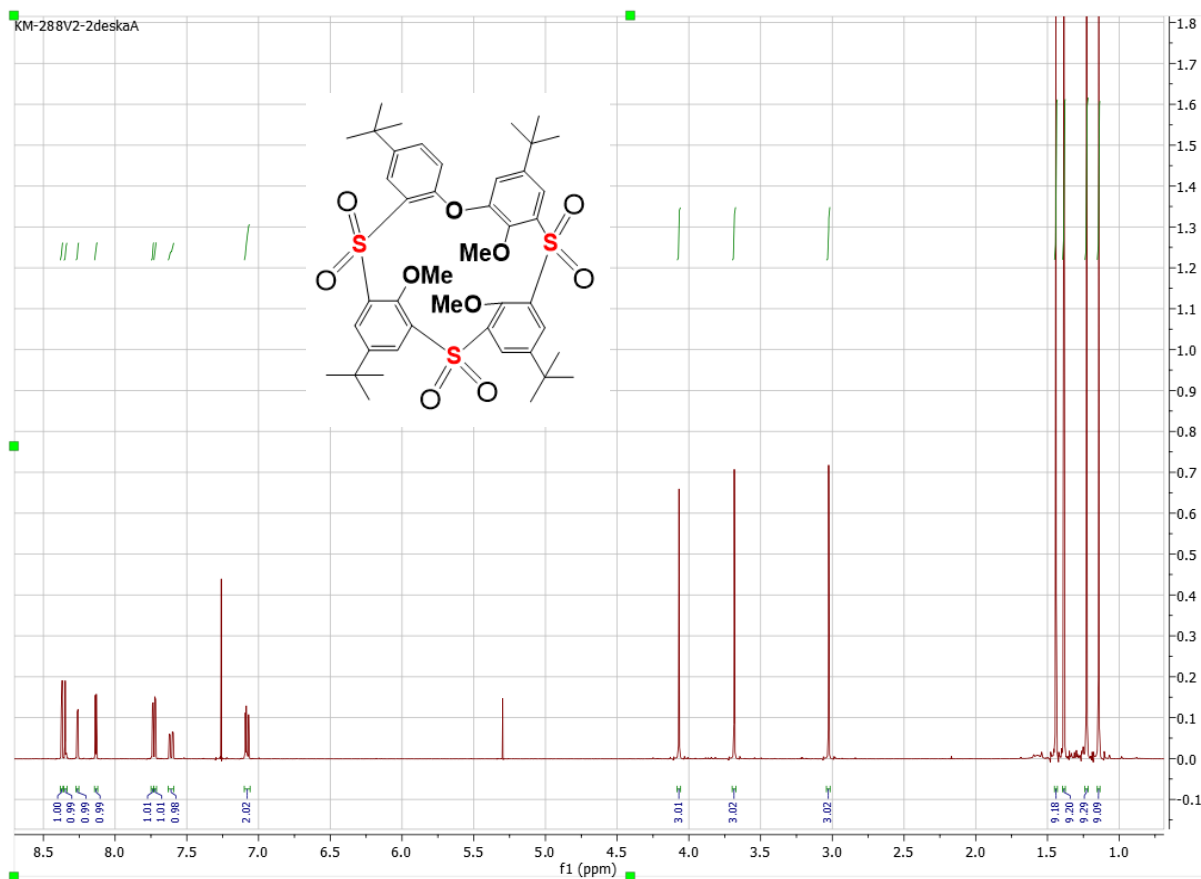
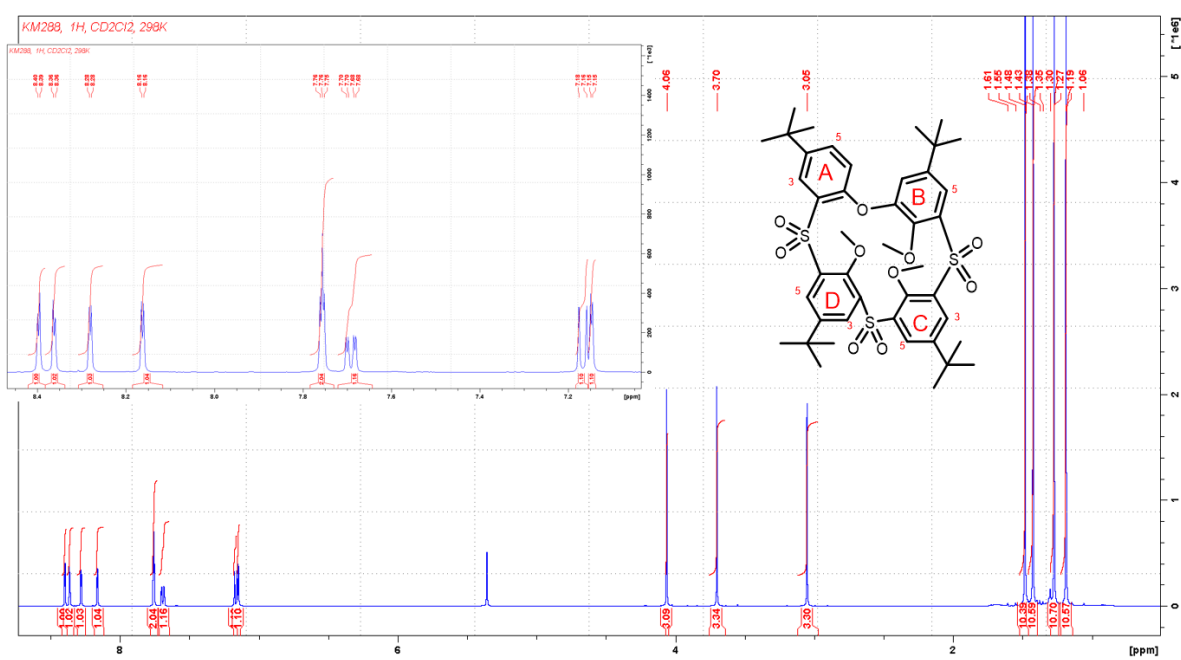


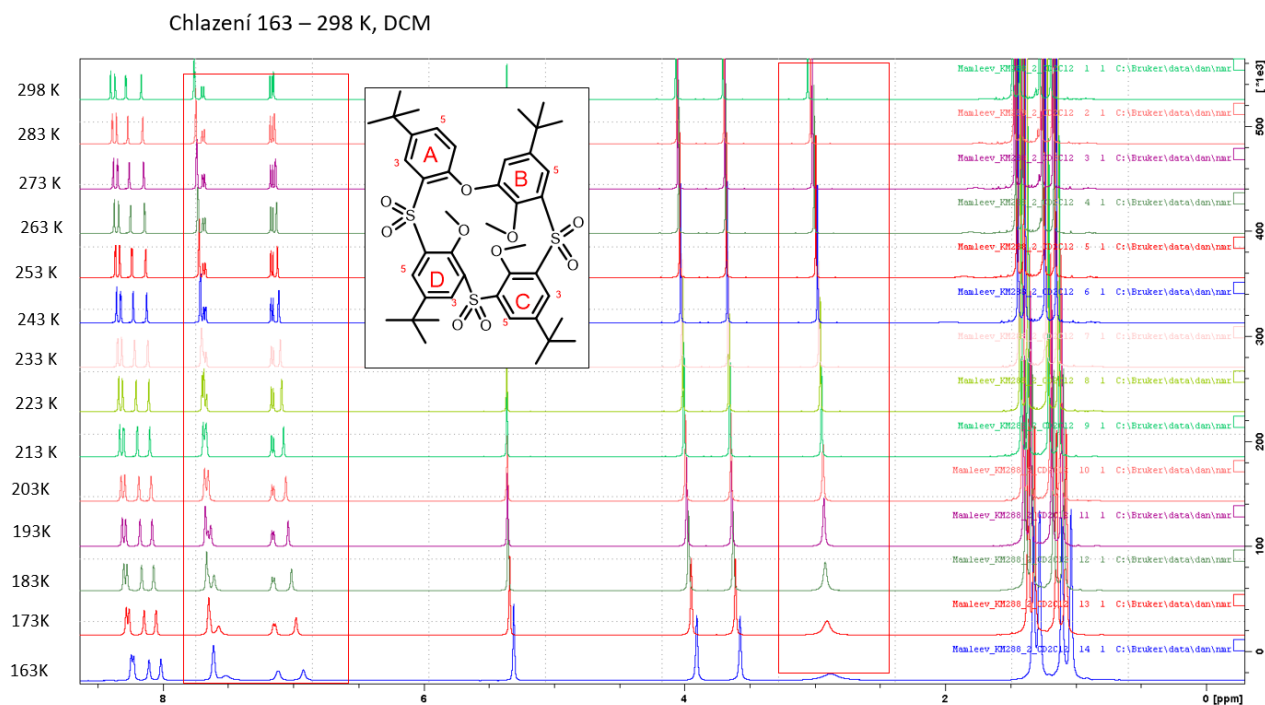
Figure S25: HRMS of compound 14 (ESI<sup>+</sup>).



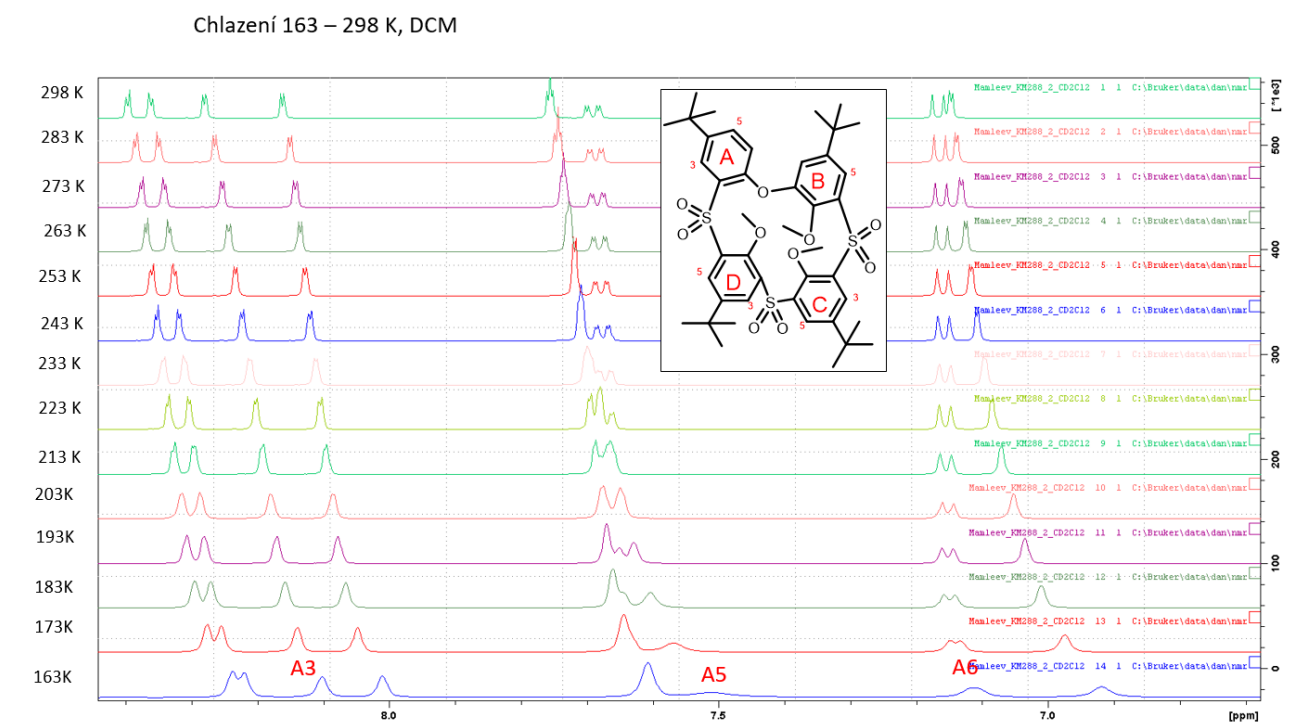
**Figure S26:** <sup>1</sup>H NMR of compound 15 (CDCl<sub>3</sub>, 400 MHz).



**Figure S27:** <sup>1</sup>H NMR of compound 15 (CD<sub>2</sub>Cl<sub>2</sub>, 500 MHz, 298 °K).



**Figure S28:**  $^1\text{H}$  NMR of compound 15 ( $\text{CD}_2\text{Cl}_2$ , 500 MHz).



**Figure S29:**  $^1\text{H}$  NMR of compound 15 ( $\text{CD}_2\text{Cl}_2$ , 500 MHz).

Zahřívání 298 – 403 K, TCE

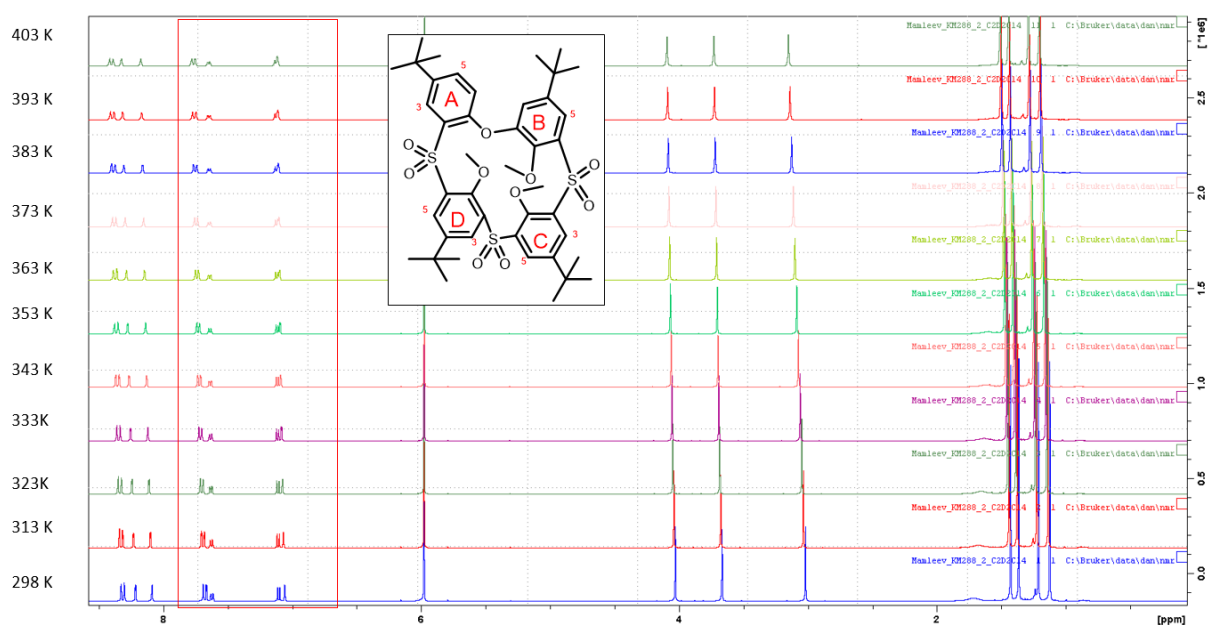


Figure S30:  $^1\text{H}$  NMR of compound 15 ( $\text{C}_2\text{D}_2\text{Cl}_4$ , 500 MHz).

Zahřívání 298 – 403 K, TCE

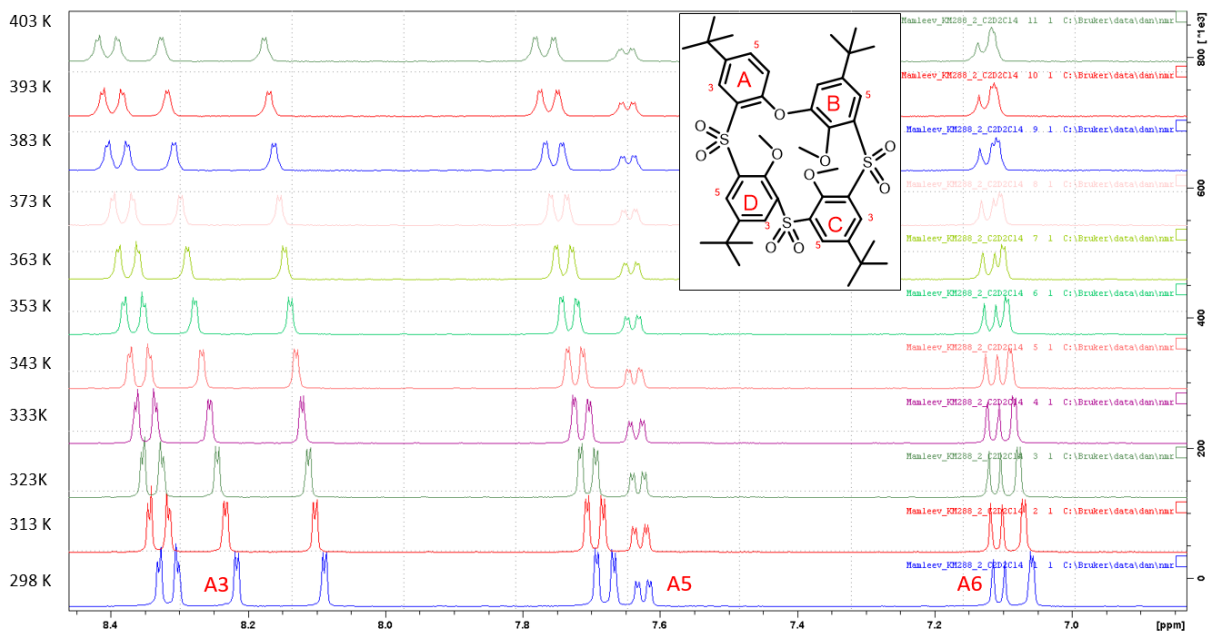
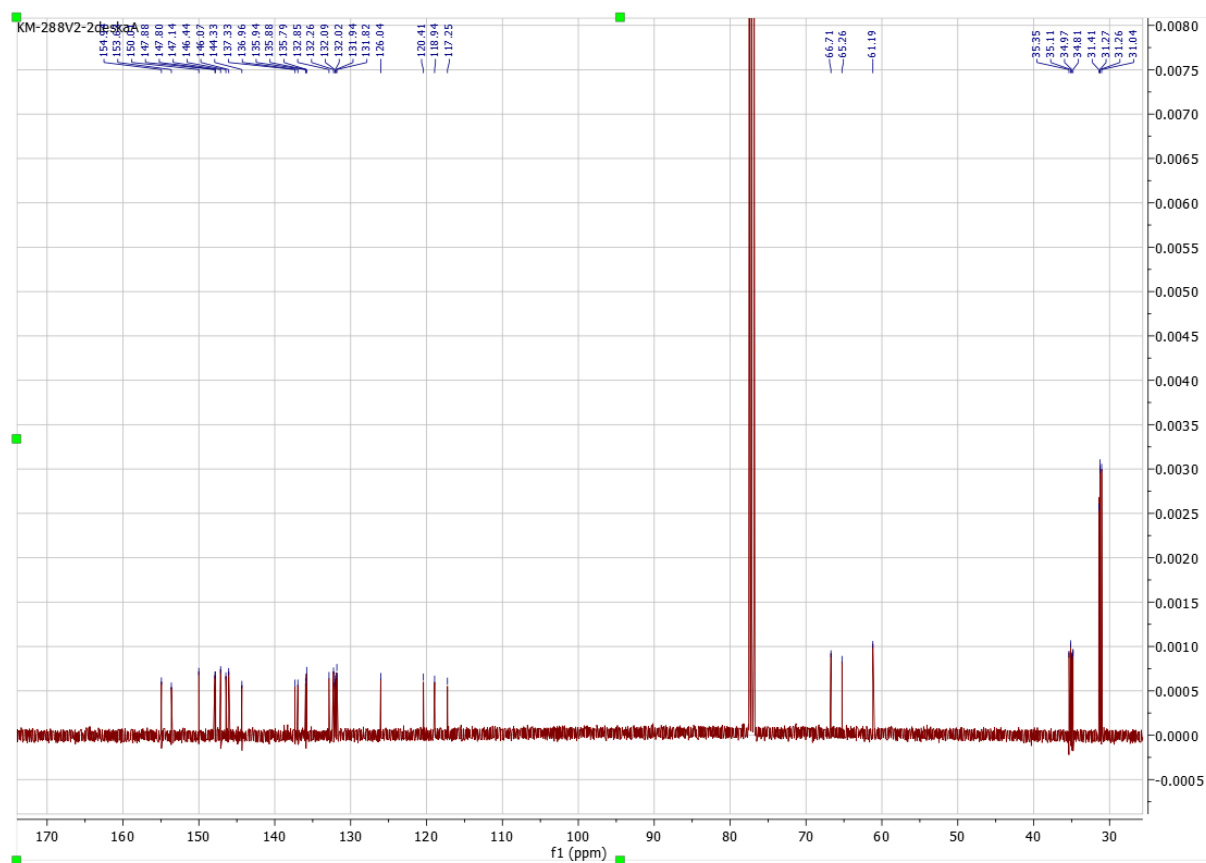


Figure S31:  $^1\text{H}$  NMR of compound 15 ( $\text{C}_2\text{D}_2\text{Cl}_4$ , 500 MHz).



**Figure S32:** <sup>13</sup>C NMR of compound **15** (CDCl<sub>3</sub>, 100 MHz)

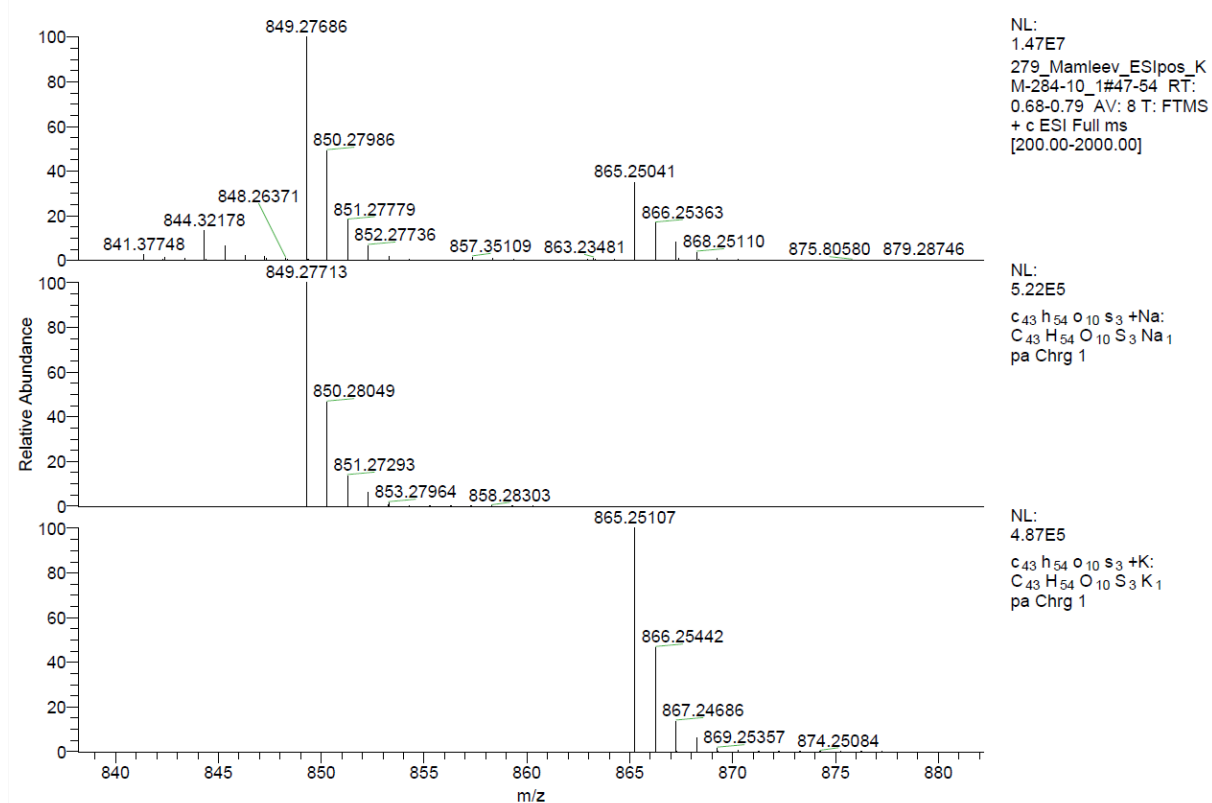
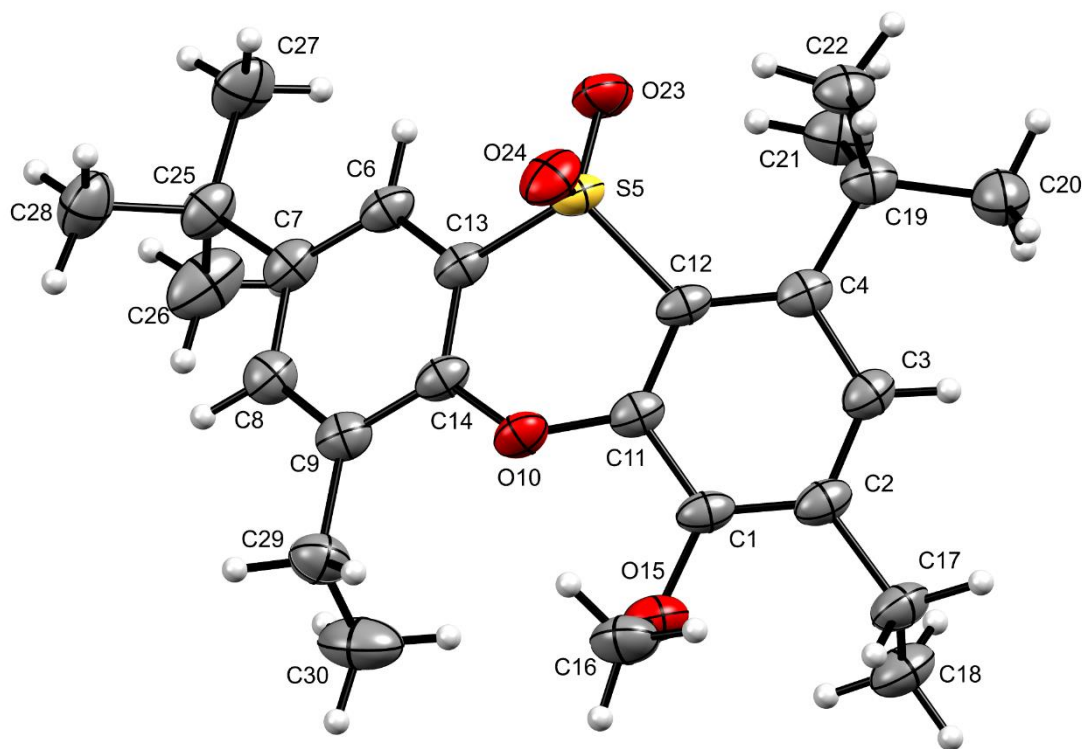
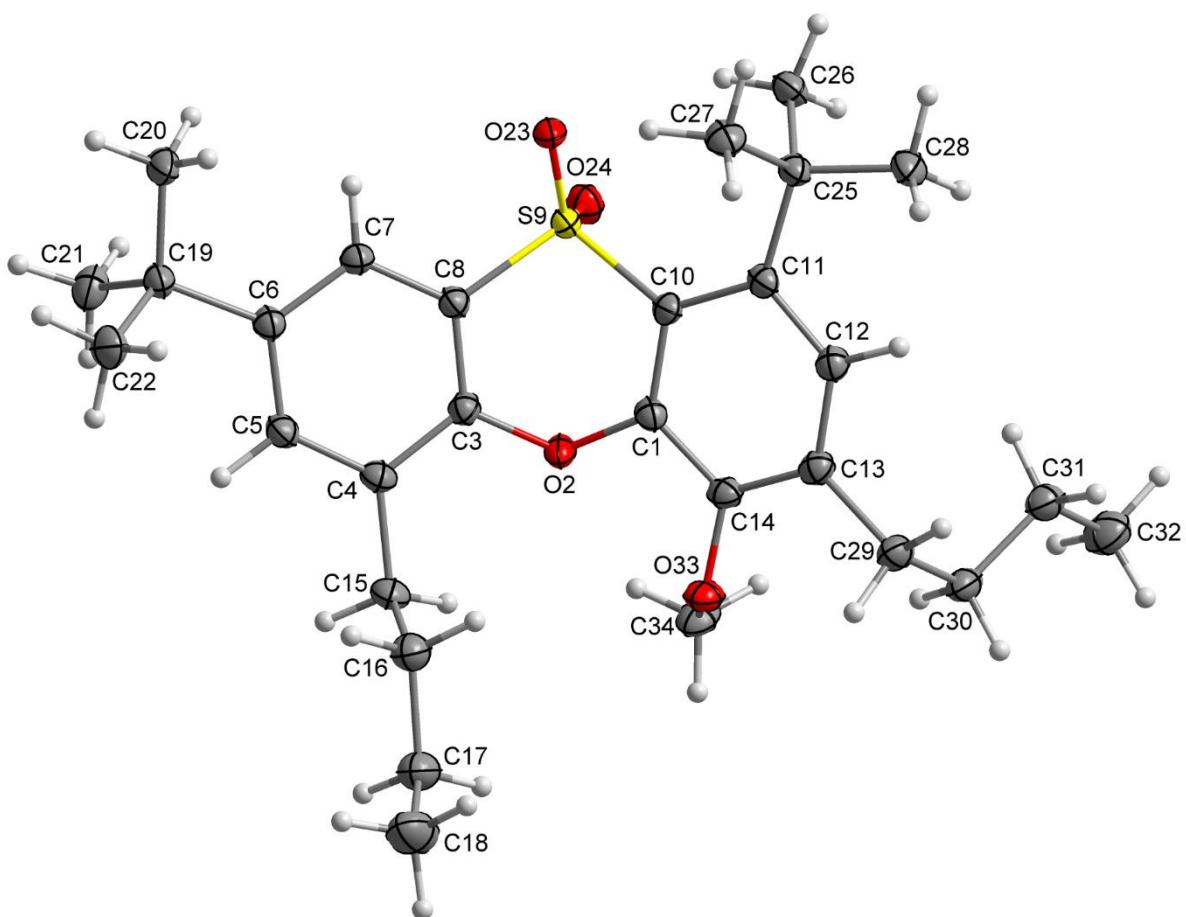


Figure S33: HRMS of compound 15 (ESI<sup>+</sup>).

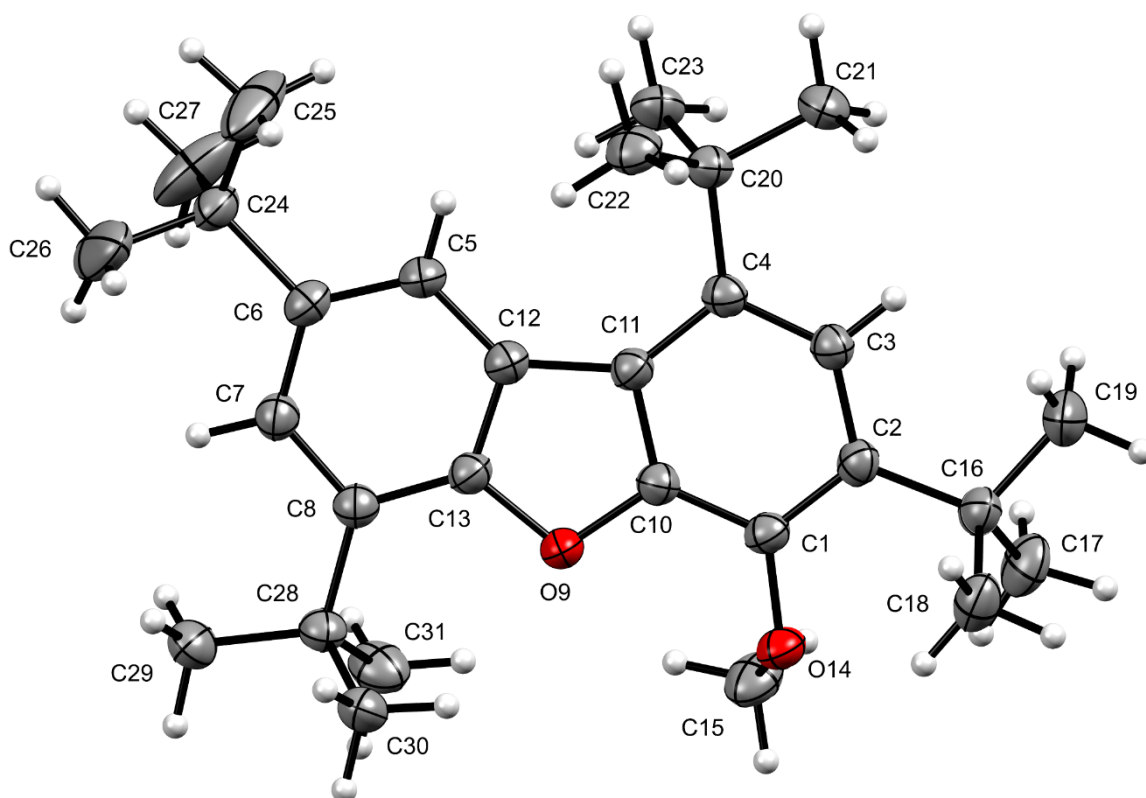
## 2. Crystallographic data



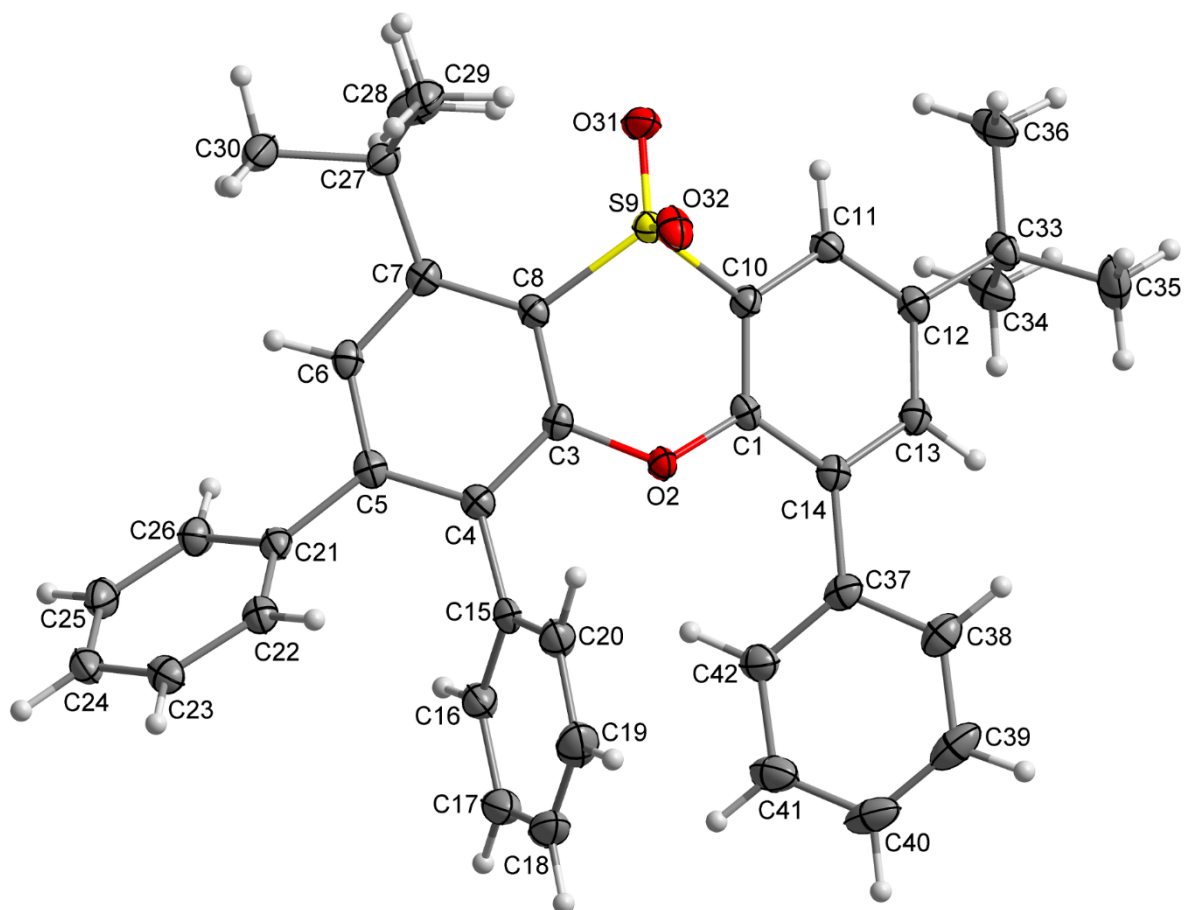
**Figure S34:** The numbering scheme of compound **10b**, drawn at 50 % probability level.



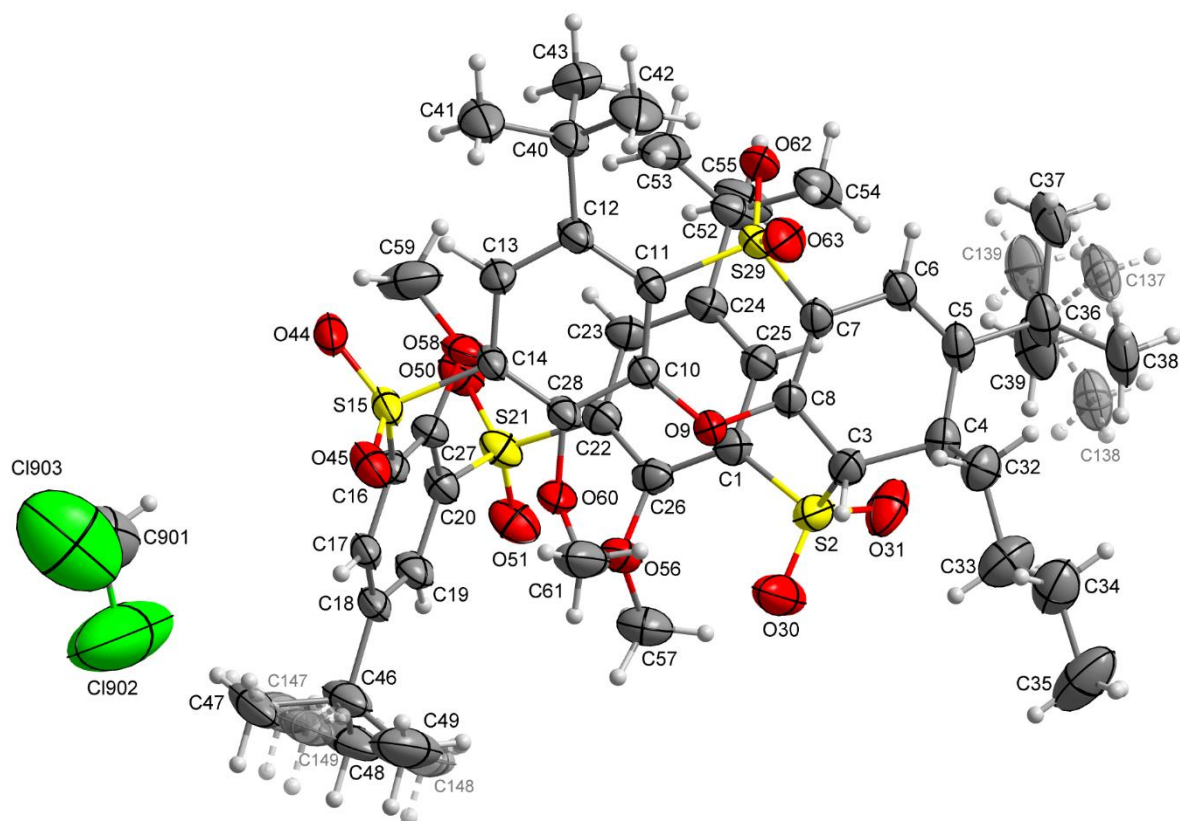
**Figure S35:** The numbering scheme of compound **10c**. The ADPs drawn at 50 % probability level.



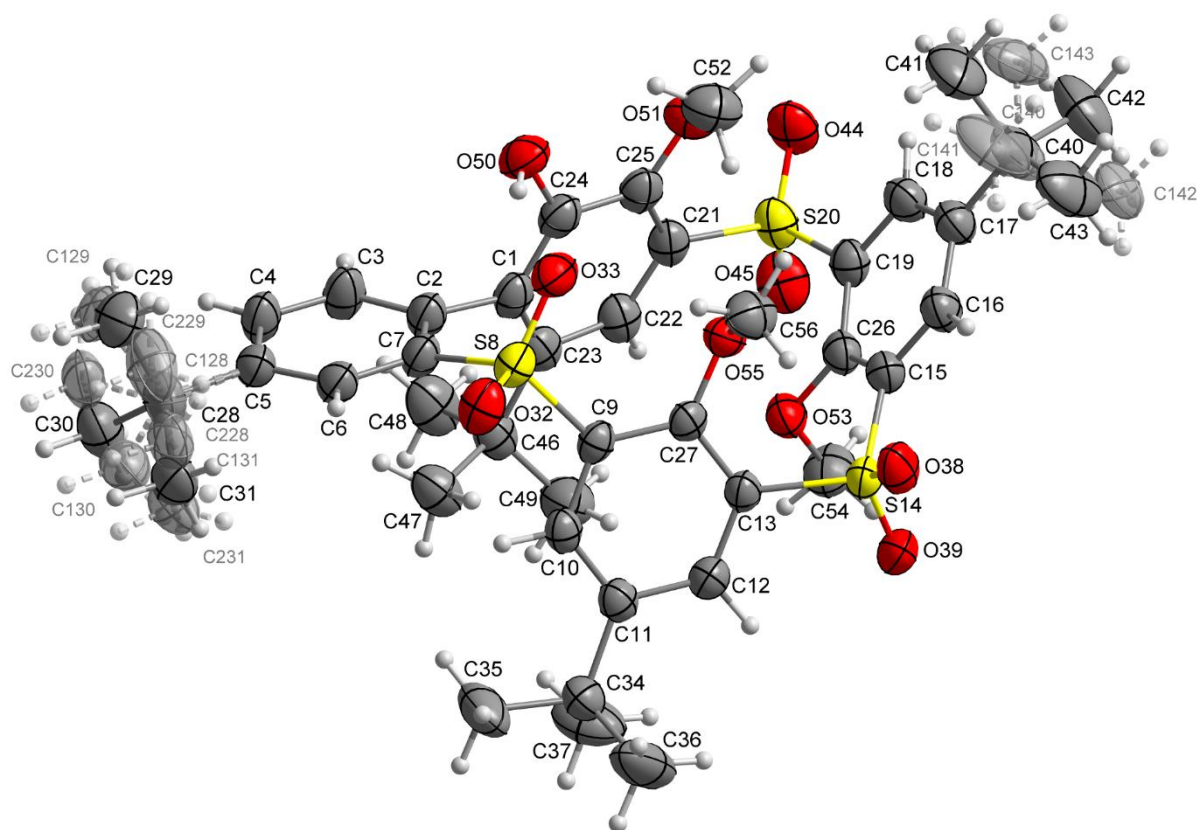
**Figure S36:** The numbering scheme of compound **11**, drawn at 50 % probability level.



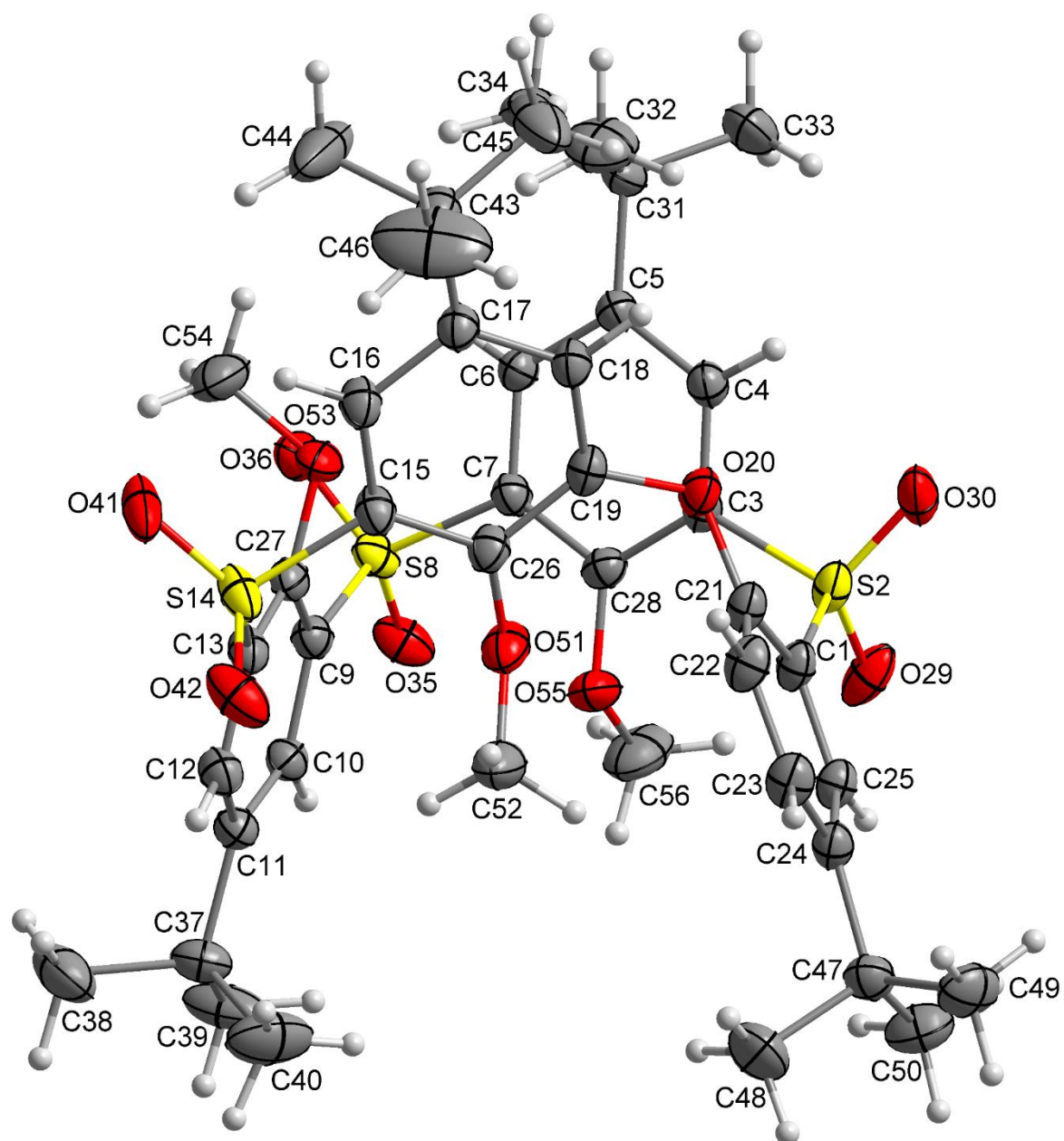
**Figure S37:** The numbering scheme of compound **12**. The ADPs drawn at 50 % probability level.



**Figure S38:** The numbering scheme of compound **13**. The ADPs drawn at 50 % probability level. The weakly occupied atoms depicted as transparent.



**Figure S39:** The numbering scheme of compound **14**. The ADPs drawn at 50 % probability level. The weakly occupied atoms depicted as transparent.



**Figure S40:** The numbering scheme of compound **15**. The ADPs drawn at 50 % probability level.

### 3. Computations

#### Cartesian coordinates of transition states

##### MeLi C1

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -1.35782718580429 | 0.42542254899761  | 1.40873967143725  |
| C | 0.04454595288813  | 0.34146323843746  | 1.30029401669025  |
| C | 0.84714699713719  | 1.37845524500638  | 1.79902128283144  |
| C | 0.30811518803266  | 2.41317539020456  | 2.58166423225550  |
| C | -1.07523452460184 | 2.41366209943072  | 2.74934444276699  |
| C | -1.87742645941203 | 1.48515154546520  | 2.12626653630296  |
| S | 2.41936333927075  | 1.28653298243279  | 0.91582784504884  |
| C | 2.84474760934350  | -0.39920302165685 | 1.09930877745773  |
| C | 1.78070242881990  | -1.23987877377140 | 0.72609933415843  |
| O | 0.49730267549554  | -0.73498703680170 | 0.59211876522591  |
| C | 4.07222034772398  | -0.89298400890918 | 1.47098344277114  |
| C | 4.28710599562995  | -2.27098512544111 | 1.59364947715936  |
| C | 3.17069266041716  | -3.09900421060080 | 1.43522676857505  |
| C | 1.93887456319047  | -2.59795799580720 | 1.08651736114219  |
| C | 5.66708188234387  | -2.79250218527882 | 1.95003392972480  |
| C | 5.71580067529265  | -4.32206336237738 | 1.97240774926618  |
| S | 0.47984243951911  | -3.61553848676551 | 1.15756549723813  |
| O | 0.87792510575865  | -4.98426422832759 | 1.36252014467796  |
| S | -3.65143210492707 | 1.76491729180032  | 1.99944588647530  |
| O | -4.03588922739682 | 2.69493976212013  | 3.02874461578491  |
| C | 1.13546182500683  | 3.53913265163910  | 3.18775009462092  |
| C | 2.32157154212230  | 2.97032452961005  | 3.97762155048493  |
| O | 1.98108063613963  | 1.48797992679784  | -0.45847341027149 |
| O | -2.24529969439759 | -0.44688958902583 | 0.87705691803562  |
| C | -2.10308379936406 | -0.84943054158833 | -0.48496553529741 |
| C | -0.32479412822918 | -3.05658354164355 | 2.69152448382778  |
| C | 0.53120229563358  | -2.41162368938504 | 3.57406729297807  |
| C | 0.13157234294704  | -1.90474935980846 | 4.80039604535148  |
| C | -1.19921336456821 | -2.11331640825387 | 5.15262799194809  |
| C | -2.04896250840061 | -2.76799208245455 | 4.29947223054861  |
| C | -1.66223394590450 | -3.24693572654157 | 3.04086000975514  |
| C | 1.06554456313240  | -1.15172122294114 | 5.73043085318297  |
| C | 2.41904008678660  | -0.85067191536259 | 5.07805984304463  |
| S | -3.78335706336598 | -2.89295061280253 | 4.74079056694549  |
| O | -4.28266855868496 | -4.22946610931380 | 4.58795355783655  |
| O | -2.64922531981208 | -3.80412496601933 | 2.32884007378205  |
| C | -2.39744812329700 | -4.82258921059296 | 1.37044002357927  |
| O | -0.35363383704708 | -3.34492085040132 | 0.01465100135528  |
| C | -4.51505803254244 | -1.83887655945248 | 3.48581484545616  |
| C | -5.44184176725595 | -2.34636627491832 | 2.59669135654383  |
| C | -5.90971296980088 | -1.58771535640498 | 1.52832606038455  |
| C | -5.38094511152291 | -0.30557392915201 | 1.37645103657762  |
| C | -4.45601285712833 | 0.18813664974217  | 2.26849295816614  |
| C | -4.00373340088048 | -0.55863278307554 | 3.34466863383374  |
| C | -6.91326273696579 | -2.11191571958199 | 0.51610840838233  |
| C | -8.12859797224545 | -1.17502067006951 | 0.48662529938134  |
| O | -3.02319062174183 | -0.05577339219930 | 4.15667113307441  |
| C | -3.50518038686546 | 0.65769758728213  | 5.29907756425292  |
| O | -3.95656960583857 | -2.28930915339698 | 6.03806627611081  |
| O | -3.89638144457986 | 2.16760451346858  | 0.64008394205830  |
| C | 6.06605365417267  | -2.26830488406751 | 3.33711756393628  |
| C | 6.66821726588064  | -2.29241520032169 | 0.89879642577451  |
| C | 1.29773355604414  | -2.00093612226061 | 6.98742596577359  |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | 0.40357826315991  | 0.17887325762919  | 6.11701139696491  |
| C | -7.39491820969188 | -3.52430591315651 | 0.85529400477816  |
| C | -6.24233743729106 | -2.14248021912055 | -0.86480509194286 |
| C | 0.31312353769664  | 4.38971686285340  | 4.16671053792988  |
| C | 1.61268543162336  | 4.46199236559223  | 2.05724978805046  |
| H | 4.85111972207271  | -0.17845965983975 | 1.68759529863013  |
| H | 3.21448319405486  | -4.15753711617042 | 1.63268493422154  |
| H | 1.55820912319456  | -2.31056432748592 | 3.26977581428317  |
| H | -1.61230320468764 | -1.78232175433374 | 6.09137518756701  |
| H | -5.75613301962820 | -3.36258070308094 | 2.76724463507526  |
| H | -5.65059236558780 | 0.33311292117400  | 0.54990318494784  |
| H | -1.58349279483721 | 3.17995624201285  | 3.30746359759322  |
| H | -1.48570186523625 | -5.37590900337006 | 1.59670150359794  |
| H | -3.25828164413129 | -5.48917964711438 | 1.42806924774641  |
| H | -2.31415267321040 | -4.39733766062335 | 0.36928399312389  |
| H | -4.12973452596866 | 1.49856955198881  | 4.98868384087005  |
| H | -2.61389924143884 | 1.02902601254645  | 5.79938932970855  |
| H | -4.05388977149448 | -0.01715240787857 | 5.96025443328780  |
| H | -1.48034479291200 | -1.74047498364926 | -0.57201723838532 |
| H | -1.69767945671964 | -0.03728517816527 | -1.09608114877799 |
| H | -3.11679292813068 | -1.07441398014920 | -0.81322560861565 |
| H | 5.36514708455945  | -2.62070457143773 | 4.09063752423590  |
| H | 6.07827349708146  | -1.18236716377961 | 3.36170642958856  |
| H | 7.05867052576032  | -2.62752169332562 | 3.59793564185222  |
| H | 6.37451162829216  | -2.63557875310073 | -0.09027686267830 |
| H | 6.71887787362045  | -1.20765918529796 | 0.88316563081978  |
| H | 7.66162021226644  | -2.67746911946699 | 1.11702567855038  |
| H | 6.73381760841117  | -4.64836492927220 | 2.17316099136514  |
| H | 5.07507326528454  | -4.72653658119704 | 2.75179098098351  |
| H | 5.41060615208057  | -4.73331841977609 | 1.01393831300215  |
| H | 0.35724234915643  | -2.22237998558885 | 7.48368893830156  |
| H | 1.77433782245249  | -2.94225433697011 | 6.72420237620609  |
| H | 1.94112001973869  | -1.47006751017587 | 7.68532659416678  |
| H | -0.47589384217136 | 0.01265877559529  | 6.73136135086618  |
| H | 1.10048033147943  | 0.79060975464771  | 6.68658810784730  |
| H | 0.10114365588171  | 0.72180826020798  | 5.22297727076520  |
| H | 2.95867821978267  | -1.76584642323396 | 4.84761193274510  |
| H | 3.03102109041721  | -0.26981877369999 | 5.76466411393482  |
| H | 2.29599003056128  | -0.27340383324819 | 4.16307401580367  |
| H | -8.12329847091862 | -3.84519458428175 | 0.11373934071402  |
| H | -7.87348595651062 | -3.54979383008880 | 1.83075448856962  |
| H | -6.57010134751194 | -4.23161458506200 | 0.84519439004611  |
| H | -5.35809074778228 | -2.77528912187643 | -0.83785590177925 |
| H | -6.93232973279164 | -2.54443700510017 | -1.60317961256768 |
| H | -5.94625213629530 | -1.14663976739652 | -1.18198699866843 |
| H | -7.84614109886127 | -0.16690758087488 | 0.19845791920302  |
| H | -8.59487391008760 | -1.13295156529495 | 1.46812169298600  |
| H | -8.86219387014828 | -1.54151323190116 | -0.22766603334234 |
| H | 0.97151701954294  | 5.11967682432779  | 4.63218866030049  |
| H | -0.47638094968343 | 4.93770944187748  | 3.66014534836149  |
| H | -0.12071526593506 | 3.77854539856846  | 4.95436301119348  |
| H | 0.75998048538427  | 4.82874730275002  | 1.48970137966374  |
| H | 2.14012816959169  | 5.31373090930692  | 2.47977464620699  |
| H | 2.28626114468845  | 3.94661060079959  | 1.38249995327091  |
| H | 1.96672517037224  | 2.29616289930267  | 4.75282819062447  |
| H | 2.86245869802758  | 3.78498043200477  | 4.45297775442247  |
| H | 3.01494424765342  | 2.44359134423532  | 3.33432389414117  |
| O | 3.49800765023514  | 2.11860707506695  | 1.35166061286163  |
| C | 2.14416549658997  | -1.76718499860406 | -1.63834029347011 |
| H | 1.53791176549176  | -2.64906960776880 | -1.48108569676395 |
| H | 3.16744395614863  | -2.01277514844816 | -1.37890654876258 |

|    |                  |                   |                   |
|----|------------------|-------------------|-------------------|
| H  | 2.13296210656504 | -1.55192820914849 | -2.71456119109443 |
| Li | 1.34178587462932 | -0.03695356859743 | -1.04535268354581 |

# MeLi C2

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -0.93279900081470 | 0.70876817781551  | 0.77391208736594  |
| C | 0.46087668991985  | 0.60884124540141  | 0.67631956069594  |
| C | 1.30318979581618  | 1.63510375664848  | 1.12464186007035  |
| C | 0.78725484704090  | 2.65477719494526  | 1.93480000002481  |
| C | -0.59850260908098 | 2.70073095888615  | 2.09329665722886  |
| C | -1.42819389979445 | 1.80453423288724  | 1.46248158302318  |
| S | 2.78240959475676  | 1.60070990539770  | 0.01746783014204  |
| C | 3.23266467203846  | -0.04276697496761 | 0.51918174768213  |
| C | 2.19154947892710  | -0.95509580872793 | 0.40427695615305  |
| O | 0.92965491973855  | -0.56468149950295 | 0.11750702173602  |
| C | 4.48661737504507  | -0.44337598775277 | 0.95206440466338  |
| C | 4.77467092805587  | -1.78841451111212 | 1.16950097324869  |
| C | 3.74319166087050  | -2.70759112912696 | 0.98432823956093  |
| C | 2.46569896337339  | -2.29167272551587 | 0.64690118243071  |
| C | 6.17664927104966  | -2.19574917664037 | 1.59229814487842  |
| C | 6.30444661510920  | -3.70690140586271 | 1.79812685662612  |
| S | 1.08190353487972  | -3.43817522954031 | 0.72579284128735  |
| O | 1.60422958105047  | -4.75489353651453 | 0.98901601297346  |
| S | -3.19522417443731 | 2.10496664493710  | 1.38437718634691  |
| O | -3.54664998898467 | 3.02660847710814  | 2.43639081017817  |
| C | 1.64834530487209  | 3.69433017069123  | 2.64196027354095  |
| C | 2.90679607435318  | 3.03146335758496  | 3.21665670301285  |
| O | 1.98307617584185  | 1.94294720694150  | -1.17216037371455 |
| O | -1.83365260642612 | -0.15876490226175 | 0.26129830601606  |
| C | -1.57522750974154 | -0.75830766995521 | -1.00619191289140 |
| C | 0.22211522534421  | -2.88320966561811 | 2.22209630031661  |
| C | 1.07023088689893  | -2.30642867637651 | 3.15742147257219  |
| C | 0.62837312708481  | -1.77452234294455 | 4.35831317707590  |
| C | -0.73327833183117 | -1.89308563052115 | 4.62689412047531  |
| C | -1.57133480517865 | -2.49755623980289 | 3.72629646538016  |
| C | -1.14064882974100 | -2.99820544925126 | 2.49215308996097  |
| C | 1.54388927653075  | -1.06836600442612 | 5.34142580584147  |
| C | 2.97219521335674  | -0.92630128041014 | 4.80663184356955  |
| S | -3.32517828102622 | -2.58860486982773 | 4.09865359497272  |
| O | -3.81685170738045 | -3.92806360626525 | 3.93359681210715  |
| O | -2.10328732112221 | -3.50915299949600 | 1.71255757790567  |
| C | -1.84492880631592 | -4.62990307340604 | 0.87697248636171  |
| O | 0.27770724272605  | -3.28881413594410 | -0.45600795662965 |
| C | -4.03859833761529 | -1.53375245389289 | 2.83823637297108  |
| C | -4.99198161949151 | -2.01767533979471 | 1.96504334898027  |
| C | -5.48213126587323 | -1.22814767207141 | 0.92999570104462  |
| C | -4.94896690228530 | 0.05433589969836  | 0.79931040582610  |
| C | -3.99495059068387 | 0.52449826421407  | 1.67385110291971  |
| C | -3.51922413413069 | -0.25496580157606 | 2.71727825083558  |
| C | -6.51603213687912 | -1.71793910933674 | -0.06896663899554 |
| C | -7.71596950476040 | -0.76112088596084 | -0.05801432811474 |
| O | -2.51215512493678 | 0.19238503209367  | 3.52803056023529  |
| C | -2.94614081142313 | 0.96586273873227  | 4.64949811667756  |
| O | -3.53190054101735 | -1.98699261298036 | 5.39225469909297  |
| O | -3.51290671658827 | 2.51764478236179  | 0.04341330732830  |
| C | 6.53125431971819  | -1.49324097865685 | 2.91004027840613  |
| C | 7.16065374189178  | -1.76957650389696 | 0.49389743911026  |
| C | 1.58348590602393  | -1.86673837520362 | 6.65120833972049  |
| C | 0.97480773837826  | 0.33429530137519  | 5.60123797894165  |
| C | -7.01509173176098 | -3.12760983286581 | 0.25671123220348  |
| C | -5.87377633690128 | -1.73559839109164 | -1.46344320465830 |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| C  | 0.89806296136870  | 4.33579291206510  | 3.81966416810796  |
| C  | 2.02110435199016  | 4.80694477155908  | 1.65409550285756  |
| H  | 5.22687182819008  | 0.32493717353769  | 1.10144845217498  |
| H  | 3.87430773604858  | -3.76525552461116 | 1.13996309378872  |
| H  | 2.11759004023652  | -2.27900415636246 | 2.91409071572419  |
| H  | -1.17925938184845 | -1.53378471124242 | 5.54004921615816  |
| H  | -5.31180199977769 | -3.03426512657219 | 2.12258028083306  |
| H  | -5.23538446980234 | 0.71526510275844  | -0.00382426109433 |
| H  | -1.08105613509929 | 3.48320099966547  | 2.65296061140021  |
| H  | -0.92779449926345 | -5.14623626918824 | 1.16283028720603  |
| H  | -2.69908400018206 | -5.29668135087392 | 1.00542426399024  |
| H  | -1.76349364862026 | -4.31468148937349 | -0.16401879599178 |
| H  | -3.52608520434698 | 1.83114638281675  | 4.32104488673012  |
| H  | -2.03210423530008 | 1.30076529634510  | 5.13450490131080  |
| H  | -3.52711552676710 | 0.33991559636119  | 5.33174305276266  |
| H  | -0.95337799871977 | -1.65005733444003 | -0.91385844540019 |
| H  | -1.09881052294229 | -0.04442716361989 | -1.68035462397432 |
| H  | -2.55868058329184 | -1.02637294426916 | -1.39055081330665 |
| H  | 5.83501654242676  | -1.78337486842403 | 3.69301775542640  |
| H  | 6.49792961263686  | -0.41283673677162 | 2.80692626819492  |
| H  | 7.53465052180377  | -1.77535809023692 | 3.21983179532769  |
| H  | 6.88756475154559  | -2.22816207800019 | -0.45335026042260 |
| H  | 7.16423468073764  | -0.69145898137034 | 0.36355724694926  |
| H  | 8.16818178147653  | -2.08593313438639 | 0.75342614556486  |
| H  | 7.32240827662803  | -3.94476050105106 | 2.09862658650569  |
| H  | 5.63332300037137  | -4.05582814182348 | 2.57874731921394  |
| H  | 6.09072226511865  | -4.24603047936617 | 0.87923748809452  |
| H  | 0.58760813322342  | -1.97769535689468 | 7.06984265185797  |
| H  | 1.99207530566658  | -2.85912150075588 | 6.47570537454743  |
| H  | 2.21001772471816  | -1.35818069895427 | 7.38041969818545  |
| H  | 0.03634347672272  | 0.27808974973830  | 6.14429332858657  |
| H  | 1.67527756605626  | 0.91916971680208  | 6.19393151094859  |
| H  | 0.79466884486010  | 0.84632313258958  | 4.65757462003794  |
| H  | 3.42884087294785  | -1.90130398212195 | 4.65430652217371  |
| H  | 3.57698913138560  | -0.38382958486654 | 5.53025859318621  |
| H  | 2.98994014856226  | -0.37559664745088 | 3.86799958806374  |
| H  | -7.76646517253665 | -3.42246961917649 | -0.47276405229657 |
| H  | -7.47041120041609 | -3.16171782108295 | 1.24304379162762  |
| H  | -6.20380149853864 | -3.84931766862045 | 0.21474696389058  |
| H  | -5.01134707699562 | -2.39842477787295 | -1.46946174038172 |
| H  | -6.59083674597850 | -2.09461080636845 | -2.19838709709630 |
| H  | -5.54769390752146 | -0.74268540097593 | -1.75933805944474 |
| H  | -7.42355367657369 | 0.24540628674237  | -0.34133087570860 |
| H  | -8.15731915313702 | -0.72311000543711 | 0.93514203920415  |
| H  | -8.47287111259066 | -1.10680135798590 | -0.75842839189098 |
| H  | 1.59581250771087  | 4.93963061097707  | 4.39586757982374  |
| H  | 0.10071775320152  | 4.99145392487285  | 3.48210813769913  |
| H  | 0.48042137779871  | 3.57833007800205  | 4.47824209744934  |
| H  | 1.12149717291894  | 5.23220621135862  | 1.21491495222952  |
| H  | 2.56310635080017  | 5.59418988073210  | 2.17307957250982  |
| H  | 2.65102132657765  | 4.41653311796590  | 0.86151746328102  |
| H  | 2.63193652243030  | 2.22492589179611  | 3.89187481632492  |
| H  | 3.48448151096341  | 3.76488711855920  | 3.77463104485299  |
| H  | 3.53498783168058  | 2.63707900000114  | 2.42791513626472  |
| O  | 3.76659671633371  | 2.59841214565803  | 0.37017988561602  |
| C  | 4.40911009832871  | 0.76345440584492  | -1.76189523187635 |
| H  | 5.28853330594377  | 0.70497886177761  | -1.13262478028220 |
| H  | 4.75864391909546  | 1.04809920331502  | -2.77322195892756 |
| H  | 3.98574962448661  | -0.23071975633147 | -1.86384021477471 |
| Li | 3.35776508278453  | 2.58308092637393  | -2.04248394858710 |

**MeLi C3**

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -0.94369171628191 | 0.89582235360422  | 0.32774342055248  |
| C | 0.41395180876280  | 0.63575383894336  | 0.71508202861106  |
| C | 1.17350034311677  | 1.65919708395625  | 1.26896406416778  |
| C | 0.58138554853000  | 2.84117318511595  | 1.77723676112720  |
| C | -0.81265876433966 | 2.87264983445819  | 1.75487349200271  |
| C | -1.54303284242429 | 1.93064162626166  | 1.07866000846137  |
| S | 2.95370817650678  | 1.42533675891529  | 1.14359278381047  |
| C | 3.16931638318924  | -0.30945255065134 | 0.79863804370775  |
| C | 2.06357586848339  | -1.11568842507517 | 0.60331648101218  |
| O | 0.80602780375003  | -0.66143562831069 | 0.47313744855920  |
| C | 4.44640349092769  | -0.83172362595460 | 0.85728314258282  |
| C | 4.68579544169480  | -2.19610183941764 | 0.72291014063356  |
| C | 3.56338243221308  | -3.01714718302364 | 0.62519229424874  |
| C | 2.28844999281561  | -2.49566099635050 | 0.57322681910578  |
| C | 6.10601708100886  | -2.72868915144623 | 0.76611700370036  |
| C | 6.16381421857215  | -4.23965511064021 | 0.52935682885496  |
| S | 0.89184765333834  | -3.59502286994086 | 0.81389130006026  |
| O | 1.40428929184988  | -4.90120533493540 | 1.13682186283094  |
| S | -3.29122725144037 | 2.07892758789082  | 0.93724732950336  |
| O | -3.77476288471804 | 3.11742647306924  | 1.79956826202286  |
| C | 1.32326544710049  | 4.01596427905433  | 2.41106553318922  |
| C | 1.80149844707629  | 3.62456749926341  | 3.81708635945735  |
| O | 3.45065513731321  | 2.14427626021340  | 0.00512071290085  |
| O | -1.85421210314117 | -0.02837929589092 | -0.11312522790019 |
| C | -1.49165576116252 | -0.97999321557522 | -1.10435780914961 |
| C | 0.18353443886491  | -2.90023954135721 | 2.32138916251355  |
| C | 1.09405931500476  | -2.40508193657800 | 3.24061955004283  |
| C | 0.69740367774013  | -1.79356142648926 | 4.42302389975865  |
| C | -0.67186537038347 | -1.75942158202263 | 4.68587645999925  |
| C | -1.56958350351337 | -2.28747688872719 | 3.78993858357129  |
| C | -1.17976960409211 | -2.84575306357275 | 2.57670885139166  |
| C | 1.67693959011022  | -1.16968177245102 | 5.40020404888516  |
| C | 3.11881959948080  | -1.18741771764949 | 4.88426335167319  |
| S | -3.32582367971647 | -2.30275324178993 | 4.14265648468499  |
| O | -3.79770747885297 | -3.66069083201631 | 4.11305955818036  |
| O | -2.14422155755766 | -3.24595613957061 | 1.70863515248614  |
| C | -2.23406400426729 | -4.64886108547252 | 1.47424306367957  |
| O | -0.02174969078450 | -3.52405660035354 | -0.29235812193198 |
| C | -4.05867728226580 | -1.40608468279239 | 2.77576219397066  |
| C | -5.05490110817741 | -1.96856180106831 | 2.00440546887573  |
| C | -5.57727625784019 | -1.28901140090219 | 0.90875002180552  |
| C | -5.04798182272855 | -0.02981737620408 | 0.62738066387584  |
| C | -4.05002339182525 | 0.52160752395616  | 1.40196343265653  |
| C | -3.52903537897122 | -0.15861485495639 | 2.49366064984320  |
| C | -6.64446581374615 | -1.87309481392050 | 0.00022679006975  |
| C | -7.85051830945619 | -0.92472219419730 | -0.03589377809951 |
| O | -2.46774782055030 | 0.33630436083670  | 3.20108848552701  |
| C | -2.80423464414370 | 1.24390486014059  | 4.25248916890902  |
| O | -3.55229912753593 | -1.56355840490109 | 5.35776748653723  |
| O | -3.60488019639855 | 2.25021057722129  | -0.48146552632011 |
| C | 6.70222347081764  | -2.42171370163546 | 2.14720561438254  |
| C | 6.93091605173993  | -2.03304425953253 | -0.32518125730576 |
| C | 1.61148299336215  | -1.94286559540455 | 6.72459672025468  |
| C | 1.26860454725923  | 0.29326310114973  | 5.62131104969731  |
| C | -7.12028449811653 | -3.24771801850818 | 0.47581685335443  |
| C | -6.05067409397599 | -2.02125091741974 | -1.40856546882369 |
| C | 0.39924619735507  | 5.23758272061596  | 2.55695566987547  |
| C | 2.51546644060877  | 4.46710726121022  | 1.55890432956800  |
| H | 5.24365243337388  | -0.12735783501901 | 1.03221351444009  |
| H | 3.63650016945387  | -4.09232291514534 | 0.62252342414503  |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| H  | 2.14022027812990  | -2.50208636097350 | 3.00391902048978  |
| H  | -1.07590752627270 | -1.33368633437280 | 5.59054488400743  |
| H  | -5.38228077941705 | -2.95525279350586 | 2.28684721716657  |
| H  | -5.38568847255137 | 0.54839608470037  | -0.21802403547607 |
| H  | -1.37294591388910 | 3.64524962424144  | 2.25109662408481  |
| H  | -1.25212694616833 | -5.09644269025532 | 1.31130494139090  |
| H  | -2.73268950653708 | -5.12112563668999 | 2.32644436847764  |
| H  | -2.83552009142841 | -4.75921542859312 | 0.57500546196183  |
| H  | -3.39600122592950 | 2.07964267837369  | 3.87177421279901  |
| H  | -1.85033172472131 | 1.60644401618807  | 4.62930098163065  |
| H  | -3.34564454042304 | 0.71435218722606  | 5.04095678149923  |
| H  | -0.95798756693285 | -1.83154949943065 | -0.68474282560573 |
| H  | -0.88806837719906 | -0.51037299461189 | -1.88266488402772 |
| H  | -2.42893268603418 | -1.33156406137375 | -1.53471693580892 |
| H  | 6.11969075235524  | -2.90828027624733 | 2.92621877669908  |
| H  | 6.71106133754546  | -1.35383339147120 | 2.34455824173870  |
| H  | 7.72391063255058  | -2.79002700101780 | 2.20011610510896  |
| H  | 6.49760998413131  | -2.22502528721599 | -1.30388114187225 |
| H  | 6.96680476796220  | -0.95879978152670 | -0.17217777821196 |
| H  | 7.94978974139143  | -2.41299829206502 | -0.31867388358931 |
| H  | 7.20191142090397  | -4.56403936455944 | 0.52218125896209  |
| H  | 5.64913836335429  | -4.78300097937891 | 1.31748204415886  |
| H  | 5.72127559586819  | -4.50024783278163 | -0.42861925376227 |
| H  | 0.60678848064094  | -1.93052518999667 | 7.13725789647661  |
| H  | 1.90576254995696  | -2.97864249899307 | 6.57168118910216  |
| H  | 2.28684367364272  | -1.49526334332248 | 7.44969807999711  |
| H  | 0.29323564787305  | 0.36735263721410  | 6.09331441774653  |
| H  | 1.99628133949482  | 0.78816297731408  | 6.25970088922700  |
| H  | 1.23739698092184  | 0.81637105459536  | 4.66858656605286  |
| H  | 3.46759156559456  | -2.20298647093670 | 4.71250260330180  |
| H  | 3.76845766884678  | -0.73563444685591 | 5.63029857272945  |
| H  | 3.21814737127292  | -0.60879104973020 | 3.96788207072512  |
| H  | -7.89089957341053 | -3.61617376857619 | -0.19772846393022 |
| H  | -7.54576123835007 | -3.18955610388683 | 1.47421081235736  |
| H  | -6.30434429239443 | -3.96541134271088 | 0.47824201415496  |
| H  | -5.17450943042556 | -2.66515654415465 | -1.37954012751507 |
| H  | -6.78525226466077 | -2.46764191975137 | -2.07477690587094 |
| H  | -5.75795554416533 | -1.05827196523080 | -1.81875581089340 |
| H  | -7.57804868214420 | 0.05284995151409  | -0.42226926556571 |
| H  | -8.25797031497876 | -0.79640798522891 | 0.96410420800569  |
| H  | -8.62813807251869 | -1.33849862028458 | -0.67361349098526 |
| H  | 0.99022188218348  | 6.08734375903610  | 2.89124104101864  |
| H  | -0.05959323969624 | 5.49671357463930  | 1.60612009770351  |
| H  | -0.37815384677341 | 5.07618394078426  | 3.29911390029494  |
| H  | 2.24283025518906  | 4.51535989359716  | 0.50790040995958  |
| H  | 2.83961692736975  | 5.45575833374714  | 1.87697956301574  |
| H  | 3.35873139011724  | 3.79754588337039  | 1.66319346998983  |
| H  | 0.95905262307311  | 3.31155364753971  | 4.43098139660674  |
| H  | 2.27528231547794  | 4.48046970017385  | 4.29190223997291  |
| H  | 2.52605209348541  | 2.81893479344098  | 3.76378392413015  |
| O  | 3.62922923927296  | 1.62221314263713  | 2.40350930970627  |
| C  | -0.29817629798206 | 1.94488115689187  | -1.73395984947993 |
| H  | 0.06710620946008  | 2.82161821671100  | -1.20806261559509 |
| H  | -0.55252372031162 | 2.27041684833124  | -2.75481431746182 |
| H  | 0.54511129955402  | 1.27197441301979  | -1.83520645692103 |
| Li | -2.23193815529668 | 1.55960432150682  | -1.28312257613287 |

#### MeLi C4

|   |                   |                  |                   |
|---|-------------------|------------------|-------------------|
| C | -0.46640975046947 | 1.25040630633801 | -1.49665416812388 |
| C | 0.86058181452952  | 1.17932890036377 | -0.99175293655017 |
| C | 1.46697522327078  | 2.20609204978717 | -0.28473409310397 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | 0.71928006665432  | 3.35412588057272  | 0.04513079428597  |
| C | -0.61798602185445 | 3.32995337039034  | -0.32102644412560 |
| C | -1.21778382665164 | 2.32922327067623  | -1.07499357876614 |
| S | 3.25231979375322  | 1.98381142368383  | -0.00956572673674 |
| C | 3.59074999613024  | 0.27419388454024  | -0.36533824829445 |
| C | 2.58819262521012  | -0.49118534085909 | -0.88751935128613 |
| O | 1.38154946295823  | -0.03685187479781 | -1.27876109140951 |
| C | 4.84982961114199  | -0.26709363328081 | -0.12926450740173 |
| C | 5.11740480503909  | -1.60332371334856 | -0.45290294341711 |
| C | 4.07665159530433  | -2.38660482426070 | -0.93207234451670 |
| C | 2.80850294221996  | -1.84901390894826 | -1.19422799683086 |
| C | 6.51905503680468  | -2.14744516461998 | -0.23005612302666 |
| C | 6.65141265382398  | -3.61205365882841 | -0.65404115547656 |
| S | 1.36572776214208  | -2.88695087795983 | -1.02314629098667 |
| O | 1.76084906453242  | -4.25747702864119 | -0.87517080079474 |
| S | -3.01180237586986 | 2.52544682423969  | -1.19051434935280 |
| O | -3.38138147738481 | 3.60030127049940  | -0.31013089931095 |
| C | 1.23915860569000  | 4.55139066238636  | 0.83497089709463  |
| C | 1.39715215771140  | 4.14058141831256  | 2.30642789818669  |
| O | 3.95805939150452  | 2.76956716820888  | -0.98168665531941 |
| O | -0.73458799613110 | 0.23094878094901  | -2.34096605139163 |
| C | -2.01391466563038 | -0.00392095487584 | -2.89842947761064 |
| C | 0.70199098936756  | -2.29717446631943 | 0.55419056140775  |
| C | 1.62095129442030  | -1.96012218556855 | 1.53857292246820  |
| C | 1.23903318253167  | -1.39978851365425 | 2.75147278415325  |
| C | -0.12958264584796 | -1.23109791557608 | 2.96655319629950  |
| C | -1.04066901813279 | -1.61457037225198 | 2.01097741415093  |
| C | -0.65842368709756 | -2.13250278897089 | 0.77926069207762  |
| C | 2.23285646681905  | -0.98434377503544 | 3.82056681119441  |
| C | 3.67768615812515  | -1.30985774148259 | 3.43467920837138  |
| S | -2.79558763996253 | -1.61490492491370 | 2.37370222231112  |
| O | -3.23444445938710 | -2.98435357979087 | 2.40562815391835  |
| O | -1.63484429805058 | -2.39883955360488 | -0.13461865064119 |
| C | -1.86339087196012 | -3.78182937364793 | -0.39862850050299 |
| O | 0.35930868269875  | -2.62894789439675 | -2.02788464931831 |
| C | -3.62397808529949 | -0.80337906478282 | 1.00430839708543  |
| C | -4.73180495903969 | -1.37311306487599 | 0.41166941960366  |
| C | -5.37309077895991 | -0.74499821614627 | -0.65252870631554 |
| C | -4.82804048518620 | 0.45721127275372  | -1.10229155371042 |
| C | -3.70726145388864 | 1.00823178494566  | -0.51474925790243 |
| C | -3.09212715865184 | 0.39876761734863  | 0.56965145753451  |
| C | -6.59220401999891 | -1.32358344336013 | -1.34723895800214 |
| C | -7.73858703558495 | -0.30613618974718 | -1.26936678074161 |
| O | -1.95755926645017 | 0.90302348691668  | 1.14819695243728  |
| C | -2.19842720256963 | 1.85200753759537  | 2.19056699713599  |
| O | -3.01333903744422 | -0.82913680947955 | 3.56048535404103  |
| O | -3.44618281903654 | 2.63807245676474  | -2.56009796052762 |
| C | 6.87432997704135  | -2.03837558930266 | 1.25918955200337  |
| C | 7.50118298136678  | -1.31327477436474 | -1.06446440129627 |
| C | 1.89449559844704  | -1.72357855401916 | 5.12368300829677  |
| C | 2.12170893563337  | 0.53221465621010  | 4.03083051292743  |
| C | -7.05713587083323 | -2.63274007487227 | -0.70555950214443 |
| C | -6.23358810551468 | -1.59629081147609 | -2.81541145910557 |
| C | 0.26004436320374  | 5.73483018081857  | 0.77944669788651  |
| C | 2.58083286133736  | 5.05207817870314  | 0.28887331093752  |
| H | 5.59424331124495  | 0.38086078620762  | 0.30003786880498  |
| H | 4.20157392545066  | -3.43718722639526 | -1.13032249584419 |
| H | 2.66018252017706  | -2.15218957028704 | 1.32926566441344  |
| H | -0.52260871035377 | -0.82537222798287 | 3.88539807217357  |
| H | -5.05886024488304 | -2.31952984068029 | 0.80929495866463  |
| H | -5.24478168582018 | 0.98910847538952  | -1.94329063401489 |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| H  | -1.28085005918635 | 4.12385665661628  | -0.02728429538095 |
| H  | -0.93417934047602 | -4.30165745655802 | -0.63661806127237 |
| H  | -2.34809496849547 | -4.23919769677885 | 0.46921971938228  |
| H  | -2.52523135797931 | -3.80870626633393 | -1.26065193658493 |
| H  | -2.78559438410806 | 2.69382237675427  | 1.81536483459797  |
| H  | -1.21122240370318 | 2.18998249959874  | 2.49725720860348  |
| H  | -2.70879606380288 | 1.36859958406079  | 3.02757275641858  |
| H  | -1.82842494209428 | -0.60224114118133 | -3.79021641751953 |
| H  | -2.52181877471388 | 0.92192222052122  | -3.17046902645492 |
| H  | -2.62245724680134 | -0.58775741526316 | -2.20571214522273 |
| H  | 6.18409782152520  | -2.62975086490965 | 1.85626775183253  |
| H  | 6.83054299159426  | -1.00975463952743 | 1.60420191192892  |
| H  | 7.88159015533003  | -2.41223064903066 | 1.42716819271772  |
| H  | 7.23232772005971  | -1.36239408581907 | -2.11678452585621 |
| H  | 7.49533591009118  | -0.27120096457560 | -0.75969676549432 |
| H  | 8.51109424635033  | -1.69936151756337 | -0.94655859379703 |
| H  | 7.67715113497407  | -3.94000907906011 | -0.50025009891168 |
| H  | 6.00180141758892  | -4.25386832485278 | -0.06433185639909 |
| H  | 6.41203446706094  | -3.73443463739828 | -1.70692319658876 |
| H  | 0.91066006333702  | -1.45037091306207 | 5.49280147859070  |
| H  | 1.91481009912842  | -2.79928796959488 | 4.96416900161423  |
| H  | 2.62560978151878  | -1.47522345211825 | 5.88923984436009  |
| H  | 1.09761025452270  | 0.83034119908316  | 4.23722581391794  |
| H  | 2.74185907504528  | 0.83154906106946  | 4.87229366781827  |
| H  | 2.47269912571139  | 1.06225678486919  | 3.14814284221469  |
| H  | 3.81057381521738  | -2.37738627467462 | 3.27436378321622  |
| H  | 4.33944764462757  | -1.00536047850660 | 4.24203170233852  |
| H  | 3.97452957231528  | -0.76821857648700 | 2.53957650317979  |
| H  | -7.93860622106935 | -2.99693689753658 | -1.22825443454778 |
| H  | -7.32260339335752 | -2.48376254718611 | 0.33777452832527  |
| H  | -6.28790386828872 | -3.39766890223513 | -0.77161914577011 |
| H  | -5.40163546151438 | -2.29398897046506 | -2.87784863796376 |
| H  | -7.08745171103049 | -2.03197601351740 | -3.32836968779813 |
| H  | -5.95425837815522 | -0.68295268050752 | -3.33240466680951 |
| H  | -7.47865502810215 | 0.62475156772401  | -1.76423529147122 |
| H  | -7.97841049370844 | -0.08774223446482 | -0.23149291288344 |
| H  | -8.62576229036055 | -0.71150824834511 | -1.74973702578062 |
| H  | 0.71880424962892  | 6.59095751158162  | 1.26863130783778  |
| H  | 0.03837490445289  | 6.01300908266164  | -0.24762068833072 |
| H  | -0.66820078862810 | 5.52360264488555  | 1.30374048104661  |
| H  | 2.55114347411541  | 5.13693873713524  | -0.79430952465902 |
| H  | 2.80039446635660  | 6.03248139968805  | 0.70541203063960  |
| H  | 3.39405738015352  | 4.39115607217001  | 0.55771952540561  |
| H  | 0.45094944301074  | 3.78396532252463  | 2.70841954048904  |
| H  | 1.71587340722678  | 5.00093525625861  | 2.88951456727507  |
| H  | 2.14538145318510  | 3.36245412023567  | 2.40887488765735  |
| O  | 3.58213622303995  | 2.18569280441425  | 1.38016625597867  |
| C  | 2.61295336499325  | -1.40425182497730 | -3.86014280553216 |
| H  | 3.09183253905147  | -2.37424469758773 | -3.87201603967822 |
| H  | 3.37239849570803  | -0.65785293611646 | -3.65341287022234 |
| H  | 2.22900604325707  | -1.22389478180658 | -4.86571397692796 |
| Li | 0.85278837305696  | -1.10439632502324 | -2.76420296549972 |

#### MeLi C5

|   |                   |                  |                  |
|---|-------------------|------------------|------------------|
| C | -1.00568916908885 | 0.88079079387765 | 0.23155080053503 |
| C | 0.26288883845918  | 0.60595779077536 | 0.72028854634923 |
| C | 0.98480462149199  | 1.60736653935476 | 1.41698389492331 |
| C | 0.36973169181139  | 2.82896765686643 | 1.78245224584488 |
| C | -0.93324709875441 | 3.02060422030502 | 1.37305002986754 |
| C | -1.55856093724191 | 2.15246086616599 | 0.47410175962702 |
| S | 2.75779797492907  | 1.38160298633826 | 1.40525536091810 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | 3.01971293343083  | -0.31977525286792 | 0.93834879774374  |
| C | 1.93547297873736  | -1.14356674176190 | 0.70878285869587  |
| O | 0.66884867748348  | -0.71200732923449 | 0.56975931974965  |
| C | 4.30927244207994  | -0.81138527799885 | 0.98078769975762  |
| C | 4.58262944336860  | -2.16316312672256 | 0.79329860473634  |
| C | 3.48081986942573  | -3.00592431277806 | 0.66431251694130  |
| C | 2.19209902626441  | -2.51527837650123 | 0.62605604351005  |
| C | 6.01487334881839  | -2.66354077911800 | 0.82437410584210  |
| C | 6.10992342294499  | -4.16170207556283 | 0.52620530449259  |
| S | 0.83080956339434  | -3.65909447076768 | 0.87830170224097  |
| O | 1.38688345204373  | -4.95641956561909 | 1.16040893165388  |
| S | -3.34850913602741 | 2.17267844650706  | 0.43427208487852  |
| O | -3.84426605634638 | 3.25450269374044  | 1.23347143559396  |
| C | 1.02048200259267  | 3.88943278102840  | 2.67071792928250  |
| C | 1.33814352525852  | 3.28227433583704  | 4.04362948544202  |
| O | 3.32594930366798  | 2.19545965185695  | 0.36537102353102  |
| O | -1.75692065811623 | 0.19499754824881  | -0.69190432720680 |
| C | -1.70954227394151 | -1.21910365646535 | -0.79387915377082 |
| C | 0.20413813035938  | -2.96838461192495 | 2.42420186574364  |
| C | 1.18250826692220  | -2.61177888564321 | 3.33807768300844  |
| C | 0.88892626226550  | -1.93615851448275 | 4.51526316851822  |
| C | -0.45337544968980 | -1.62802349483241 | 4.74764504178198  |
| C | -1.42751763294490 | -2.03539582189898 | 3.86729758570870  |
| C | -1.13184408395346 | -2.72067898471571 | 2.69421118813861  |
| C | 1.95371842132156  | -1.54069776313199 | 5.52157961512574  |
| C | 3.35085188552098  | -2.01439083635431 | 5.11126767116333  |
| S | -3.17172765163581 | -1.83399974885096 | 4.23192689903362  |
| O | -3.72972828036974 | -3.14966485844332 | 4.39948082718104  |
| O | -2.15915472990726 | -3.06309683389054 | 1.86693600468923  |
| C | -2.38227166637156 | -4.46146484064071 | 1.70932134095476  |
| O | -0.13263135004388 | -3.59020971764875 | -0.18350110453979 |
| C | -3.90084109854583 | -1.10624881722268 | 2.76276792763503  |
| C | -4.92133534586925 | -1.76743160699410 | 2.11031589945350  |
| C | -5.47052822655230 | -1.24998363967148 | 0.94325934909526  |
| C | -4.95233914825801 | -0.04116570602269 | 0.48125151165291  |
| C | -3.93320075515607 | 0.61718447328211  | 1.13859608430579  |
| C | -3.37501167539069 | 0.08846104191015  | 2.29711946406634  |
| C | -6.56431345267390 | -1.94811425814579 | 0.15592007949188  |
| C | -7.77768288206593 | -1.01492633802120 | 0.04589179057588  |
| O | -2.30144143130436 | 0.66330163065160  | 2.92165772330912  |
| C | -2.63562234729225 | 1.69515511221801  | 3.85369398459037  |
| O | -3.31201398626826 | -0.92292014056412 | 5.33671484948577  |
| O | -3.82477889533443 | 2.13752050252928  | -0.94016581494335 |
| C | 6.59489581958413  | -2.40020837131355 | 2.22138041986831  |
| C | 6.82980213404404  | -1.90418748975875 | -0.23130308103490 |
| C | 1.60022557452772  | -2.16606290030292 | 6.87891085697635  |
| C | 1.98393919557335  | -0.01161903200979 | 5.63498086706502  |
| C | -7.01040976030433 | -3.25302876624133 | 0.81939148039804  |
| C | -6.02225857323230 | -2.27001314820521 | -1.24453916943830 |
| C | 0.08676829215732  | 5.08690238793212  | 2.90883469590149  |
| C | 2.29792207367093  | 4.44752230675107  | 2.03099828924026  |
| H | 5.08747480947965  | -0.09458032291627 | 1.18821125335467  |
| H | 3.58038954231510  | -4.07835261340109 | 0.62509597174271  |
| H | 2.19705300326445  | -2.88142229657614 | 3.09801479433365  |
| H | -0.77729324380448 | -1.09205931873624 | 5.62589376073264  |
| H | -5.24593898910969 | -2.69727923496952 | 2.54672840697991  |
| H | -5.32338404111213 | 0.42165872696987  | -0.41922871854485 |
| H | -1.50117586597379 | 3.88817831424453  | 1.65300588321433  |
| H | -1.45698248211971 | -4.99198203550931 | 1.47781249182226  |
| H | -2.83530476257246 | -4.85814093699740 | 2.62286714516366  |
| H | -3.07171663394920 | -4.55466691297084 | 0.87358543853802  |

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| H  | -3.24694005841812 | 2.46543922684103  | 3.37788833125607  |
| H  | -1.68208036758608 | 2.11563190070482  | 4.16357457871299  |
| H  | -3.15540151549163 | 1.26401073698032  | 4.71321224723540  |
| H  | -1.90610285784489 | -1.69417520050350 | 0.16608056168837  |
| H  | -0.75615624493504 | -1.57763117108470 | -1.17709591135660 |
| H  | -2.49959669707326 | -1.48863998926719 | -1.49291219311695 |
| H  | 6.01899160530001  | -2.93119069551057 | 2.97607212325201  |
| H  | 6.57891528215582  | -1.34116974227209 | 2.46172063240623  |
| H  | 7.62440012315122  | -2.74714670372860 | 2.26641831820416  |
| H  | 6.40917249537647  | -2.06794130706037 | -1.22065405681903 |
| H  | 6.83700717342257  | -0.83631173576273 | -0.03555136235477 |
| H  | 7.85800243279483  | -2.25812179573703 | -0.23106018538246 |
| H  | 7.15558686192365  | -4.46033807028185 | 0.50980385816971  |
| H  | 5.60652801295553  | -4.74924104631342 | 1.28951625012111  |
| H  | 5.67660577149644  | -4.39348567960856 | -0.44335846383412 |
| H  | 0.65023053911097  | -1.79462041557223 | 7.25092711836752  |
| H  | 1.53503161640901  | -3.24824956233808 | 6.79126127651760  |
| H  | 2.36959192983751  | -1.92510523153487 | 7.60851989455316  |
| H  | 1.00163068361677  | 0.38971740849320  | 5.86548067120598  |
| H  | 2.66979253882254  | 0.28578417654876  | 6.42450096492277  |
| H  | 2.33150356504905  | 0.42469853153617  | 4.70174894406928  |
| H  | 3.38800676277721  | -3.09685932817820 | 5.01153813886327  |
| H  | 4.06457116652948  | -1.72190893036012 | 5.87790844858659  |
| H  | 3.65959873817254  | -1.55084683123277 | 4.17666172453789  |
| H  | -7.79598822809963 | -3.71141775754026 | 0.22277053016162  |
| H  | -7.40758708053150 | -3.06943304257785 | 1.81423034308037  |
| H  | -6.18660626901846 | -3.95834953029410 | 0.89066091730637  |
| H  | -5.13930629857560 | -2.90110413058346 | -1.17013819164566 |
| H  | -6.77732109214201 | -2.79960160196591 | -1.82077791956517 |
| H  | -5.75541045835980 | -1.36476493717500 | -1.78274382283212 |
| H  | -7.52489478611288 | -0.09226824519643 | -0.46796279047225 |
| H  | -8.15047553615654 | -0.76430748401788 | 1.03621170973661  |
| H  | -8.57428689204555 | -1.50670695605322 | -0.50742146221997 |
| H  | 0.60312359591887  | 5.80919058162726  | 3.53762993726745  |
| H  | -0.16748503745384 | 5.58100451008414  | 1.97504540291344  |
| H  | -0.82393996382855 | 4.79455541861234  | 3.42566479659696  |
| H  | 2.12506009965005  | 4.69322966340750  | 0.98633532202903  |
| H  | 2.60212767922277  | 5.35141114900532  | 2.55441137031871  |
| H  | 3.11609296069794  | 3.74156349915112  | 2.08471673163621  |
| H  | 0.44831993821291  | 2.83167312796674  | 4.47878317734155  |
| H  | 1.69251883247998  | 4.06103378552162  | 4.71469755332171  |
| H  | 2.11137322084802  | 2.52942674133429  | 3.96009620660327  |
| O  | 3.36200400159096  | 1.47048597425191  | 2.71420970034524  |
| C  | -1.01572527704296 | 3.43260836239805  | -1.57257313205225 |
| H  | 0.01683477882601  | 3.30337457859619  | -1.27604558541147 |
| H  | -1.42047033123206 | 4.29617931763909  | -1.06417695143896 |
| H  | -1.03813677120162 | 3.64419505336858  | -2.64612860638819 |
| Li | -2.23417677905502 | 1.80503510466827  | -1.66455808928766 |

# MeLi C6

|   |                   |                   |                  |
|---|-------------------|-------------------|------------------|
| C | -1.56889909601686 | -0.22160200295644 | 2.76486348258550 |
| C | -0.17861894299349 | -0.23856529854668 | 2.43237070325884 |
| C | 0.66094846135761  | 0.77879618410768  | 2.98586710587788 |
| C | 0.09850318964109  | 1.96850228786910  | 3.48966854717942 |
| C | -1.28665514409469 | 2.03056492733328  | 3.59025251265019 |
| C | -2.08601615388300 | 0.92755386128071  | 3.27636555924513 |
| S | 2.38686558522477  | 0.59128425394359  | 2.53181613059317 |
| C | 2.59290849804624  | -1.16802273326808 | 2.28915507877984 |
| C | 1.47663866408656  | -1.97739851699552 | 2.23133964109744 |
| O | 0.21087406928562  | -1.54345810904387 | 2.20691735796198 |
| C | 3.86280868815471  | -1.71157708026620 | 2.28868986725284 |

|   |                   |                   |                  |
|---|-------------------|-------------------|------------------|
| C | 4.07206196359728  | -3.08768033451435 | 2.23134707722153 |
| C | 2.94000775808936  | -3.90183792279139 | 2.25022766621929 |
| C | 1.67364190775006  | -3.35849643999125 | 2.25746299938362 |
| C | 5.48767894517610  | -3.63655697595187 | 2.20730015014362 |
| C | 5.51561594175543  | -5.16192116469940 | 2.08453573240474 |
| S | 0.21954569296319  | -4.39507214007075 | 2.46778412595796 |
| O | 0.66954912470102  | -5.72164586032239 | 2.81034189464883 |
| S | -3.79375795205698 | 1.19428175953515  | 2.90583949630250 |
| O | -4.32575477036020 | 2.32233000564101  | 3.61103273017556 |
| C | 0.90513822649793  | 3.17540569371022  | 3.96893666453974 |
| C | 1.63519737486636  | 2.81347700555249  | 5.27058637177036 |
| O | 2.67678084739485  | 1.24549965011432  | 1.28387403033249 |
| O | -2.43167681384096 | -1.24523447580845 | 2.51030010931080 |
| C | -2.48741390129525 | -1.85827656080915 | 1.22611939503413 |
| C | -0.57452447827220 | -3.69818839514121 | 3.93932642212456 |
| C | 0.27833590482469  | -3.08145395791381 | 4.83859032991933 |
| C | -0.17985645029688 | -2.43926459200130 | 5.98150587378052 |
| C | -1.54662538577164 | -2.51792746151812 | 6.24003620828196 |
| C | -2.38846310355266 | -3.17180740560804 | 5.37310596081943 |
| C | -1.94426026165300 | -3.74769950420179 | 4.18385998219819 |
| C | 0.72899471604435  | -1.65984139141265 | 6.91408444248056 |
| C | 2.16418099477430  | -1.55475410869654 | 6.38952927621615 |
| S | -4.13749178877785 | -3.27886912302549 | 5.75875384640849 |
| O | -4.59379240370197 | -4.63351975943823 | 5.61223119164638 |
| O | -2.87170013836632 | -4.25428338652758 | 3.33919570943589 |
| C | -2.78347574893724 | -5.64184051274964 | 3.02654547242633 |
| O | -0.61983220317777 | -4.28621102917830 | 1.30710479922623 |
| C | -4.88720600907597 | -2.27163326416281 | 4.47713226800630 |
| C | -5.75067151684856 | -2.81510699124075 | 3.54529456543127 |
| C | -6.17316934751527 | -2.08202735804144 | 2.44122419829073 |
| C | -5.63222485610837 | -0.80470196193723 | 2.27347159565610 |
| C | -4.77349567006331 | -0.27390681551209 | 3.20944521751158 |
| C | -4.40719873350081 | -0.98211993956109 | 4.34682381142242 |
| C | -7.11854322524268 | -2.63841450753831 | 1.39072496723942 |
| C | -8.31278691774312 | -1.68585994011494 | 1.23951863679569 |
| O | -3.49551648458399 | -0.44386318708476 | 5.21141025413340 |
| C | -4.06313250548861 | 0.32997092152910  | 6.26871151851855 |
| O | -4.35968315515005 | -2.65813670113181 | 7.03942238148152 |
| O | -3.71621881770721 | 1.34857147708380  | 1.44619811841908 |
| C | 6.19380004210220  | -3.23465441976885 | 3.50983032301335 |
| C | 6.23065381220521  | -3.03875762138180 | 1.00472560544189 |
| C | 0.74983047266947  | -2.35372261336191 | 8.28301064456650 |
| C | 0.16276996578921  | -0.23953199061216 | 7.05282810337477 |
| C | -7.64822911382197 | -4.02441516745701 | 1.76605788248818 |
| C | -6.36395022989808 | -2.74740255791305 | 0.05770155303179 |
| C | 0.00606820174291  | 4.38437872409746  | 4.27607416812324 |
| C | 1.90590988482142  | 3.63518339177093  | 2.90210175141851 |
| H | 4.68280660376571  | -1.01491797679602 | 2.35511523467070 |
| H | 3.00191321900363  | -4.97694621617857 | 2.28665295178934 |
| H | 1.33194426278889  | -3.09957423713755 | 4.61474842850235 |
| H | -1.99320075481079 | -2.08806897253416 | 7.12213982040822 |
| H | -6.04653393358183 | -3.83815510818257 | 3.70787695741291 |
| H | -5.83892072484125 | -0.21447931190553 | 1.39472036790266 |
| H | -1.79913797350198 | 2.88760014990482  | 3.98770655110907 |
| H | -1.75172058813041 | -5.97897189688192 | 2.92730944413743 |
| H | -3.29255155871197 | -6.20849412259008 | 3.81255764392342 |
| H | -3.29730812114152 | -5.77210187233080 | 2.07645318339457 |
| H | -4.68947921710845 | 1.13228692633548  | 5.86942200358220 |
| H | -3.21498435596673 | 0.75795193822851  | 6.79858035375458 |
| H | -4.63676237560762 | -0.31583660850079 | 6.93871263284008 |
| H | -1.57697444420089 | -2.40329404892090 | 0.98537442445026 |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| H  | -2.71363796971203 | -1.11529035845010 | 0.45290401136908  |
| H  | -3.30710243229399 | -2.56873226287012 | 1.31205686331039  |
| H  | 5.67009656980312  | -3.65235361750337 | 4.36669180543915  |
| H  | 6.22774506195012  | -2.15524192021306 | 3.62373214472995  |
| H  | 7.21326784628729  | -3.61303373813570 | 3.51105777033223  |
| H  | 5.71845235700667  | -3.29617978864324 | 0.08070148291690  |
| H  | 6.28988429449259  | -1.95682074528676 | 1.07248517615125  |
| H  | 7.24273096600871  | -3.43417731552050 | 0.95987679785133  |
| H  | 6.54801916058019  | -5.50054173684587 | 2.03386785525208  |
| H  | 5.04991882630264  | -5.63549622112904 | 2.94485868754052  |
| H  | 5.00799128920681  | -5.48910036247410 | 1.18085293055741  |
| H  | -0.25100247496995 | -2.43086505903972 | 8.69819010567981  |
| H  | 1.15970154722884  | -3.35682529202484 | 8.19106822774743  |
| H  | 1.36887004445429  | -1.78995331468259 | 8.97681975798994  |
| H  | -0.79904882951319 | -0.24609094855229 | 7.55702659926649  |
| H  | 0.84865273954263  | 0.37590611660513  | 7.63025928013322  |
| H  | 0.03478413099039  | 0.20805477298086  | 6.06923302224573  |
| H  | 2.62465681849235  | -2.53524176742218 | 6.29405326374749  |
| H  | 2.76013424952236  | -0.97688342001638 | 7.09213570218512  |
| H  | 2.20247538749462  | -1.04445782575671 | 5.42897172363947  |
| H  | -8.34741505960613 | -4.36189580315430 | 1.00419310955722  |
| H  | -8.17298858300888 | -3.99701177063830 | 2.71749012882555  |
| H  | -6.84156208817650 | -4.74990337564603 | 1.82568145209244  |
| H  | -5.50930793109047 | -3.41187637141307 | 0.16119383641599  |
| H  | -7.02321238867386 | -3.15144302194705 | -0.70702796572162 |
| H  | -6.00551977562128 | -1.77825562630678 | -0.27733405823777 |
| H  | -7.99764520489235 | -0.69933433691664 | 0.91300747479363  |
| H  | -8.83471046812224 | -1.58295915249429 | 2.18800163166247  |
| H  | -9.01039233803316 | -2.08033542217566 | 0.50454080548147  |
| H  | 0.63904948234222  | 5.22137618354053  | 4.56259075586191  |
| H  | -0.56906268899866 | 4.68238783970081  | 3.40234632305188  |
| H  | -0.66718724441947 | 4.19176305090839  | 5.10754256625505  |
| H  | 1.43710680058137  | 3.65708437108316  | 1.92046840987033  |
| H  | 2.25995560626543  | 4.63589413555783  | 3.13997851518961  |
| H  | 2.76817503522280  | 2.98417586689672  | 2.85540062090369  |
| H  | 0.91829233928909  | 2.53642877558713  | 6.04011513413918  |
| H  | 2.20063973181549  | 3.67454052720250  | 5.61864900847615  |
| H  | 2.32568071490616  | 1.99333531029944  | 5.11068295523595  |
| O  | 3.27002826200377  | 0.88919113365851  | 3.63512704319658  |
| C  | -0.24462312693912 | 0.36022867528505  | 0.17702246369537  |
| H  | -0.11713832824373 | -0.66959026630086 | -0.13020328226675 |
| H  | 0.73311684492263  | 0.81745326959754  | 0.23317320343721  |
| H  | -0.78905599148647 | 0.86685450030132  | -0.65098955548135 |
| Li | -1.98021614464591 | 1.14621464654307  | 1.07629066835055  |

# PhLi C1

|   |                   |                   |                  |
|---|-------------------|-------------------|------------------|
| C | -1.27752530676090 | 0.63098324899428  | 1.30606781524060 |
| C | 0.13001392263042  | 0.57324255118614  | 1.31865298617925 |
| C | 0.86369181818050  | 1.60102315604581  | 1.93248139323988 |
| C | 0.24858118655338  | 2.56778829631518  | 2.74225601874662 |
| C | -1.14271813644748 | 2.52755850126703  | 2.80618555838973 |
| C | -1.86942273664255 | 1.63419836461521  | 2.05560038529547 |
| S | 2.48826013142518  | 1.60301289145600  | 1.14990935784607 |
| C | 2.96492026293778  | -0.06648553886116 | 1.35311821523767 |
| C | 1.96420187848052  | -0.93358352060333 | 0.89942484160624 |
| O | 0.68799262104327  | -0.47613250034233 | 0.63328963389512 |
| C | 4.20160770516080  | -0.52209657070184 | 1.76014301460301 |
| C | 4.46625322341196  | -1.88869779132251 | 1.83603504009860 |
| C | 3.38958063659499  | -2.75519230101757 | 1.59615986007397 |
| C | 2.16096470529994  | -2.29882509473514 | 1.19379079732471 |
| C | 5.81288197228898  | -2.45104340755183 | 2.24978649358016 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | 6.20285804513639  | -3.58469590439992 | 1.29235047992978  |
| S | 0.75806253703833  | -3.39399430379596 | 1.20150304959045  |
| O | 1.22491262773698  | -4.73843874295581 | 1.41645316302540  |
| S | -3.64445254935289 | 1.85514825979268  | 1.86565618688487  |
| O | -4.10143981537474 | 2.70836856287553  | 2.93242449004485  |
| C | 1.00604825752731  | 3.64846429244673  | 3.50191104330691  |
| C | 2.15946719462659  | 3.02802908568916  | 4.30210522988331  |
| O | 2.12934429098667  | 1.81274201266658  | -0.24311160953909 |
| O | -2.12392080062014 | -0.18371523227659 | 0.64800659586769  |
| C | -1.79064027595831 | -0.70752568503849 | -0.63402484645988 |
| C | -0.08128465125725 | -2.88619810726273 | 2.72501575833713  |
| C | 0.70488502945392  | -2.34429420911301 | 3.72791590520435  |
| C | 0.18139989593284  | -1.93457942770203 | 4.94808372265817  |
| C | -1.17924882447471 | -2.14826220819643 | 5.15469434994124  |
| C | -1.95678823124168 | -2.69671771257349 | 4.16371517203429  |
| C | -1.44839300678592 | -3.05446930242004 | 2.91853603519177  |
| C | 1.02064837896862  | -1.27071912356705 | 6.02506750161150  |
| C | 2.44139681640272  | -0.95779505265045 | 5.54452504173980  |
| S | -3.71953780500980 | -2.91973420790425 | 4.40468317714704  |
| O | -4.08316932041544 | -4.28264747180424 | 4.13133010484350  |
| O | -2.31802332042794 | -3.46981723371486 | 1.96716471440195  |
| C | -2.21256937824639 | -4.82690196693692 | 1.54194442379490  |
| O | -0.09433973744504 | -3.16933773004801 | 0.06829074201894  |
| C | -4.41690428543595 | -1.85456117098247 | 3.14429571588177  |
| C | -5.30016668384487 | -2.34791099784484 | 2.20516944897967  |
| C | -5.75586402905925 | -1.55088622029607 | 1.15984157471295  |
| C | -5.26673962372814 | -0.24611507224260 | 1.09181727806261  |
| C | -4.38459688667549 | 0.23272584182476  | 2.03407430085603  |
| C | -3.93897636817916 | -0.55614938395695 | 3.08260250152681  |
| C | -6.70423137972271 | -2.05450116339306 | 0.08616761087945  |
| C | -7.94849638887482 | -1.15651925895148 | 0.05494071134557  |
| O | -2.99322463717766 | -0.08599002425203 | 3.95486518389019  |
| C | -3.52084682637084 | 0.57875982725727  | 5.10682648346907  |
| O | -4.06187112345412 | -2.40943157175076 | 5.70793716001814  |
| O | -3.87275625776968 | 2.32042617945359  | 0.52483619083193  |
| C | 5.70052351722815  | -2.99497703224681 | 3.68197655696468  |
| C | 6.91082170068811  | -1.38496633215269 | 2.20621413196272  |
| C | 1.10325388265344  | -2.20852928498894 | 7.23684767150113  |
| C | 0.33894162981577  | 0.04515621373457  | 6.42943665537626  |
| C | -7.15053648400586 | -3.49682320620032 | 0.33633194563715  |
| C | -5.97975738415409 | -1.99344750782285 | -1.26640273913432 |
| C | 0.10097401759006  | 4.37501107261657  | 4.50745748812888  |
| C | 1.52456544156331  | 4.69130064935693  | 2.50188626934311  |
| H | 4.93740622696532  | 0.218756670715598 | 2.02766322232279  |
| H | 3.47567487377983  | -3.81798481011959 | 1.75764367737629  |
| H | 1.75879785774830  | -2.24429583104513 | 3.52980817559509  |
| H | -1.67207778699049 | -1.89634550531792 | 6.07990895972271  |
| H | -5.59039354979666 | -3.37947758119737 | 2.31587084648479  |
| H | -5.53369211071752 | 0.42557856671583  | 0.29106111992889  |
| H | -1.71153538345137 | 3.23693013307406  | 3.38094623792892  |
| H | -1.17463967795016 | -5.13757452959501 | 1.41790097751261  |
| H | -2.71672876117511 | -5.46449256548962 | 2.27481950120109  |
| H | -2.72383486349188 | -4.87677671775970 | 0.58341729162277  |
| H | -4.12978288113842 | 1.43525987544348  | 4.80858691051696  |
| H | -2.64969222864283 | 0.92149708665657  | 5.66055679868562  |
| H | -4.09993295279989 | -0.12180323830591 | 5.71337029350141  |
| H | -1.22328788811269 | -1.63489911740068 | -0.55046139886385 |
| H | -1.24100547802416 | 0.02604209335792  | -1.23407980196700 |
| H | -2.75254011597552 | -0.90906704378936 | -1.10288849412531 |
| H | 4.93650697767181  | -3.76554828947872 | 3.74532737452016  |
| H | 5.44423045732569  | -2.19395460228731 | 4.37259073682323  |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| H  | 6.64955058189996  | -3.42603440309639 | 3.99155788421184  |
| H  | 6.95593760432600  | -0.92483086047521 | 1.22262489461292  |
| H  | 6.74718469730921  | -0.61306812315918 | 2.95395323499575  |
| H  | 7.87381509465537  | -1.84666455806530 | 2.41185577812711  |
| H  | 7.21204358357121  | -3.92537591316393 | 1.51216936594025  |
| H  | 5.53284665716642  | -4.43387819197629 | 1.38398450698095  |
| H  | 6.16669419028986  | -3.23332891076058 | 0.26465111070389  |
| H  | 0.11263466393696  | -2.44310403038598 | 7.61539919381184  |
| H  | 1.59255630624259  | -3.13943264136440 | 6.96053509744413  |
| H  | 1.67576863060532  | -1.73968636333455 | 8.03373002373298  |
| H  | -0.59713300489084 | -0.14113688216311 | 6.94699377495871  |
| H  | 0.98580773795776  | 0.61128895251752  | 7.09636868982411  |
| H  | 0.12892563326368  | 0.64585082764815  | 5.54596576379103  |
| H  | 2.98622543394772  | -1.86940388884824 | 5.31216371497909  |
| H  | 2.98263261340990  | -0.43870818511505 | 6.33260980402604  |
| H  | 2.42871993524000  | -0.31780331031351 | 4.66382902134687  |
| H  | -7.83926189625701 | -3.80277011289125 | -0.44816388535781 |
| H  | -7.66478126781113 | -3.58670963008669 | 1.28965438682297  |
| H  | -6.30275807043656 | -4.17643166249667 | 0.32369860658879  |
| H  | -5.07394428191512 | -2.59451518507969 | -1.23332764520937 |
| H  | -6.62518020009213 | -2.38234681023938 | -2.05065740796055 |
| H  | -5.70796832282868 | -0.97347772015303 | -1.52236769603306 |
| H  | -7.68972661679690 | -0.12677588406975 | -0.17234883840412 |
| H  | -8.45283128579043 | -1.17861622071824 | 1.01812647688103  |
| H  | -8.64168724937169 | -1.50998601630401 | -0.70480640063755 |
| H  | 0.70809988467068  | 5.06493781430785  | 5.08914860409300  |
| H  | -0.66869774879848 | 4.95732463751448  | 4.00892734025821  |
| H  | -0.36691616285234 | 3.67571580787620  | 5.19617956973989  |
| H  | 0.69880338061213  | 5.09036491476244  | 1.91678100097463  |
| H  | 1.99600331181714  | 5.51016851383989  | 3.03981551251770  |
| H  | 2.25647091517292  | 4.26166370454807  | 1.82777909378393  |
| H  | 1.78207349893350  | 2.25900898496153  | 4.97194771508539  |
| H  | 2.63914919099075  | 3.79789875057643  | 4.90156909944471  |
| H  | 2.91081568232018  | 2.59882960063659  | 3.65131138715916  |
| O  | 3.49700680773332  | 2.47561961013354  | 1.66605898550132  |
| Li | 1.61928640704465  | 0.28057365475777  | -0.94226391763802 |
| C  | 2.75129646583591  | -1.25148268331357 | -1.36602876400757 |
| C  | 2.41345948910599  | -2.52896920697479 | -1.82263448685982 |
| C  | 4.11342971792270  | -0.93978039918933 | -1.37086186347753 |
| C  | 3.37029799706768  | -3.43849537716981 | -2.24254051730545 |
| H  | 1.37743187182652  | -2.83636885717294 | -1.81763483131721 |
| C  | 5.08124245347323  | -1.83365787006265 | -1.80289652532990 |
| H  | 4.43513800617564  | 0.03279674101216  | -1.00811927110006 |
| C  | 4.71093435838084  | -3.09442751099740 | -2.23492831144928 |
| H  | 3.06897440094249  | -4.42063114128387 | -2.58003397722173 |
| H  | 6.12570034079212  | -1.54706919773824 | -1.79985366264500 |
| H  | 5.46039501547675  | -3.80366234055266 | -2.55907026818061 |

# PhLi S2

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | -0.92777648496182 | 0.73951704181113  | 0.77481151822785  |
| C | 0.46313676366658  | 0.66342661711490  | 0.62041968744415  |
| C | 1.29788687557047  | 1.69887433291946  | 1.06275601985705  |
| C | 0.80153926784741  | 2.69463045531648  | 1.91064858397307  |
| C | -0.57671398193045 | 2.70737952351229  | 2.13051739692827  |
| C | -1.41336730021807 | 1.80865177739609  | 1.51175183129162  |
| S | 2.73171586471971  | 1.68912983725554  | -0.08148307898924 |
| C | 3.25755479464790  | 0.05776732392102  | 0.30643687214912  |
| C | 2.21521325434893  | -0.86138275636542 | 0.23192724035643  |
| O | 0.93381536004764  | -0.47419652898152 | 0.00096302419329  |
| C | 4.51707131379420  | -0.33310883506646 | 0.74478824979867  |
| C | 4.81003903244042  | -1.67080625929455 | 0.97584364185600  |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| C | 3.78750061995468  | -2.60284656674936 | 0.77731461066281  |
| C | 2.50633434513825  | -2.19743455309008 | 0.44729991477006  |
| C | 6.19704712751767  | -2.07086668311987 | 1.45309423007601  |
| C | 6.30141961978560  | -3.57044917588707 | 1.74235082395464  |
| S | 1.13350188313892  | -3.35589370786136 | 0.52366999286882  |
| O | 1.66537561883866  | -4.67650276681341 | 0.74283382428469  |
| S | -3.18601811292396 | 2.09960428837700  | 1.48574787648986  |
| O | -3.51830544923331 | 2.98090873206324  | 2.57691126795927  |
| C | 1.68150333715047  | 3.74150802130821  | 2.57962194640808  |
| C | 2.97131289556227  | 3.08857753349688  | 3.09372844178559  |
| O | 1.91871433869983  | 1.96995393790448  | -1.26915851539817 |
| O | -1.83304970957229 | -0.12549344124667 | 0.26795369712627  |
| C | -1.61260044345794 | -0.68003683471239 | -1.02756529981294 |
| C | 0.29553684350372  | -2.84938180935984 | 2.05114636629586  |
| C | 1.15054489232299  | -2.27375824520423 | 2.98081616859520  |
| C | 0.72456591675091  | -1.78382734760648 | 4.20525126354652  |
| C | -0.62628686948701 | -1.94491991554766 | 4.50325729889656  |
| C | -1.47043825240915 | -2.54804140146908 | 3.60736968320111  |
| C | -1.05755581711613 | -3.00475648362290 | 2.35010751404705  |
| C | 1.64415393399995  | -1.07569386477868 | 5.18309738400296  |
| C | 3.06446521217556  | -0.91501495881053 | 4.63331822430415  |
| S | -3.21184042032874 | -2.68642295793253 | 4.02086327441040  |
| O | -3.68955879754310 | -4.02470393125661 | 3.81344276746478  |
| O | -2.02687722170084 | -3.51622299021923 | 1.57940070686901  |
| C | -1.76404523346462 | -4.60498213785769 | 0.70355747086103  |
| O | 0.30358022091924  | -3.18043249817626 | -0.63691777767939 |
| C | -3.96873018798714 | -1.59230494317423 | 2.82000537030318  |
| C | -4.92797176661748 | -2.05810473829010 | 1.94315613085077  |
| C | -5.44645492446107 | -1.23942278577720 | 0.94506965002063  |
| C | -4.93239324896985 | 0.05408124185483  | 0.85040789100075  |
| C | -3.97258226735972 | 0.50574891798566  | 1.72821539988460  |
| C | -3.47174678493207 | -0.30163682910060 | 2.73783790779543  |
| C | -6.49050114231672 | -1.70861341629107 | -0.05327501797264 |
| C | -7.70129573022880 | -0.76751744363341 | 0.00895534251161  |
| O | -2.46283059011561 | 0.14076848682366  | 3.54905156695925  |
| C | -2.90127820285581 | 0.84975073159059  | 4.71086511008987  |
| O | -3.39534954618632 | -2.13968302936504 | 5.34197817014418  |
| O | -3.52589402872020 | 2.56106786409099  | 0.16635108249780  |
| C | 6.52849301571867  | -1.30561665758031 | 2.74212120491770  |
| C | 7.21682956315520  | -1.71337081142983 | 0.36561215423610  |
| C | 1.70935426209382  | -1.88191119244170 | 6.48702588524182  |
| C | 1.06257355607919  | 0.31874580879924  | 5.45894564657943  |
| C | -6.96755159027214 | -3.13431983290082 | 0.23318501171071  |
| C | -5.87142200949325 | -1.67214548030350 | -1.45783330181771 |
| C | 0.97725052737232  | 4.37604287189040  | 3.78803014005918  |
| C | 2.00037332312458  | 4.85407923292987  | 1.57283512487934  |
| H | 5.26060309787841  | 0.43844704745948  | 0.85678879862676  |
| H | 3.93078996232394  | -3.65981725633740 | 0.92411045709087  |
| H | 2.19066949421916  | -2.21289770973933 | 2.71389861714179  |
| H | -1.05845948606039 | -1.62114437399447 | 5.43609549456447  |
| H | -5.22941206737405 | -3.08490318617844 | 2.06724836173178  |
| H | -5.23890662501495 | 0.73791796588493  | 0.07435053463848  |
| H | -1.04998289651362 | 3.46794704632803  | 2.72721657086167  |
| H | -0.83257725602146 | -5.11289012603253 | 0.95579248047151  |
| H | -2.60358572291515 | -5.29092973178150 | 0.82668358911718  |
| H | -1.70813828351553 | -4.25582076470660 | -0.32825204650705 |
| H | -3.51188299106542 | 1.71057264857326  | 4.42968339305874  |
| H | -1.99014061032761 | 1.19210773103805  | 5.19597019369209  |
| H | -3.45175353775819 | 0.17706089372124  | 5.37353018786351  |
| H | -0.96734946917001 | -1.55894559187608 | -0.98851316591071 |
| H | -1.18070524328424 | 0.06590849072828  | -1.69700265958394 |

|    |                   |                   |                   |
|----|-------------------|-------------------|-------------------|
| H  | -2.60482681165268 | -0.95947647939097 | -1.37967609001905 |
| H  | 5.80650819740120  | -1.53979188779258 | 3.52020393305556  |
| H  | 6.52113358915020  | -0.23218569803507 | 2.58011850583255  |
| H  | 7.51749652307611  | -1.58950910014364 | 3.09392480299073  |
| H  | 6.97728334749082  | -2.23226840416962 | -0.55882834217897 |
| H  | 7.21438840284597  | -0.64721706375783 | 0.16119681859058  |
| H  | 8.21583486370599  | -2.00504169508676 | 0.68156245073675  |
| H  | 7.30364900737484  | -3.79909270642354 | 2.09795731118328  |
| H  | 5.59422308494891  | -3.87432841023757 | 2.51006986976792  |
| H  | 6.12364291849061  | -4.15482339436953 | 0.84388583914115  |
| H  | 0.72124358007813  | -2.00460283630250 | 6.92023712528193  |
| H  | 2.12426415837506  | -2.86934829377354 | 6.29907706056812  |
| H  | 2.34211820516314  | -1.37250122490366 | 7.21024725700930  |
| H  | 0.12698517254175  | 0.24643865623108  | 6.00493525788126  |
| H  | 1.75970935828170  | 0.90431122884607  | 6.05495860066014  |
| H  | 0.87265158810710  | 0.83901143747752  | 4.52160516167864  |
| H  | 3.52379806860675  | -1.88529734498164 | 4.46013260112889  |
| H  | 3.67451122797842  | -0.38033811880742 | 5.35845293736840  |
| H  | 3.06812279674001  | -0.34928618107609 | 3.70336183515717  |
| H  | -7.72824145977407 | -3.41348282335635 | -0.49276839717147 |
| H  | -7.40501643415536 | -3.20695789187417 | 1.22548422022708  |
| H  | -6.14905313396785 | -3.84452302167618 | 0.15284261420182  |
| H  | -5.00287996577105 | -2.32557761048257 | -1.50073110971734 |
| H  | -6.59715973288259 | -2.01360661457334 | -2.19258264376691 |
| H  | -5.56040807746306 | -0.66637759606345 | -1.72526940060340 |
| H  | -7.42590451633996 | 0.25125531634353  | -0.24627463691007 |
| H  | -8.12610783803339 | -0.76727326183174 | 1.01000639333683  |
| H  | -8.46586965402537 | -1.09970328101877 | -0.68961100899511 |
| H  | 1.69001748829294  | 4.99588798976459  | 4.32747251166612  |
| H  | 0.15293047479705  | 5.01455696021711  | 3.48415223797993  |
| H  | 0.60517119288040  | 3.61479215798362  | 4.46913963460920  |
| H  | 1.07889537419099  | 5.27310727202594  | 1.17517315662835  |
| H  | 2.56085010999643  | 5.64587219855760  | 2.06440508224725  |
| H  | 2.59500451212147  | 4.46704416531270  | 0.75207764248847  |
| H  | 2.73580523971132  | 2.27431991742544  | 3.77481374108613  |
| H  | 3.56458271360698  | 3.82482117101967  | 3.63111267960381  |
| H  | 3.56985901038145  | 2.70640625162601  | 2.27587442833883  |
| O  | 3.73982344971409  | 2.68234023495870  | 0.18074418272269  |
| C  | 4.28428436756388  | 0.73461833313005  | -1.89215850362218 |
| Li | 3.24095363601081  | 2.37607350847515  | -2.32744576856404 |
| C  | 5.64484692379498  | 1.06419850642854  | -1.85416512067452 |
| C  | 6.62083864773568  | 0.23630264021060  | -2.38852509405057 |
| C  | 6.26432036707346  | -0.96662814562037 | -2.97243431008205 |
| C  | 4.92890318992425  | -1.32701426643436 | -3.02722542832481 |
| C  | 3.96255323706074  | -0.47789566091749 | -2.51240062676751 |
| H  | 5.95050271253704  | 1.97809688218886  | -1.35401181183261 |
| H  | 7.66298924922446  | 0.52689131183591  | -2.35008408523437 |
| H  | 7.02332198775387  | -1.61934627493870 | -3.38155838091265 |
| H  | 4.64192019575447  | -2.26951795901450 | -3.47451292029041 |
| H  | 2.92353762289825  | -0.79394974312414 | -2.54706163329050 |

#### PhLi C3

|   |                   |                   |                  |
|---|-------------------|-------------------|------------------|
| C | -1.00041676204304 | 0.92450288222160  | 0.54717891728627 |
| C | 0.33757997968677  | 0.70298122969562  | 1.00865277029039 |
| C | 1.06533107683041  | 1.74439705273393  | 1.57474779199807 |
| C | 0.44100617378157  | 2.92818923233665  | 2.02527090483529 |
| C | -0.94205244066374 | 2.99074749554465  | 1.84093281287024 |
| C | -1.62978059248054 | 2.02976431265484  | 1.15223656236584 |
| S | 2.84073095467415  | 1.45382187620497  | 1.64130022779023 |
| C | 3.11009068486133  | -0.09218843485207 | 0.80351976250671 |
| C | 2.04396295208385  | -0.96620049405253 | 0.72084594577390 |

|   |                   |                   |                   |
|---|-------------------|-------------------|-------------------|
| O | 0.75568341221806  | -0.59004143449934 | 0.81636230771584  |
| C | 4.40303912747981  | -0.52119521208754 | 0.58034981527261  |
| C | 4.68825682846862  | -1.85175872693751 | 0.28074293619697  |
| C | 3.62301229845170  | -2.75023774250375 | 0.33432975438684  |
| C | 2.33135738633103  | -2.31844225314769 | 0.54769748221639  |
| C | 6.11801047375755  | -2.27517836167650 | -0.00380485858466 |
| C | 6.22065320775054  | -3.75861686079655 | -0.36644303411668 |
| S | 1.00187283542262  | -3.49461062934640 | 0.82082349198409  |
| O | 1.59239109652211  | -4.76920731556916 | 1.13413123069710  |
| S | -3.36551809338313 | 2.16135360368489  | 0.87194969896268  |
| O | -3.89999681579825 | 3.26596462388396  | 1.61421694633278  |
| C | 1.02202641263832  | 4.10666905554314  | 2.80769736663995  |
| C | 0.36717735662141  | 4.10382835929243  | 4.20292254547068  |
| O | 3.59016751530972  | 2.46661581675841  | 0.95892580266902  |
| O | -1.90934770607090 | -0.02375374868555 | 0.16569451778404  |
| C | -1.63467531980480 | -1.03271858809391 | -0.78822702706231 |
| C | 0.24373708564739  | -2.84799137871779 | 2.32648831605742  |
| C | 1.13992754607590  | -2.40647699066072 | 3.28706790123552  |
| C | 0.72277150175613  | -1.81610474819034 | 4.47378684497255  |
| C | -0.65440763737697 | -1.71830231135985 | 4.67639477879915  |
| C | -1.53969288554965 | -2.19748313180195 | 3.74134117627352  |
| C | -1.12612216602081 | -2.76080226495249 | 2.53842608305317  |
| C | 1.68072935086809  | -1.29778603697725 | 5.53034551893086  |
| C | 3.14781287114326  | -1.50809674637949 | 5.14877429701106  |
| S | -3.29950004114267 | -2.21444763067387 | 4.08440793945434  |
| O | -3.75294311312157 | -3.57958482493595 | 4.05260522659118  |
| O | -2.07628510663099 | -3.14172773339452 | 1.64325854850486  |
| C | -2.18004859094446 | -4.54364326692632 | 1.41178919100643  |
| O | 0.10035990854123  | -3.46617152042659 | -0.29906168120883 |
| C | -4.07536653987077 | -1.32845622953656 | 2.73302457298624  |
| C | -5.05620761007765 | -1.91068542128024 | 1.95679864154075  |
| C | -5.61521903102438 | -1.22152377465650 | 0.88562611665306  |
| C | -5.12319623939504 | 0.05719852565567  | 0.62282159077507  |
| C | -4.13940450478051 | 0.62922410653392  | 1.40114537783097  |
| C | -3.59764047298896 | -0.05449731887129 | 2.48273454635108  |
| C | -6.67459913921066 | -1.81769335647802 | -0.02431048740570 |
| C | -7.89744279435643 | -0.89069944404522 | -0.04930247036523 |
| O | -2.55741272562010 | 0.44464273605754  | 3.21590479534057  |
| C | -2.92058683487126 | 1.40048709663795  | 4.21158427358931  |
| O | -3.53487294711311 | -1.48035898034552 | 5.30060001940768  |
| O | -3.57672871638194 | 2.21829226726500  | -0.57310431984535 |
| C | 6.96976829534241  | -2.01393120587888 | 1.24629422520067  |
| C | 6.65120540939315  | -1.44810071782062 | -1.18178626343642 |
| C | 1.39889485241832  | -2.03470861306001 | 6.84821239364870  |
| C | 1.44898224761103  | 0.20981626538268  | 5.70416090188494  |
| C | -7.12516842964698 | -3.20347180048264 | 0.44363300124144  |
| C | -6.08439780904834 | -1.94505889175594 | -1.43670325627516 |
| C | 0.67304318843986  | 5.40714271334530  | 2.06418999664261  |
| C | 2.53137688885138  | 4.11821220781919  | 3.03194723780955  |
| H | 5.17889040923501  | 0.22176166577035  | 0.67303950127573  |
| H | 3.76305244558345  | -3.81416902478091 | 0.23749921621008  |
| H | 2.18960354312293  | -2.53092801714033 | 3.07638755488149  |
| H | -1.07581800003328 | -1.28914880679855 | 5.57177699890202  |
| H | -5.34290916958198 | -2.91603089863895 | 2.21673074415094  |
| H | -5.47508033968750 | 0.63203011313665  | -0.21901507603497 |
| H | -1.52475873239904 | 3.80690554307907  | 2.23592306454130  |
| H | -1.20271080793053 | -4.99734772190955 | 1.23741458525986  |
| H | -2.67302740583806 | -5.01343187793343 | 2.26864982422995  |
| H | -2.79172248879734 | -4.65067682468517 | 0.51898093724307  |
| H | -3.50890071890714 | 2.21453403685085  | 3.78050070306701  |
| H | -1.97866135624718 | 1.78591509158340  | 4.59586389402945  |

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| H  | -3.47813905669221 | 0.90359529521103  | 5.01048869137497  |
| H  | -0.76780140453856 | -1.63974712229014 | -0.54265817931915 |
| H  | -1.51438855698428 | -0.59419342493211 | -1.78696588397496 |
| H  | -2.51349050825395 | -1.67548806154472 | -0.77711594490938 |
| H  | 6.58285817250823  | -2.57944861041659 | 2.09077388202475  |
| H  | 6.96907965539504  | -0.96100316327516 | 1.51195958078389  |
| H  | 7.99689001808619  | -2.32204890830722 | 1.06578609795245  |
| H  | 6.04163464288116  | -1.61737459178041 | -2.06636790770504 |
| H  | 6.64129496674163  | -0.38581907828711 | -0.95726349090244 |
| H  | 7.67410270850154  | -1.74014377219940 | -1.40743542559595 |
| H  | 7.25282181867778  | -3.99933116519399 | -0.61075731637520 |
| H  | 5.91812545732150  | -4.38931627946721 | 0.46530464693106  |
| H  | 5.60518048493665  | -3.99158962284339 | -1.23157870390285 |
| H  | 0.38809716083984  | -1.84975345177665 | 7.19944464801970  |
| H  | 1.52503475581518  | -3.10682293691530 | 6.71493125828159  |
| H  | 2.09329543948941  | -1.69923187255440 | 7.61485865877455  |
| H  | 0.40414290248197  | 0.43310723813395  | 5.90216055832428  |
| H  | 2.04559167340205  | 0.57828127858911  | 6.53546512101900  |
| H  | 1.76259470262567  | 0.73217255797611  | 4.80301146849020  |
| H  | 3.36819619017704  | -2.55949405614927 | 4.97912481712344  |
| H  | 3.77948168786385  | -1.15949902377904 | 5.96253466649104  |
| H  | 3.40060315820292  | -0.92725542237997 | 4.26462486000325  |
| H  | -7.89856308086800 | -3.57641254025720 | -0.22417546168536 |
| H  | -7.53883662572298 | -3.16040380365320 | 1.44774100555751  |
| H  | -6.29999620916366 | -3.91042169720976 | 0.42945878644296  |
| H  | -5.20897287136457 | -2.59056195471526 | -1.42146767573144 |
| H  | -6.82132012766745 | -2.38092887518002 | -2.10720476724044 |
| H  | -5.79095586575818 | -0.97679941536517 | -1.83341903827211 |
| H  | -7.64578057950306 | 0.09214901078566  | -0.43625188102870 |
| H  | -8.29949509096866 | -0.77158845744327 | 0.95401863415382  |
| H  | -8.67252216617853 | -1.31695825172436 | -0.68183026865192 |
| H  | 1.09362075961731  | 6.25645046797506  | 2.59770472843641  |
| H  | 1.10159648838826  | 5.38161118477811  | 1.06606367924355  |
| H  | -0.39793819025528 | 5.56164099636631  | 1.97503498552546  |
| H  | 3.06946350952325  | 4.20231356200152  | 2.09511442864449  |
| H  | 2.78563199960223  | 4.97903252126186  | 3.64825434781404  |
| H  | 2.86903924327869  | 3.22635823231375  | 3.54761342077816  |
| H  | -0.71363655853515 | 4.19776616697922  | 4.15383861703229  |
| H  | 0.75135157992552  | 4.93776799589008  | 4.78578568677477  |
| H  | 0.61304492886794  | 3.18116307389981  | 4.72398375584479  |
| O  | 3.22423146033579  | 1.14028009307704  | 3.00023113158861  |
| Li | -2.15590210544182 | 1.49370115438661  | -1.27463766831262 |
| C  | -0.20163802533545 | 1.73766532593795  | -1.43193398002284 |
| C  | 0.87921873885553  | 0.95007313277149  | -1.85770738581791 |
| C  | 0.09046393370746  | 3.09242633662680  | -1.22174918750383 |
| C  | 2.15693912354005  | 1.46040622064878  | -2.01326761808106 |
| H  | 0.73447722159536  | -0.10708039133998 | -2.04574332997071 |
| C  | 1.35734723626053  | 3.62226156866309  | -1.40671457881590 |
| H  | -0.70323972886855 | 3.75088922301361  | -0.87890642017327 |
| C  | 2.40458356181223  | 2.80280790492888  | -1.78617200809012 |
| H  | 2.96411316891589  | 0.80722111762658  | -2.32018069757952 |
| H  | 1.53490515220245  | 4.67708250295114  | -1.24618101790072 |
| H  | 3.40101924767946  | 3.20235677211740  | -1.89556631011516 |

#### PhLi C4

|   |                   |                  |                   |
|---|-------------------|------------------|-------------------|
| C | -0.41924448436080 | 1.41182848752060 | -1.35158126772176 |
| C | 0.87813517190495  | 1.35354935075326 | -0.77414262355695 |
| C | 1.42922014758184  | 2.38327712757892 | -0.02854403255576 |
| C | 0.63951943920097  | 3.50593775781799 | 0.29118029210395  |
| C | -0.67949808008540 | 3.45685150262670 | -0.13474386286064 |

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|---|-------------------|-------------------|-------------------|
| C | -1.21609450721265 | 2.46296490676402  | -0.94239456157169 |
| S | 3.21069007370002  | 2.21302129359285  | 0.29992061047185  |
| C | 3.62286769594252  | 0.53257856153906  | -0.11429257121046 |
| C | 2.65088092218775  | -0.26380616233976 | -0.65100273057687 |
| O | 1.42656810865147  | 0.14228061404861  | -1.03298738709558 |
| C | 4.91194965582034  | 0.04779864839959  | 0.06909365966786  |
| C | 5.24206779441599  | -1.25850727284366 | -0.30314601745987 |
| C | 4.22565850563988  | -2.08535325623623 | -0.76849577714672 |
| C | 2.94052796981442  | -1.59473272086492 | -0.99167434359527 |
| C | 6.67918888379628  | -1.72812301428515 | -0.16435623225207 |
| C | 6.87391573887705  | -3.15574523524042 | -0.67954922945672 |
| S | 1.52526812707632  | -2.68599697114148 | -0.98049656027019 |
| O | 1.96102162585530  | -4.04777302826483 | -0.88549120641597 |
| S | -3.00852940333844 | 2.61117250232918  | -1.13362934610670 |
| O | -3.44921491446451 | 3.63695988814304  | -0.22797223504785 |
| C | 1.08961387095906  | 4.68813970141454  | 1.14387823662198  |
| C | 1.19373428081401  | 4.22398365544474  | 2.60458582190249  |
| O | 3.91801344836280  | 3.06233216754813  | -0.61405889049642 |
| O | -0.61751610640460 | 0.41384220938304  | -2.23751114054714 |
| C | -1.85220140830014 | 0.18250270485717  | -2.88910485190908 |
| C | 0.76629137012382  | -2.20082931987932 | 0.58918044836923  |
| C | 1.62838871774376  | -1.88502082800189 | 1.63010473280749  |
| C | 1.17730328244398  | -1.37748081867301 | 2.84201791399327  |
| C | -0.20400970025993 | -1.24928728426805 | 2.99747626470143  |
| C | -1.05912489658688 | -1.61784633276843 | 1.98628970795845  |
| C | -0.60678722020746 | -2.07755676955195 | 0.75475462544959  |
| C | 2.11248142314396  | -0.97139123274463 | 3.96618341240674  |
| C | 3.58270422827661  | -1.23556789966875 | 3.63064728813900  |
| S | -2.82902851103352 | -1.67439470612444 | 2.26362161898483  |
| O | -3.23084420789254 | -3.05458518762561 | 2.21831842782419  |
| O | -1.53108598692952 | -2.32654847937115 | -0.21514065262593 |
| C | -1.69971984479117 | -3.69920844495780 | -0.56347893335562 |
| O | 0.57202083602449  | -2.39998123549102 | -2.02507529822934 |
| C | -3.61459081731546 | -0.82690224982453 | 0.89090740637858  |
| C | -4.67843508503016 | -1.40010709428818 | 0.22553426014955  |
| C | -5.29074942861774 | -0.74366664145773 | -0.83863484478347 |
| C | -4.76133828021339 | 0.49128884815736  | -1.21180087577031 |
| C | -3.68376115953015 | 1.04648777837288  | -0.55172565762807 |
| C | -3.09913813158220 | 0.40723616174314  | 0.53260484007599  |
| C | -6.46205729778878 | -1.32328011653475 | -1.61030432273398 |
| C | -7.63889494330857 | -0.34067793144190 | -1.53921599233451 |
| O | -2.00653946665107 | 0.91555397216172  | 1.18419086027302  |
| C | -2.32069838418284 | 1.81754074485548  | 2.24854997066848  |
| O | -3.12139893194351 | -0.94444549467777 | 3.46963379215667  |
| O | -3.38465776291301 | 2.76718584803649  | -2.51572430668921 |
| C | 7.09022855266583  | -1.67455567392995 | 1.31354402650117  |
| C | 7.56937046131622  | -0.79428983398279 | -0.99615263178030 |
| C | 1.74495960352077  | -1.76834593355100 | 5.22649324716927  |
| C | 1.94242903543902  | 0.53232601506397  | 4.22538818551172  |
| C | -6.91672389931017 | -2.67108758583983 | -1.04595390875624 |
| C | -6.03390845440308 | -1.52172116259144 | -3.07174456316167 |
| C | 0.07879069431805  | 5.84443602842523  | 1.08788316839494  |
| C | 2.43929015472543  | 5.24722765897833  | 0.68064407285438  |
| H | 5.63610222770184  | 0.72213855910896  | 0.49339374140663  |
| H | 4.39673979676434  | -3.12090801015185 | -1.00688500795980 |
| H | 2.68067504133278  | -2.04678160524208 | 1.46505941269360  |
| H | -0.64972784985200 | -0.88693642305976 | 3.91044902035484  |
| H | -4.99528546384840 | -2.37125565054671 | 0.56797097923891  |
| H | -5.15608364834099 | 1.04802710559222  | -2.04732993419444 |
| H | -1.37643364014063 | 4.22449888128595  | 0.15004024570061  |
| H | -0.74321068339361 | -4.17753792167820 | -0.77949712420758 |

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| H              | -2.21213524817070 | -4.21742681573425 | 0.25274004139901  |
| H              | -2.31619618971922 | -3.69970071171979 | -1.45891173887044 |
| H              | -2.91280710064750 | 2.65796550636178  | 1.87805766333844  |
| H              | -1.35826692662297 | 2.16872420484933  | 2.61374822495944  |
| H              | -2.85558903430277 | 1.28936928309184  | 3.04207867167040  |
| H              | -1.59602887033153 | -0.36634940884316 | -3.79544727821624 |
| H              | -2.36323613454632 | 1.11037500551440  | -3.14815762740478 |
| H              | -2.49065967736299 | -0.44688415344570 | -2.26671084308482 |
| H              | 6.45778766812731  | -2.33223261751964 | 1.90582568812307  |
| H              | 7.00482708309436  | -0.66792680984241 | 1.71220982113720  |
| H              | 8.12221481157533  | -1.99923837008056 | 1.42270296836884  |
| H              | 7.23508980212432  | -0.79343189682547 | -2.03067059991350 |
| H              | 7.53403001881870  | 0.22540298026712  | -0.62491189978853 |
| H              | 8.60136141940217  | -1.13583303721508 | -0.96159114322559 |
| H              | 7.92439387329136  | -3.42696441707595 | -0.60104079327660 |
| H              | 6.29896698653716  | -3.86989704849819 | -0.09534269977207 |
| H              | 6.58081099386617  | -3.22914858084457 | -1.72357517566045 |
| H              | 0.73631759730543  | -1.54324333656635 | 5.55943151804179  |
| H              | 1.81174057310644  | -2.83621211163320 | 5.03112420696381  |
| H              | 2.43197782716485  | -1.52224939947472 | 6.03248944372973  |
| H              | 0.90173168839983  | 0.78980431596572  | 4.40105308321846  |
| H              | 2.51875659661675  | 0.81994742632920  | 5.10135203548753  |
| H              | 2.30985549992974  | 1.10643752125274  | 3.37750890576569  |
| H              | 3.76045988853466  | -2.29148247945848 | 3.43976740273513  |
| H              | 4.19904250012353  | -0.93802089461493 | 4.47563623054376  |
| H              | 3.89892884646034  | -0.65272779422665 | 2.76826590744806  |
| H              | -7.76401912493760 | -3.03544980357784 | -1.62225031196298 |
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| H              | -6.12392067888273 | -3.41171867373639 | -1.11022606513530 |
| H              | -5.18207555288311 | -2.19553789271006 | -3.12799287884530 |
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| H              | -5.75703601625396 | -0.57987076270248 | -3.53623444089015 |
| H              | -7.38472647465244 | 0.61730046375679  | -1.98270712523520 |
| H              | -7.92840986929043 | -0.17391602992015 | -0.50443419487125 |
| H              | -8.49320725689972 | -0.74810080747562 | -2.07425888933544 |
| H              | 0.48858789334090  | 6.69335044167675  | 1.63015376693577  |
| H              | -0.10403532234239 | 6.15645638450891  | 0.06290795024834  |
| H              | -0.86551454126965 | 5.58643542853615  | 1.55996929818426  |
| H              | 2.46063406789190  | 5.36538247494126  | -0.39952535236330 |
| H              | 2.60587470097436  | 6.22033512883758  | 1.13689202164979  |
| H              | 3.25941170692769  | 4.60378845418357  | 0.97056257844656  |
| H              | 0.24090561120888  | 3.82726876841345  | 2.94942789169513  |
| H              | 1.46214230583474  | 5.06891080109265  | 3.23369929256167  |
| H              | 1.95823459287744  | 3.46219854235499  | 2.71158118374416  |
| O              | 3.48563655487142  | 2.36488252336361  | 1.70749686472549  |
| Li             | 1.03584019604216  | -0.81150643512060 | -2.67127227979820 |
| C              | 2.87906403652054  | -1.00510481014022 | -3.48424332127631 |
| C              | 3.38788857591227  | -2.19484225931936 | -4.01624756282887 |
| C              | 3.77522081687749  | 0.07044932069987  | -3.46059232596670 |
| C              | 4.68795998625282  | -2.31157744450384 | -4.48369735068020 |
| H              | 2.75027481868885  | -3.07068007075174 | -4.03967418848741 |
| C              | 5.07424552416049  | -0.02310983705345 | -3.93189902050074 |
| H              | 3.46156928229597  | 1.02273013827035  | -3.04110228572846 |
| C              | 5.54127455770181  | -1.22358807655902 | -4.43815444944366 |
| H              | 5.04212714691575  | -3.25672032007553 | -4.87593097745675 |
| H              | 5.72628261989570  | 0.84006028927440  | -3.89377157702283 |
| H              | 6.56132310751971  | -1.31094172013088 | -4.78960695747772 |
| <b>PhLi C5</b> |                   |                   |                   |
| C              | -0.73867215443554 | 1.85063804072252  | -1.33938068433429 |
| C              | 0.56696414668211  | 1.64031978855239  | -0.92143371478793 |

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| C | 1.25457950461249  | 2.64552933806311  | -0.20391429948193 |
| C | 0.55189416730214  | 3.75643722923180  | 0.31839195217481  |
| C | -0.77546440546248 | 3.88318629866014  | -0.03372057759471 |
| C | -1.34923399164818 | 3.08952006699966  | -1.04033650349921 |
| S | 3.03357805869744  | 2.50918831601043  | -0.24005932930374 |
| C | 3.36664758775839  | 0.87124354228570  | -0.86811750237486 |
| C | 2.32232452689978  | -0.00126674750824 | -1.10834804759708 |
| O | 1.02732479399591  | 0.35346439853441  | -1.14818756224946 |
| C | 4.68133426141781  | 0.45012785680246  | -0.90866675191208 |
| C | 5.02042198987006  | -0.86916926617721 | -1.19500564389740 |
| C | 3.96379496379774  | -1.76403036543141 | -1.35081888016433 |
| C | 2.65108702544306  | -1.34472367283591 | -1.30381626771960 |
| C | 6.47872446278483  | -1.28731513619032 | -1.24444329569609 |
| C | 6.64620681785033  | -2.75526165347903 | -1.64395351733839 |
| S | 1.33733035741564  | -2.56977500687168 | -1.22670647320025 |
| O | 1.94542919164391  | -3.86532159132868 | -1.06842560977829 |
| S | -3.13939550168237 | 3.00195028596599  | -1.08503665914349 |
| O | -3.64266203316193 | 4.04170617832835  | -0.21698739056418 |
| C | 1.14787297036496  | 4.75471127909777  | 1.31181794611031  |
| C | 1.49797389102012  | 4.01978295446664  | 2.61263846674255  |
| O | 3.58296613667481  | 3.45148763356279  | -1.17749918681376 |
| O | -1.54106497541508 | 0.98522645088908  | -2.02148717705088 |
| C | -0.98499727341679 | 0.21317639413646  | -3.08453213694043 |
| C | 0.57859653277455  | -2.10070433718058 | 0.34299241103687  |
| C | 1.53679223196146  | -1.78332916354264 | 1.29670190824553  |
| C | 1.22299404035083  | -1.23287310471747 | 2.52863385975452  |
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**PhLi C6**

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