

Supporting information

Redox-induced Diels-Alder revisited: impact of diene's oxidation on demanding cycloadditions

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1. General Information

All cycloaddition experiments were carried out in inert atmosphere (Ar glovebox). All reactions were performed in a 5 mL tube without magnetic stirring. Flash column chromatography was performed using silica gel obtained from Roth. All commercially available reagents were used without further purification.

¹H NMR and ¹³C NMR spectra were recorded on 700 MHz NMR Spectrometer and on Agilent 400-MR DD2 400 MHz spectrometer.

List of commercial reagents:

Anthracene (Sigma Aldrich),
4-nitrochalcone (Sigma Aldrich),
4-chlorochalcone (Sigma Aldrich),
9-methylantracene (Sigma Aldrich),
9-bromoanthracene (Sigma Aldrich)
9-nitroanthracene (Sigma Aldrich),
9-cyanoanthracene (Sigma Aldrich),
Dimethyl maleate (Sigma Aldrich)
Phenylbutadiene (Sigma Aldrich),
4-fluorophenylmaleimide (MIM-PhF) (ABCR),
3-(trifluoromethyl)phenylmaleimide (MIM-PhCF₃) (ABCR),

diphenylbutadiene (Sigma Aldrich),

CoF₃ (Sigma Aldrich), Ce(SO₄)₂ (Sigma Aldrich), KMnO₄ (Chempur)

Solvent for reactions:

1,2-difluorobenzene (Fluorochem), (dried over molecular sieves, 3A).

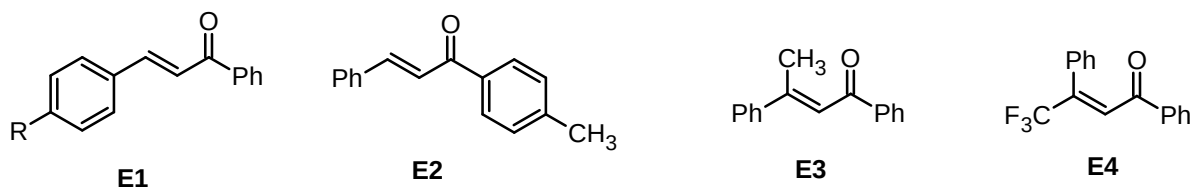
Solvents for chromatography:

hexane (Chempur),

dichloromethane (Chempur)

Non-commercial reagents: 4-methylchalcone, 4'-methylchalcone, 4-fluorochalcone, 3,5-bis(trifluoromethyl)chalcone, dypnone, (*E*)-4,4,4-Trifluoro-1,3-diphenylbut-2-en-1-one, 4-(trifluoromethyl)chalcone prepared with procedure described below.

Enones (cycloaddition substrates) synthesis



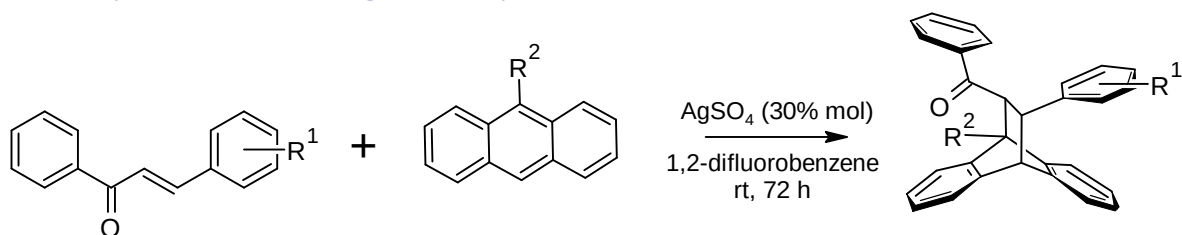
R = H, F, Br, CH₃, CF₃

Chalcones **E1**, **E2** were prepared according to the literature procedures, typically through aldol condensation of acetophenone (or 4'-methylacetophenone for chalcone **E2**) with corresponding aromatic aldehyde in ethanol/water in the presence of sodium hydroxide.¹ Chalcones **E1**, **E2** were purified by crystallization.

Dypnone (**E3**) was prepared via the self-condensation of acetophenone in ethanol mediated by tetrachlorosilane, according to the literature procedure.^{2,3} Dypnone was purified by distillation under reduced pressure.

(*E*)-4,4,4-Trifluoro-1,3-diphenylbut-2-en-1-one (**E4**) was synthesized using the Wittig reaction between 2,2,2-trifluoroacetophenone and α -(triphenylphosphoranylidene)acetophenone, according to the literature procedure.⁴ The enone **E4** was purified by column chromatography on silica gel.

2. Cycloaddition – general procedure



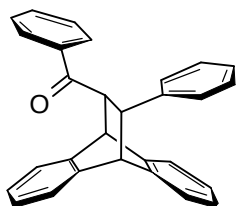
In a typical experiment, a 5 mL vial was charged with anthracene (0.2 mmol, 1.0 eq) and chalcone (0.2 mmol, 1.0 eq), AgSO₄ (0.06 mmol, 0.3 eq) and *o*-difluorobenzene (2 mL). The mixture was left at room temperature and Ar inert atmosphere for 3 days (72h). Then distilled water was added to the reaction mixture, and the solvent from organic phase was evaporated to give the crude product. The crude product was dissolved in CDCl₃ and ¹H NMR spectra were recorded to estimate yield. None of the products/substrates were soluble in water which allowed to assess the yield on the basis of NMR spectra of species isolated from organic layer.

The residue was then purified by column chromatography on silica gel using n-hexane/DCM (2:1 or 1:1) as eluent to provide the desired products. Final product was dissolved in CDCl₃ and 1D and 2D NMR spectra were recorded to assign signals.

Cycloadducts were crystallized from DCM, chloroform, DCM/hexane, *o*-difluorobenzene or acetone.

3. Characterization Data

NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, sept = septet, m = multiplet), coupling constants (Hz) and integration.

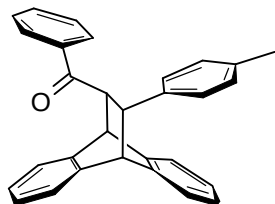


1a. White solid, 84% yield, n-hexane/DCM = 1:1;

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.79 (d, J = 7.4 Hz, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.47–7.39 (m, 3H), 7.35 (d, J = 7.3 Hz, 1H), 7.23 (td, J = 7.3 Hz, 1.3 Hz, 1H), 7.17 (td, J = 7.3 Hz, 1.3 Hz, 1H), 7.14–7.10 (m, 5H), 7.10–7.05 (m, 2H), 6.67–6.62 (m, 2H), 4.60 (d, J = 1.8 Hz, 1H), 4.31 (d, J = 2.0 Hz, 1H), 3.90 (dd, J = 5.9 Hz, 2.0 Hz, 1H), 3.80 (dd, J = 5.9 Hz, 2.1 Hz, 1H)

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 198.8, 144.2, 143.5, 143.4, 141.4, 139.1, 136.8, 133.0, 128.8, 128.6, 128.4, 128.2, 126.69, 126.66, 126.6, 126.4, 126.3, 126.0, 125.3, 123.2, 123.1, 56.0, 51.8, 48.8, 27.4

Compound known in literature⁵

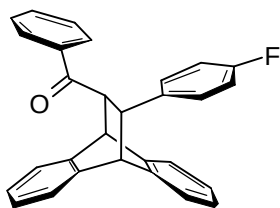


1b. White solid, 20% yield, n-hexane/DCM = 1:1;

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.84–7.79 (m, 2H), 7.58–7.53 (m, 1H), 7.47–7.41 (m, 3H), 7.38–7.35 (m, 1H), 7.27–7.23 (m, 1H), 7.20–7.13 (m, 3H), 7.12–7.05 (m, 2H), 6.98–6.94 (m, 2H), 6.58–6.53 (m, 2H), 4.61 (d, J = 2.0 Hz, 1H), 4.31 (d, J = 2.1 Hz, 1H), 3.90 (dd, J = 5.9 Hz, 2.1 Hz, 1H), 3.80 (dd, J = 5.9 Hz, 2.1 Hz, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 198.8, 144.2, 143.3, 141.5, 140.5, 139.1, 136.8, 136.2, 133.0, 129.0, 128.7, 128.5, 128.1, 126.7, 126.6, 126.3, 126.2, 126.0, 125.2, 123.2, 123.1, 56.0, 52.0, 48.8, 27.0, 21.1.

Compound known in literature⁵

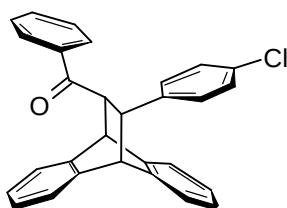


1c. White solid, 80% yield, n-hexane/DCM = 1:1;

^1H NMR (700 MHz, CDCl_3) δ [ppm] 7.83–7.78 (m, 2H), 7.59–7.54 (m, 1H), 7.49–7.43 (m, 3H), 7.37 (d, $J = 7.3$ Hz, 1H), 7.28–7.24 (m, 1H), 7.21–7.15 (m, 2H), 7.14–7.07 (m, 3H), 6.86–6.80 (m, 2H), 6.63–6.59 (m, 2H), 4.63 (d, $J = 1.9$ Hz, 1H), 4.29 (d, $J = 2.0$ Hz, 1H), 3.85 (dd, $J = 5.9$ Hz, 2.0 Hz, 1H), 3.83 (dd, $J = 5.9$ Hz, 2.0 Hz, 1H).

^{13}C NMR (175 MHz, CDCl_3) δ [ppm] 198.6, 161.7 (d, $J_{\text{C-F}} = 244.9$ Hz), 143.9, 143.3, 141.2, 139.2 (d, $J_{\text{C-F}} = 3.2$ Hz), 138.9, 136.7, 133.1, 129.6 (d, $J_{\text{C-F}} = 7.8$ Hz), 128.8, 128.5, 126.7, 126.6, 126.5, 126.3, 126.1, 125.3, 123.2, 123.2, 115.1 (d, $J_{\text{C-F}} = 21$ Hz), 56.2, 51.9, 48.7, 46.6.

HRMS (ES^+): calculated for $\text{C}_{29}\text{H}_{22}\text{FO}$ (MH^+): 405.1649, found 405.1642.

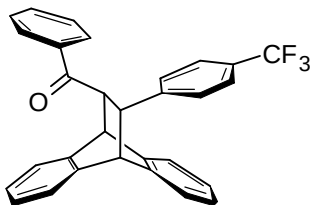


1d. White solid, 85% yield, n-hexane/DCM = 1:1;

^1H NMR (700 MHz, CDCl_3) δ [ppm] 7.82–7.79 (m, 2H), 7.59–7.54 (m, 1H), 7.47–7.42 (m, 3H), 7.36 (d, $J = 7.3$ Hz, 1H), 7.27–7.23 (m, 1H), 7.20–7.13 (m, 2H), 7.13–7.08 (m, 4H), 7.06 (d, $J = 7.1$ Hz, 1H), 6.60–6.53 (m, 2H), 4.62 (d, $J = 1.7$ Hz, 1H), 4.28 (d, $J = 1.8$ Hz, 1H), 3.84 (dd, $J = 5.8$ Hz, 1.9 Hz, 1H), 3.82 (dd, $J = 5.8$ Hz, 1.9 Hz, 1H).

^{13}C NMR (175 MHz, CDCl_3) δ [ppm] 198.5, 143.8, 143.2, 142.0, 141.0, 138.9, 136.7, 133.1, 132.5, 129.5, 128.8, 128.5, 128.5, 126.7, 126.7, 126.6, 126.4, 126.1, 125.3, 123.3, 123.2, 56.1, 51.7, 48.7, 46.7.

Compound known in literature⁵

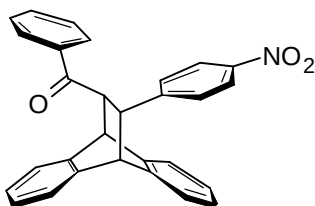


1e. White solid, 95% yield, n-hexane/DCM = 1:1;

^1H NMR (700 MHz, CDCl_3) δ [ppm] 7.85–7.79 (m, 2H), 7.61–7.54 (m, 1H), 7.49–7.43 (m, 3H), 7.41–7.36 (m, 3H), 7.29–7.26 (m, 1H), 7.21–7.14 (m, 2H), 7.14–7.08 (m, 2H), 7.05 (d, $J = 7.1$ Hz, 1H), 6.79–6.74 (m, 2H), 4.64 (d, $J = 2.0$ Hz, 1H), 4.32 (d, $J = 2.1$ Hz, 1H), 3.93 (dd, $J = 5.8$ Hz, 2.1 Hz, 1H), 3.88 (dd, $J = 5.8$ Hz, 2.1 Hz, 1H).

^{13}C NMR (175 MHz, CDCl_3) δ [ppm] 198.2, 147.6, 143.7, 143.2, 140.9, 138.8, 136.6, 133.2, 129.0 (q, $J_{\text{C-F}} = 32.5$ Hz), 128.9, 128.5, 128.5, 126.8, 126.7, 126.5, 126.2, 125.3 (q, $J_{\text{C-F}} = 3.5$ Hz), 125.3, 124.3 (q, $J_{\text{C-F}} = 271.9$ Hz), 123.3, 123.2, 56.0, 51.4, 48.7, 47.0.

HRMS (ES^+): calculated for $\text{C}_{30}\text{H}_{22}\text{F}_3\text{O}$ (MH^+): 455.1617, found 455.1619.

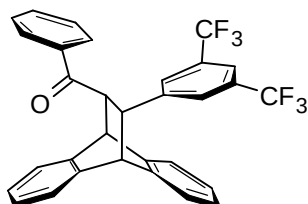


1f. White solid, 96% yield, n-hexane/DCM = 1:1;

^1H NMR (700 MHz, CDCl_3) δ [ppm] 7.99 (d, $J = 8.8$ Hz, 2H), 7.86–7.79 (m, 2H), 7.59 (t, $J = 7.4$ Hz, 1H), 7.53–7.43 (m, 3H), 7.38 (d, $J = 7.3$ Hz, 1H), 7.28 (td, $J = 7.5$ Hz, 1.0 Hz, 1H), 7.23–7.14 (m, 2H), 7.14–7.07 (m, 2H), 7.04 (d, $J = 7.4$ Hz, 1H), 6.82–6.77 (m, 2H), 4.69 (d, $J = 1.9$ Hz, 1H), 4.32 (d, $J = 2.0$ Hz, 1H), 4.02 (dd, $J = 5.6$ Hz, 2.1 Hz, 1H), 3.88 (dd, $J = 5.7$ Hz, 2.1 Hz, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 197.9, 151.2, 146.8, 143.3, 143.0, 140.5, 138.7, 136.4, 133.4, 129.0, 129.0, 128.4, 126.9, 126.6, 126.6, 126.4, 125.2, 123.6, 123.4, 55.9, 51.3, 48.7, 47.0.

HRMS (ES⁺): calculated for C₂₉H₂₂NO₃ (MH⁺): 432.1594, found 432.1592.



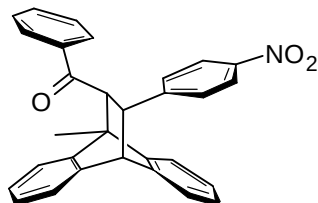
1g. White solid, 99% yield, n-hexane/DCM = 1:1;

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.87–7.83 (m, 2H), 7.68–7.65 (m, 1H), 7.63–7.58 (m, 1H), 7.54–7.47 (m, 3H), 7.42–7.38 (m, 1H), 7.31 (td, J = 7.5 Hz, 1.2 Hz, 1H), 7.24–7.15 (m, 2H), 7.11 (td, J = 7.4 Hz, 1.2 Hz, 1H), 7.09–6.99 (m, 4H), 4.70 (d, J = 2.2 Hz, 1H), 4.29 (d, J = 2.2 Hz, 1H), 4.10 (dd, J = 5.4 Hz, 2.3 Hz, 1H), 3.82 (dd, J = 5.4 Hz,

2.2 Hz, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 197.6, 146.1, 142.9, 142.7, 140.2, 138.5, 136.4, 133.4, 131.5 (q, J_{C-F} = 33.1 Hz), 129.0, 128.5, 128.5 (m), 127.1, 127.0, 126.7, 126.6, 126.5, 125.1, 123.6, 123.5, 122.2 (q, J_{C-F} = 272.8 Hz), 120.8 (sept, J_{C-F} = 3.8 Hz), 56.5, 51.3, 48.8, 46.6.

HRMS (ES⁺): calculated for C₃₁H₂₁F₆O (MH⁺): 523.1491, found 523.1494.



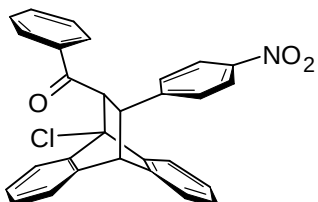
1h. White solid, 90% yield, n-hexane/DCM = 1:1;

¹H NMR (400 MHz, CDCl₃) δ [ppm] 8.03–7.98 (m, 2H), 7.71–7.65 (m, 2H), 7.54–7.41 (m, 3H), 7.39–7.26 (m, 6H), 7.21 (td, J = 7.4 Hz, 1.0 Hz, 1H), 7.14 (dd, J = 7.3 Hz, 1.0 Hz, 1H), 6.83–6.76 (m, 2H), 4.34 (d, J = 1.9 Hz, 1H), 3.88 (d, J = 6.5 Hz, 1H), 3.64 (dd, J = 6.5 Hz, 1.9 Hz, 1H), 1.93 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ [ppm] 200.7, 150.8, 146.8, 146.0, 143.7, 141.6, 140.5, 138.4, 133.3, 128.7, 128.6, 128.2, 126.7, 126.3, 126.3, 126.2, 126.1, 123.6, 123.3, 122.8, 120.7, 57.4, 52.6, 51.4, 46.6, 16.5.

HRMS (ES⁺): product decomposition during analysis, substrates found: 9-methylantracene (MH⁺ 193.10118, found 193.10117), 4-nitrochalcone (MH⁺ 254.08117, found 254.08100)

Elemental analysis: %C = 80.78% (calculated 80.88%), %N = 3.14% (calculated 3.14%), %H = 4.89% (calculated 5.20%).

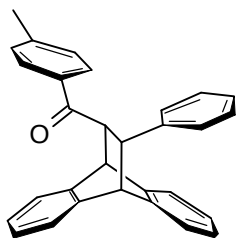


1i. White solid, 32% yield, n-hexane/DCM = 1:2;

¹H NMR (700 MHz, CDCl₃) δ [ppm] 8.01–7.98 (m, 2H), 7.87 (d, J = 7.5 Hz, 1H), 7.70 (d, J = 7.2 Hz, 1H), 7.67 (d, J = 7.6 Hz, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.43–7.36 (m, 2H), 7.36–7.29 (m, 4H), 7.26–7.22 (m, 1H), 7.10 (d, J = 7.2 Hz, 1H), 6.78–6.73 (m, 2H), 4.33–4.28 (m, 2H), 3.63 (dd, J = 6.2 Hz, 1.7 Hz, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 198.5, 149.3, 147.2, 142.7, 141.4, 138.8, 138.7, 138.2, 133.5, 128.7, 128.7, 128.6, 127.5, 127.4, 127.2, 126.8, 125.9, 124.4, 123.8, 122.7, 122.0, 72.6, 59.1, 52.9, 51.1.

HRMS (ES⁺): calculated for C₂₉H₂₁ClNO₃ (MH⁺): 466.1205, found 466.1207.

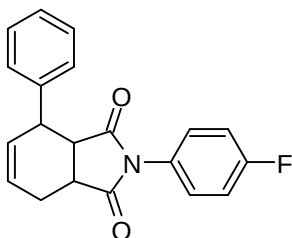


1m. White solid, 57% yield, n-hexane/DCM = 1:1;

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.74–7.71 (m, 2H), 7.45 (d, J = 7.3 Hz, 1H), 7.36 (d, J = 7.3 Hz, 1H), 7.26–7.21 (m, 3H), 7.19–7.12 (m, 6H), 7.11–7.05 (m, 2H), 6.71–6.63 (m, 2H), 4.61 (d, J = 1.8 Hz, 1H), 4.33 (d = J = 2.0 Hz, 1H), 3.90 (dd, J = 5.9 Hz, 2.0 Hz, 1H), 3.83 (dd, J = 5.9 Hz, 2.0 Hz, 1H), 2.41 (s, 3H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 198.3, 144.2, 143.8, 143.6, 143.5, 141.4, 139.2, 134.3, 129.4, 128.7, 128.3, 128.2, 126.7, 126.6, 126.5, 126.3, 126.2, 126.0, 125.3, 123.2, 123.0, 55.8, 51.8, 48.9, 47.3, 21.7.

HRMS (ES⁺): calculated for C₃₀H₂₅O (MH⁺): 401.1900, found 401.1901.

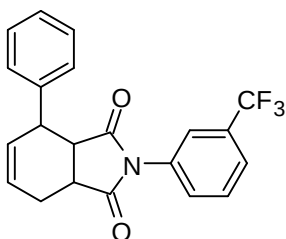


2a. White solid, 49% yield, (>99% under 0,9 GPa)

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.31–7.25 (m, 3H), 7.20–7.18 (m, 2H), 7.01–6.93 (m, 2H), 7.59–6.49 (m, 2H), 6.21–6.10 (m, 2H), (t, J = 6.3 Hz, 1H), 3.49–3.43 (m, 1H), 3.39–3.32 (m, 1H), 3.04–2.95 (m, 1H), 2.63–2.55 (m, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 178.7, 176.6, 162.2 (d, J_{C-F} = 248.2 Hz), 138.3, 129.5, 128.9, 128.7, 128.2 (d, J_{C-F} = 8.7 Hz), 127.6, 127.5 (d, J_{C-F} = 3.2 Hz), 127.0, 116.0 (d, J_{C-F} = 22.9 Hz), 44.7, 40.9, 37.9, 21.6.

HRMS (ES⁺): calculated for C₂₀H₁₇FNO₂ (MH⁺): 322.1238, found 322.1236.



2b. White solid, 56% yield, (>99% under 0,9 GPa)

¹H NMR (700 MHz, CDCl₃) δ [ppm] 7.51 (d, J = 7.8 Hz, 1H), 7.41 (t, J = 7.9 Hz, 1H), 7.30–7.25 (m, 3H), 7.18 (d, J = 6.9 Hz, 2H), 6.88 (d, J = 8.0 Hz, 1H), 6.67 (s, 1H), 6.19–6.12 (m, 2H), 4.06–3.96 (m, 1H), 3.54–3.44 (m, 1H), 3.42–3.33 (m, 1H), 3.07–2.98 (m, 1H), 2.67–2.56 (m, 1H).

¹³C NMR (175 MHz, CDCl₃) δ [ppm] 178.3, 176.4, 138.0, 132.1, 131.5 (q, J_{C-F} = 32.9 Hz), 129.8, 129.5, 129.5, 128.8, 128.6, 128.0, 126.9, 125.3 (q, J_{C-F} = 3.7 Hz), 123.6 (d, J_{C-F} = 3.8 Hz), 123.6 (d, J_{C-F} = 272.5 Hz), 44.6, 40.8, 37.8, 21.3.

HRMS (ES⁺): calculated for C₂₁H₁₇F₃NO₂ (MH⁺): 372.1206, found 372.1205.

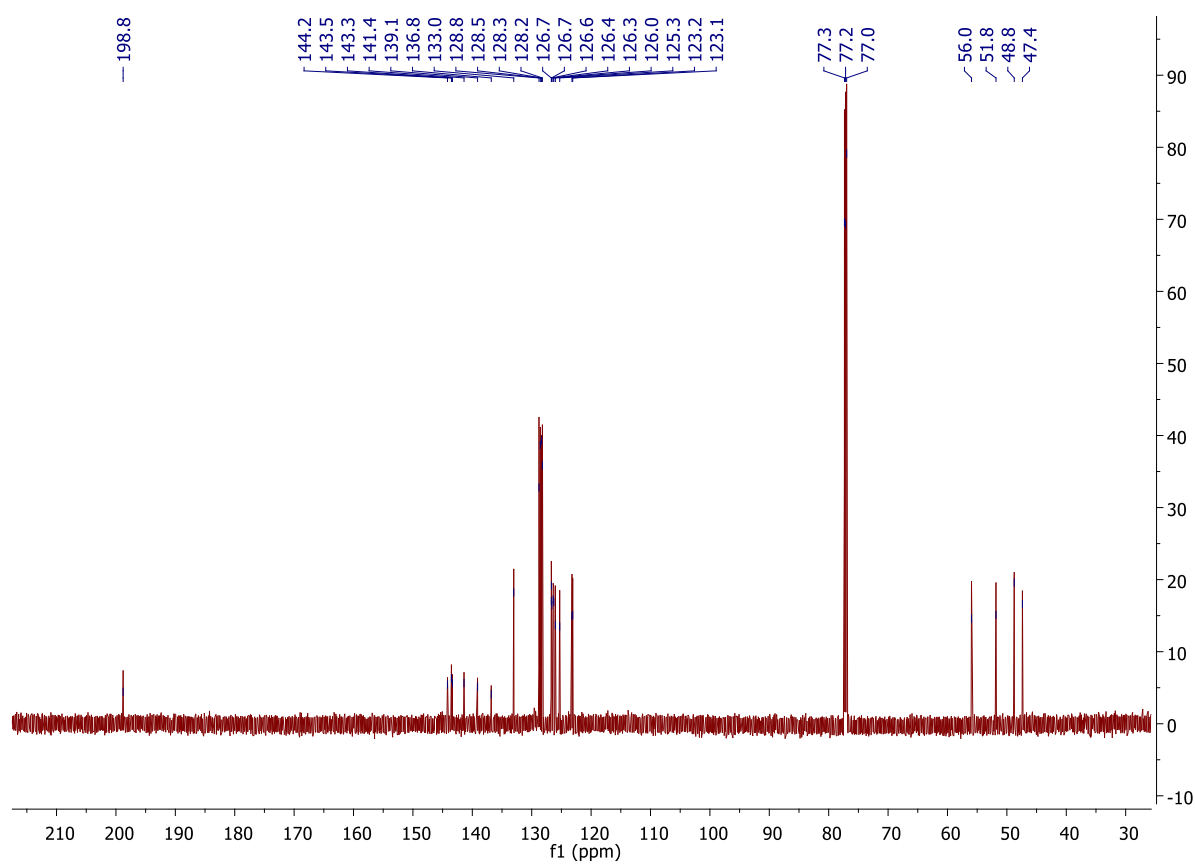
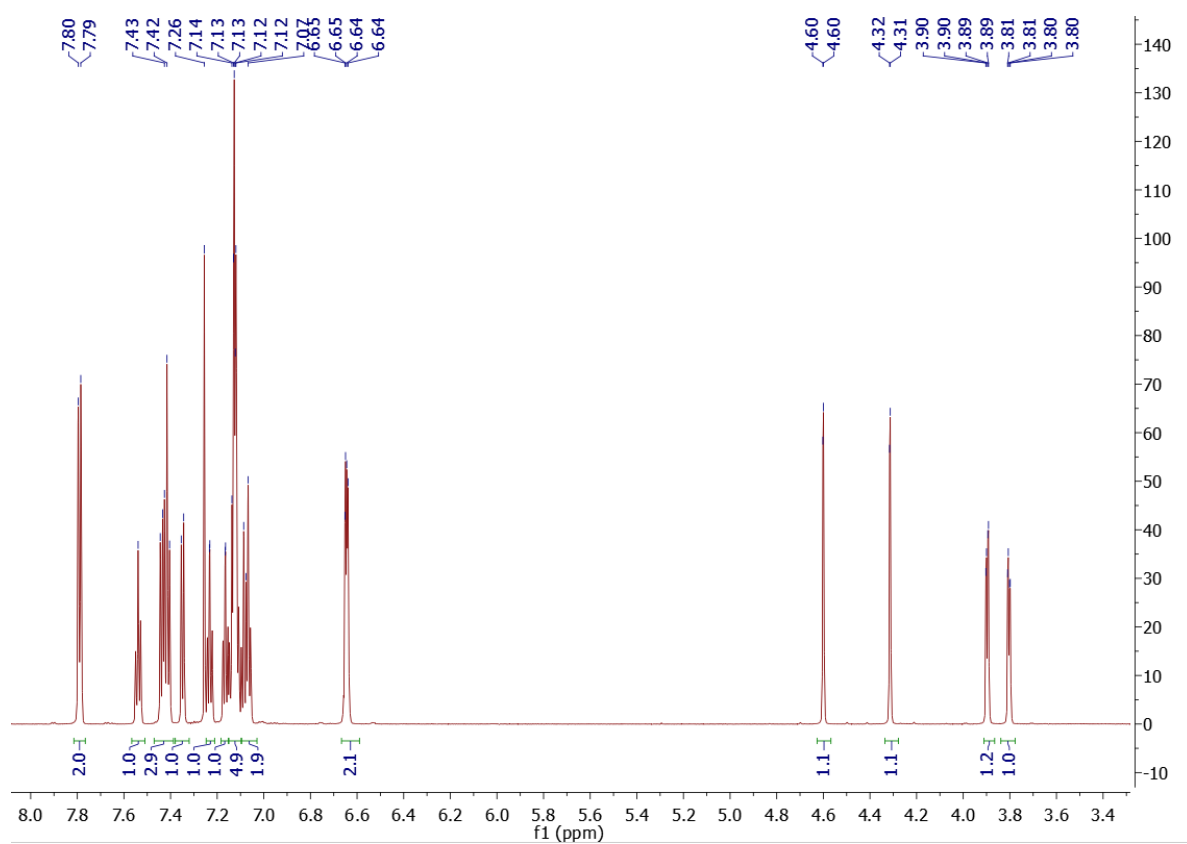
2c. 1.5% (not isolated), signals match with spectra published in patent application⁶

2d. White solid, 40% (mixture of two stereoisomers).

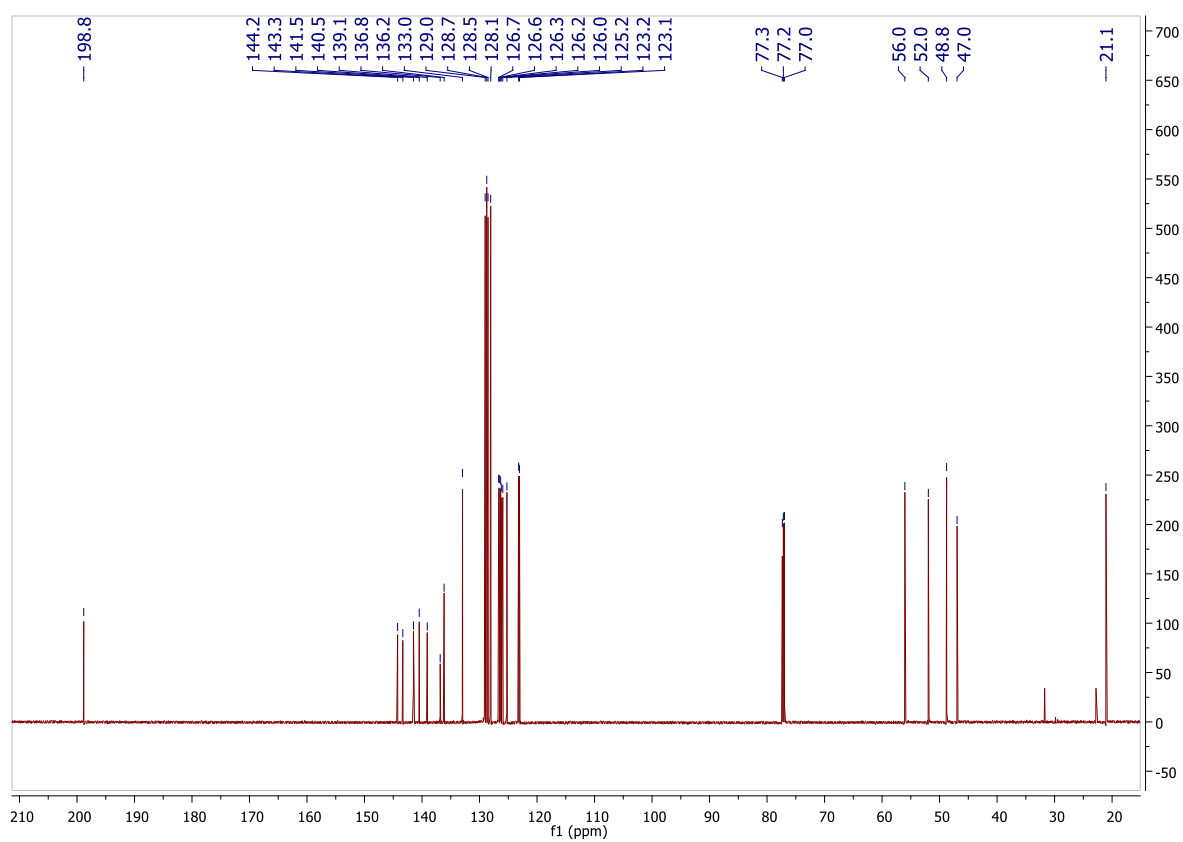
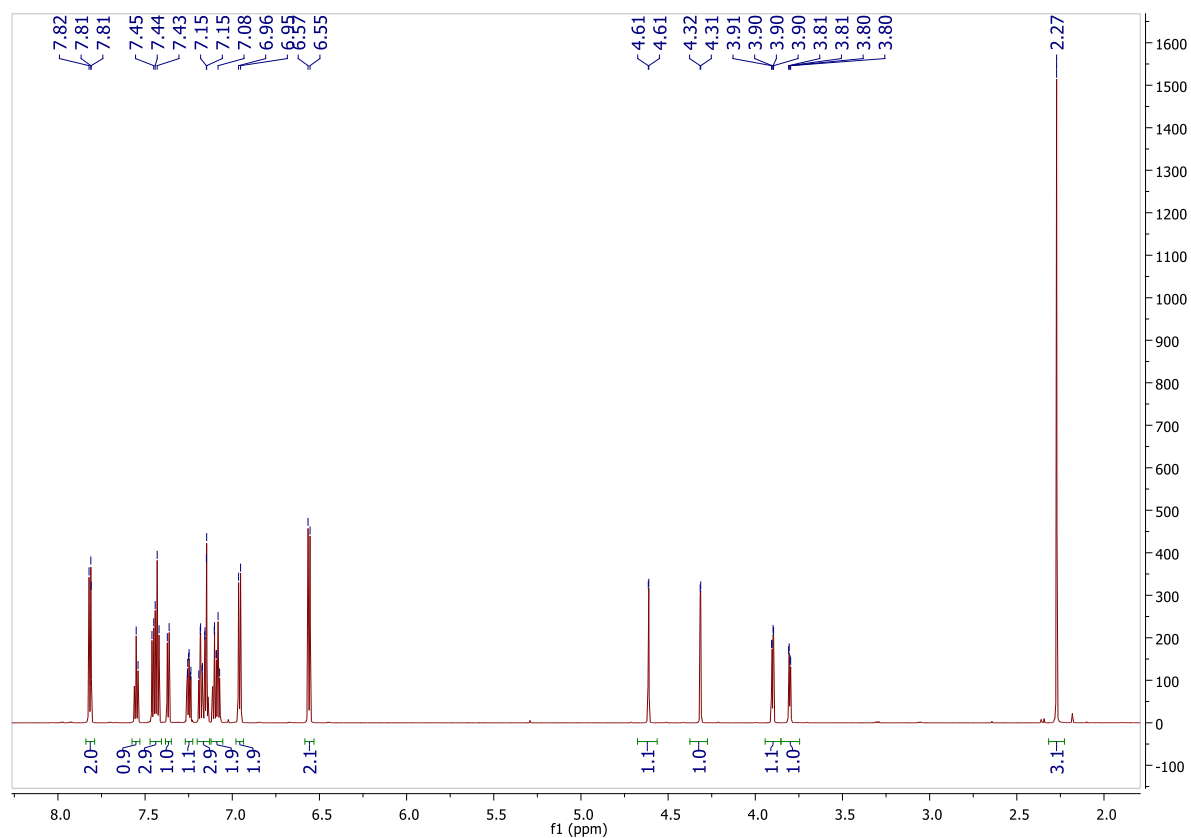
HRMS (ES⁺): calculated for C₃₁H₂₆NO₃ (MH⁺): 460.1907, found 460.1906.

Copies of NMR spectra:

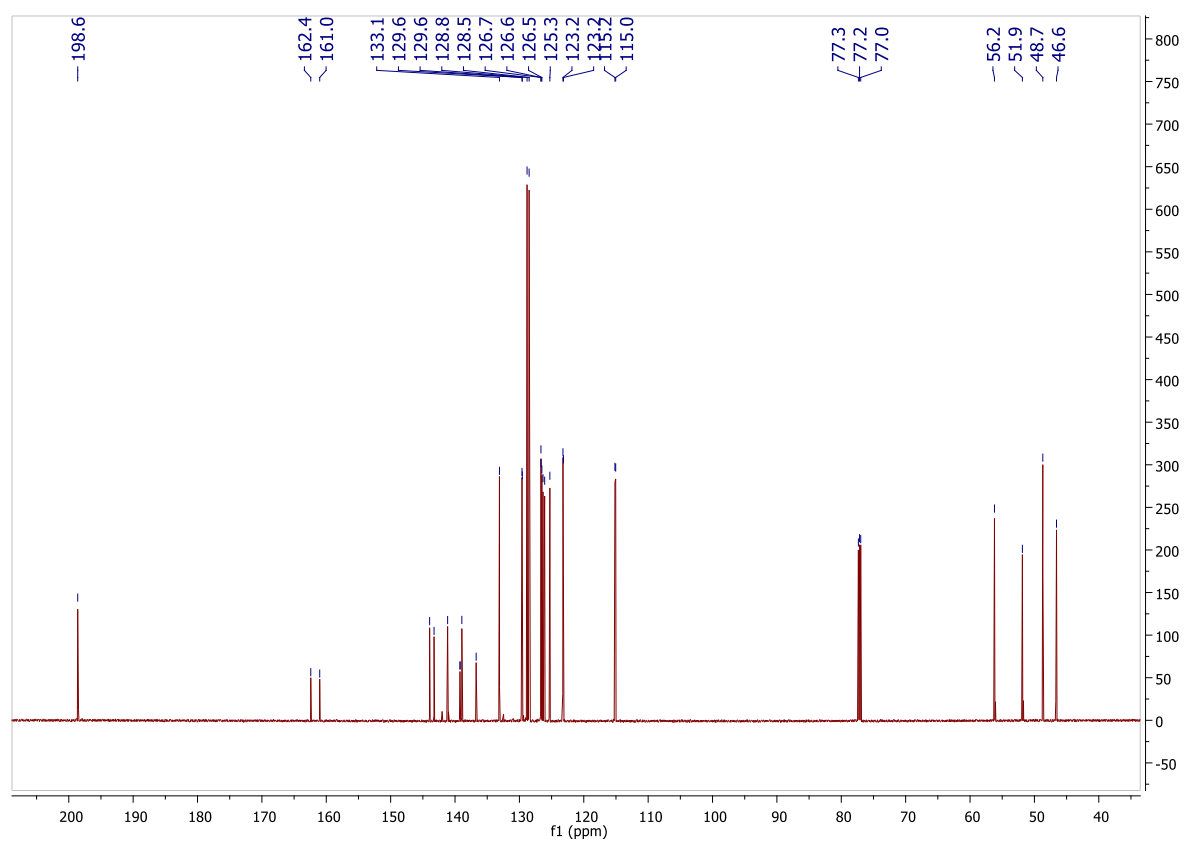
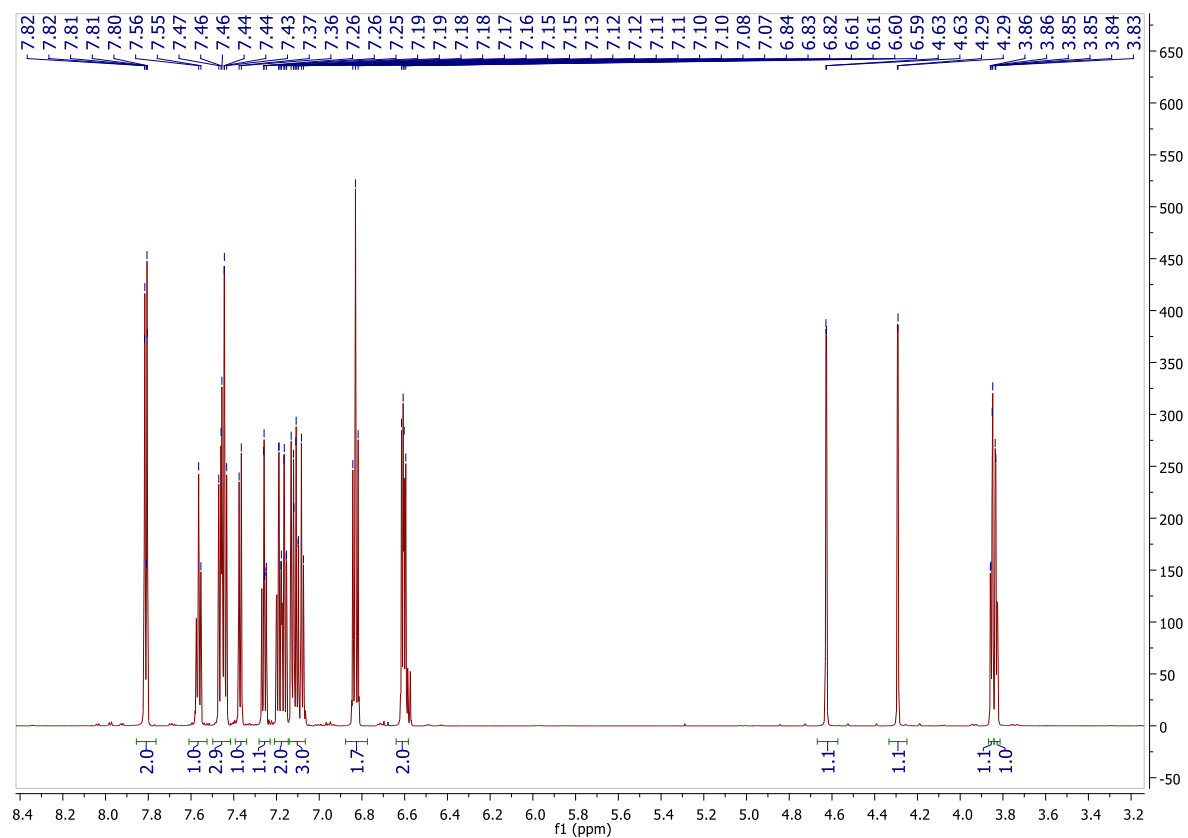
1a



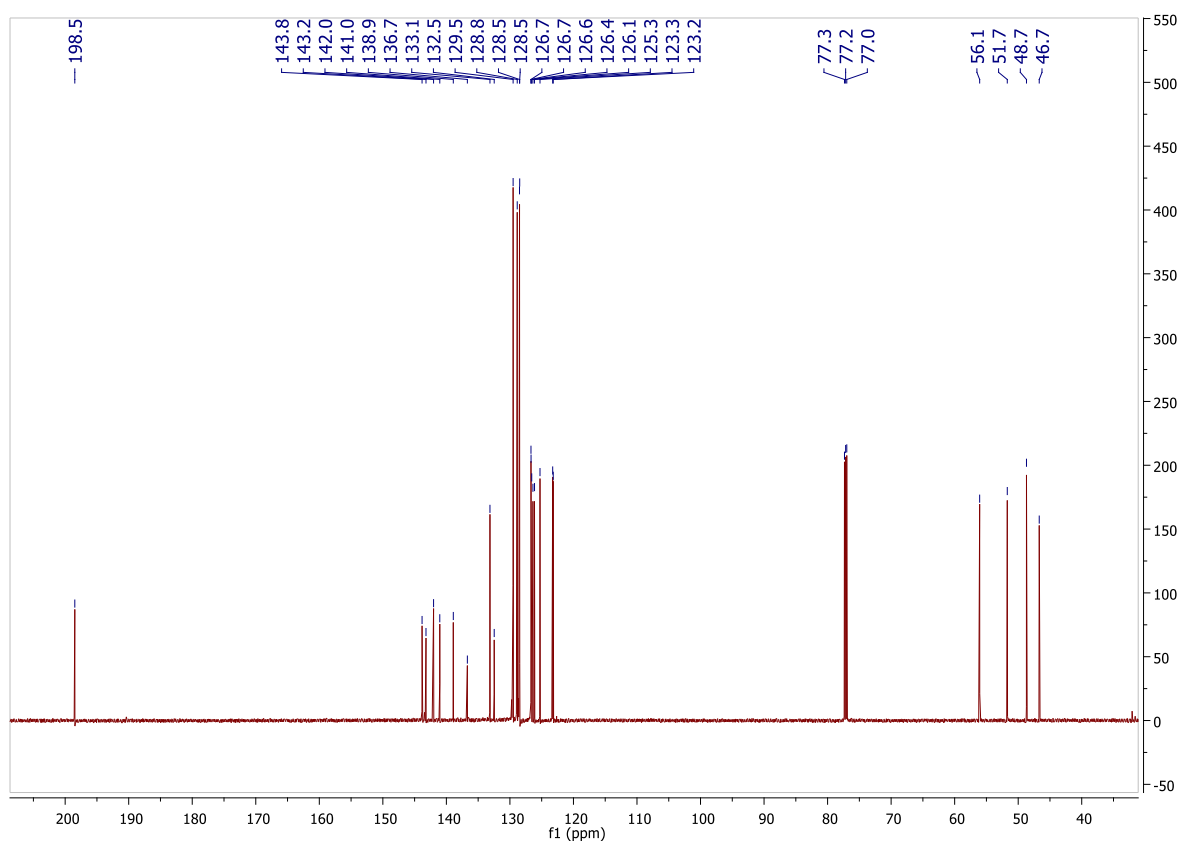
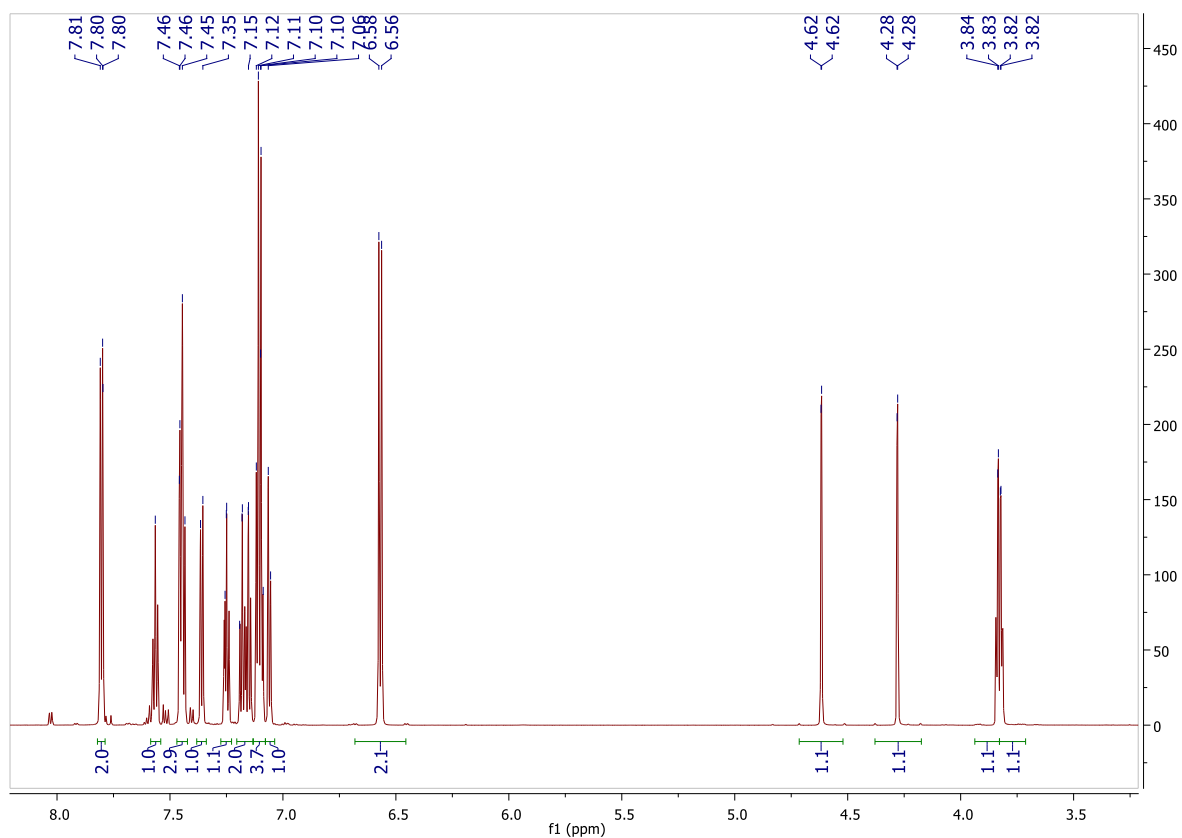
1b



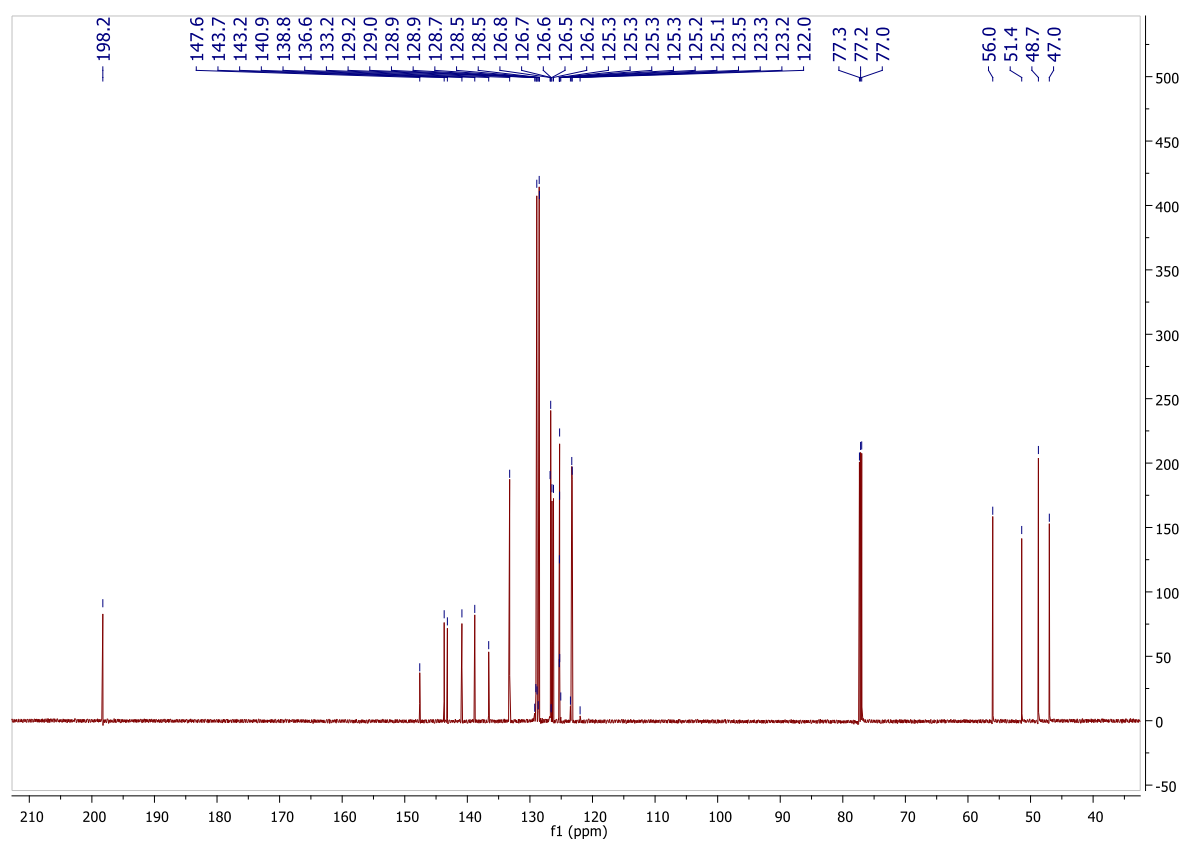
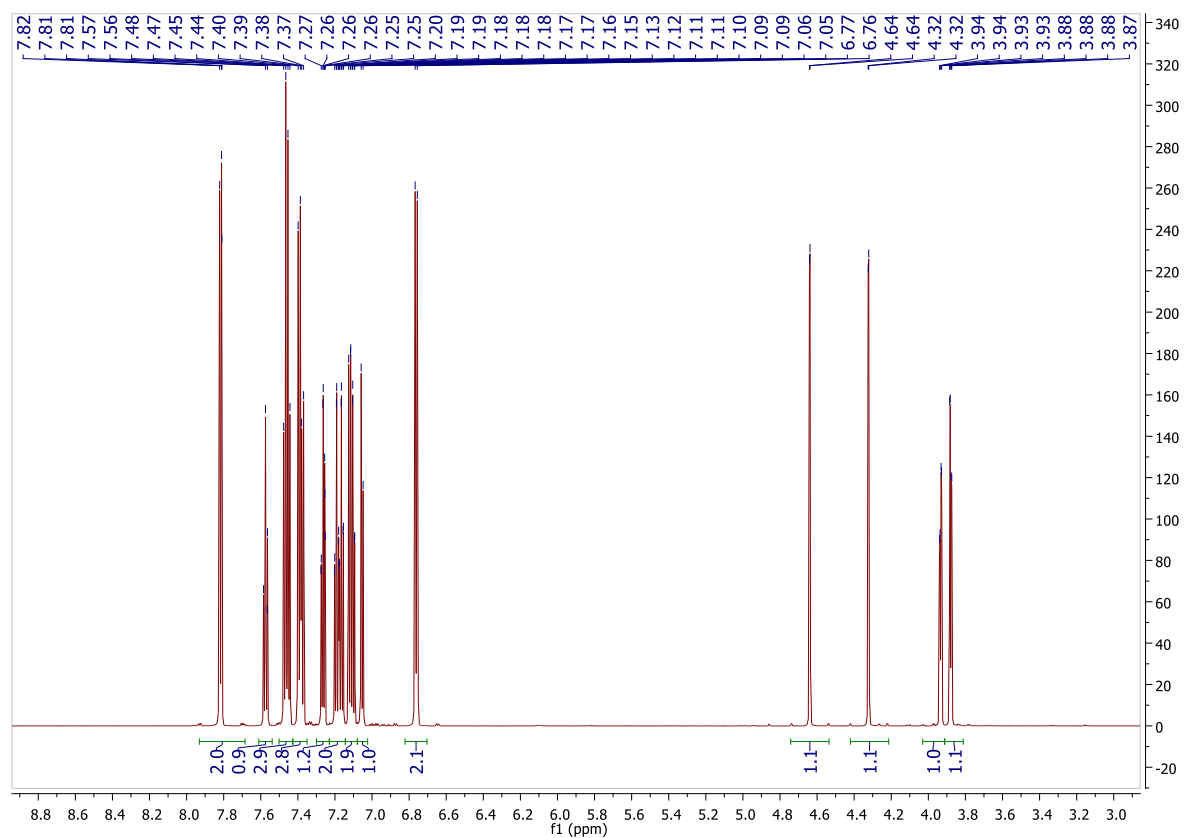
1c



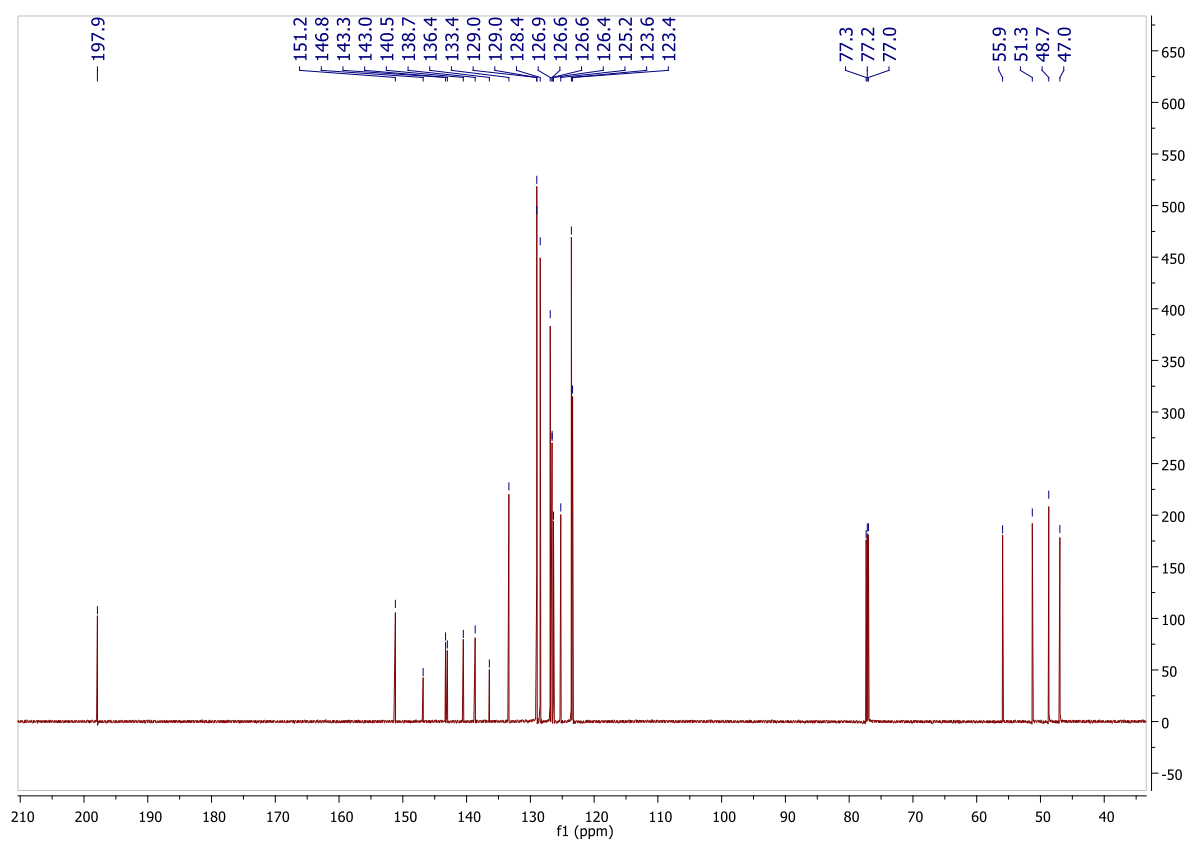
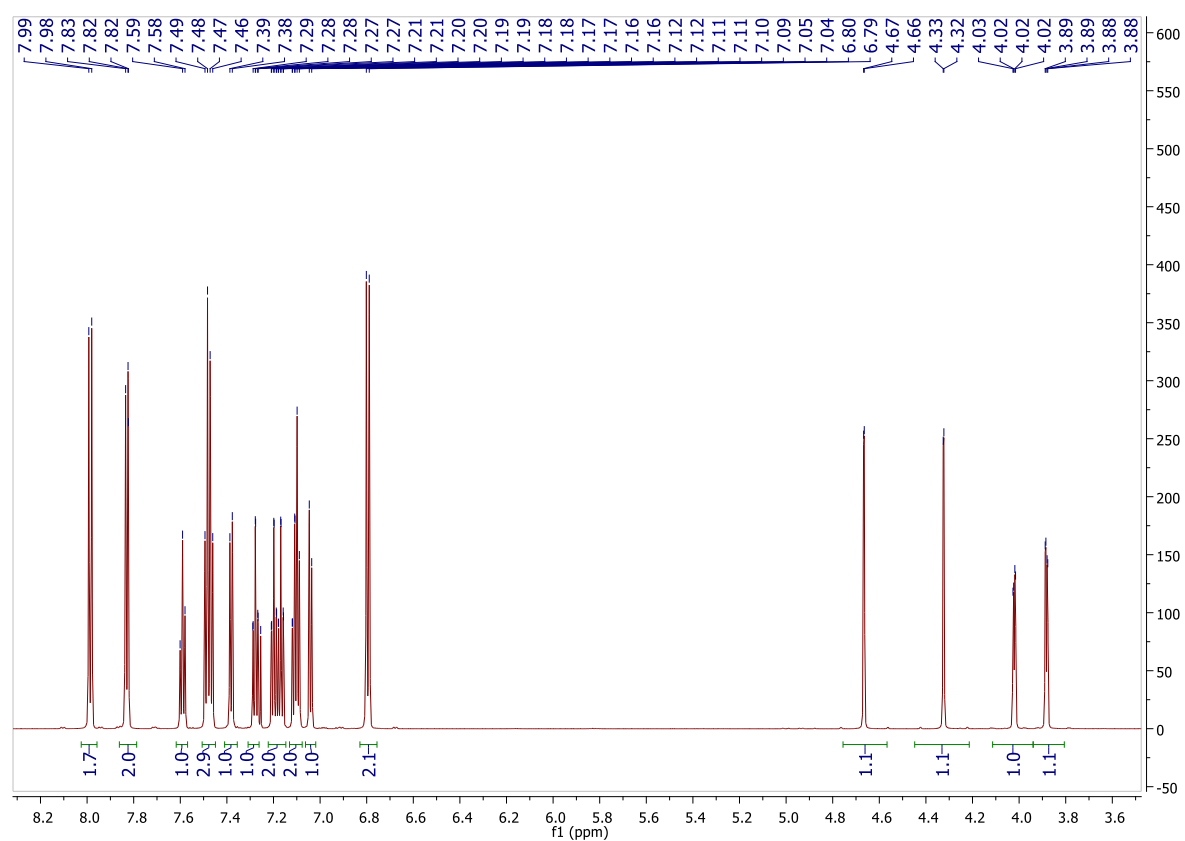
1d



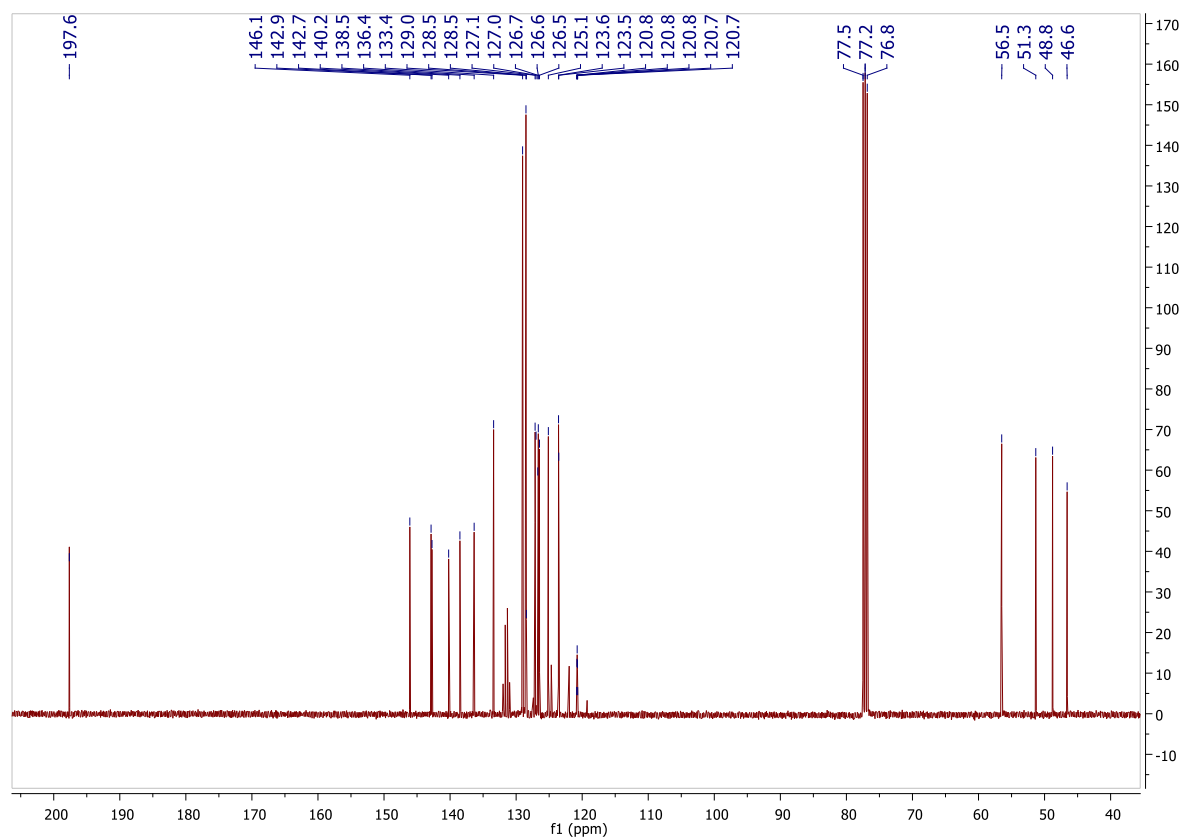
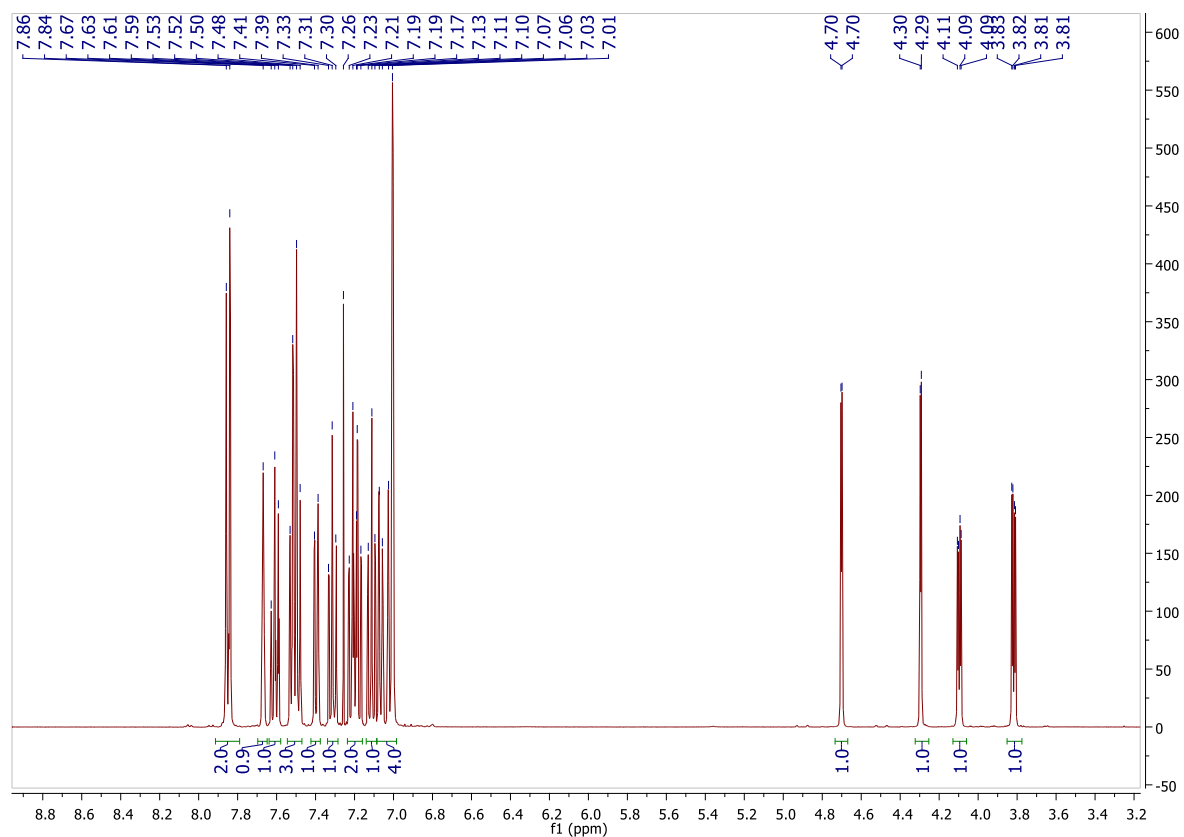
1e



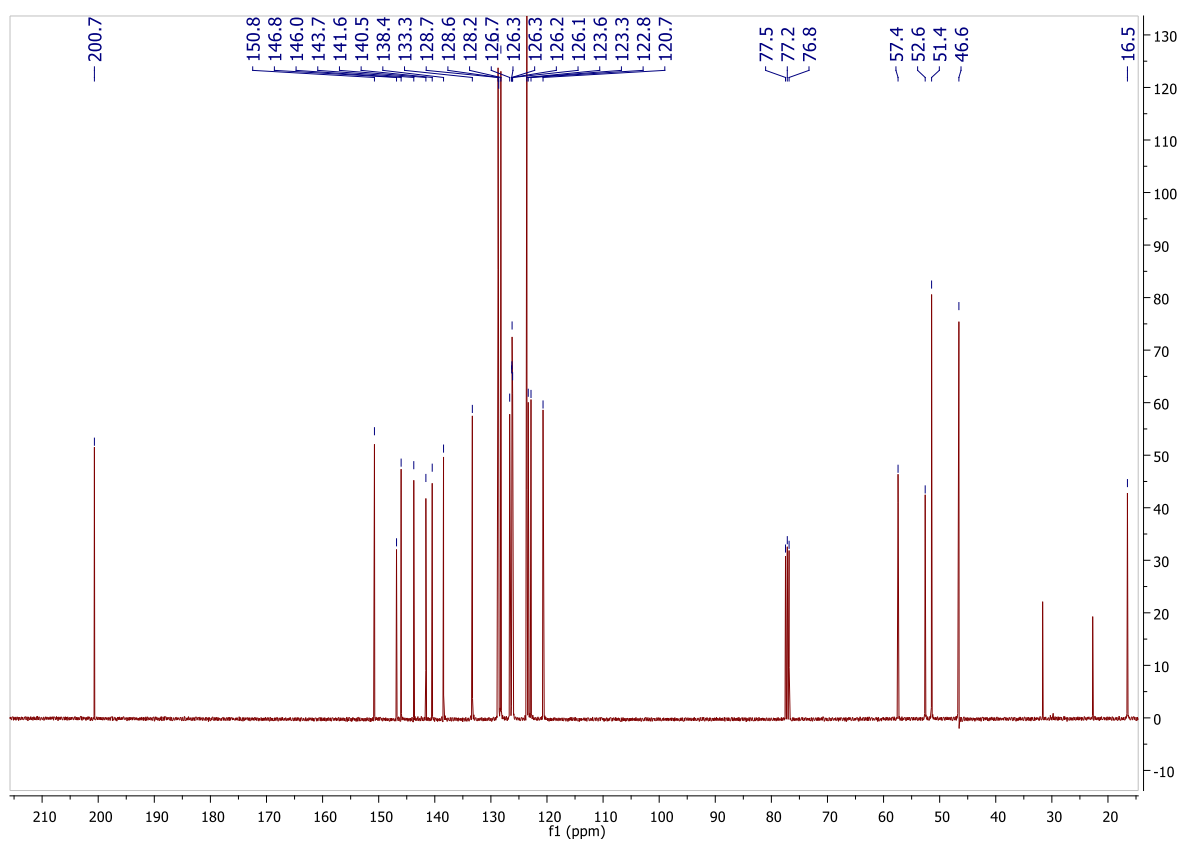
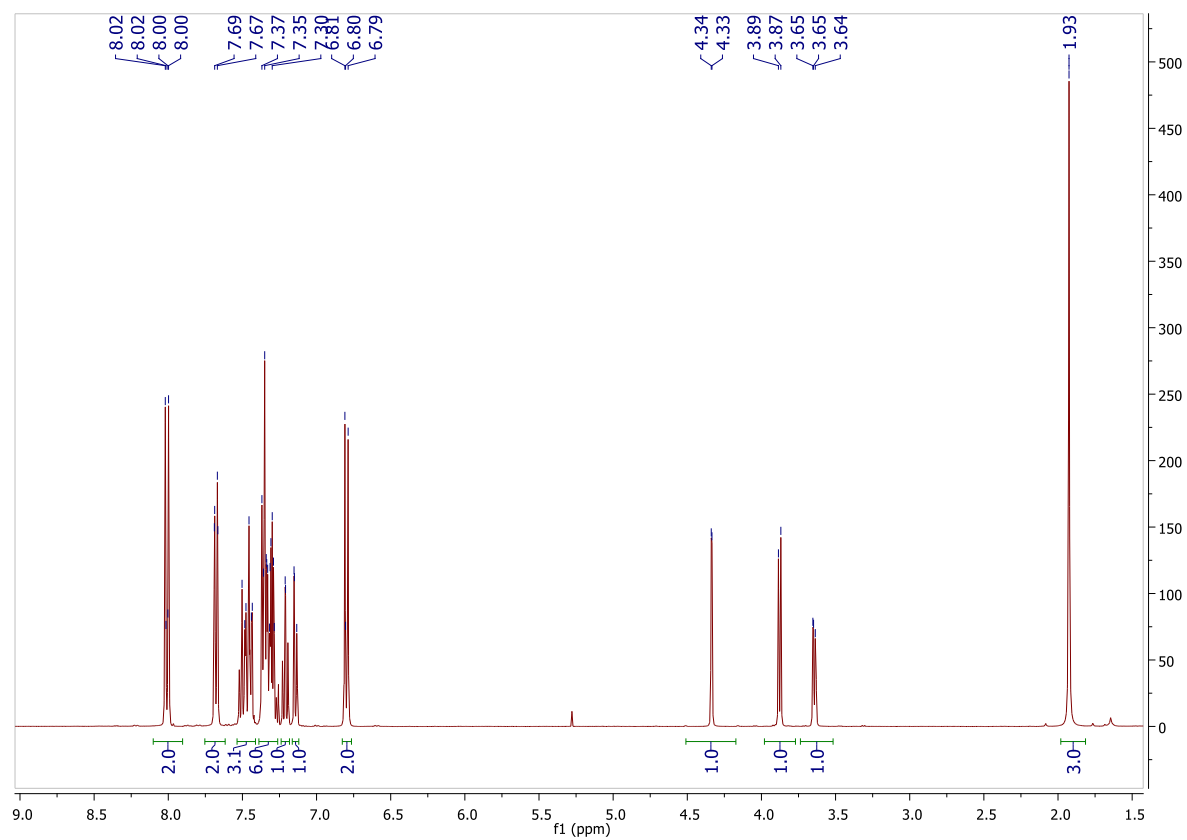
1f



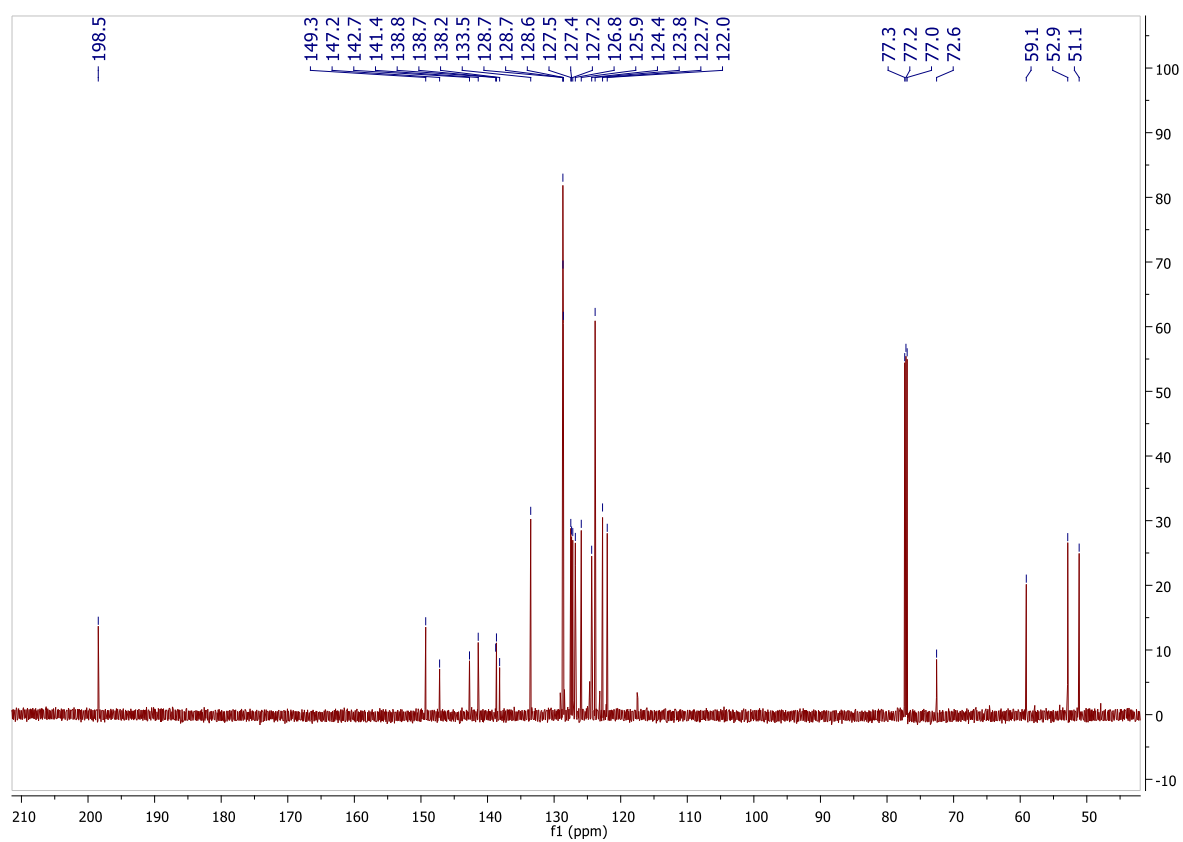
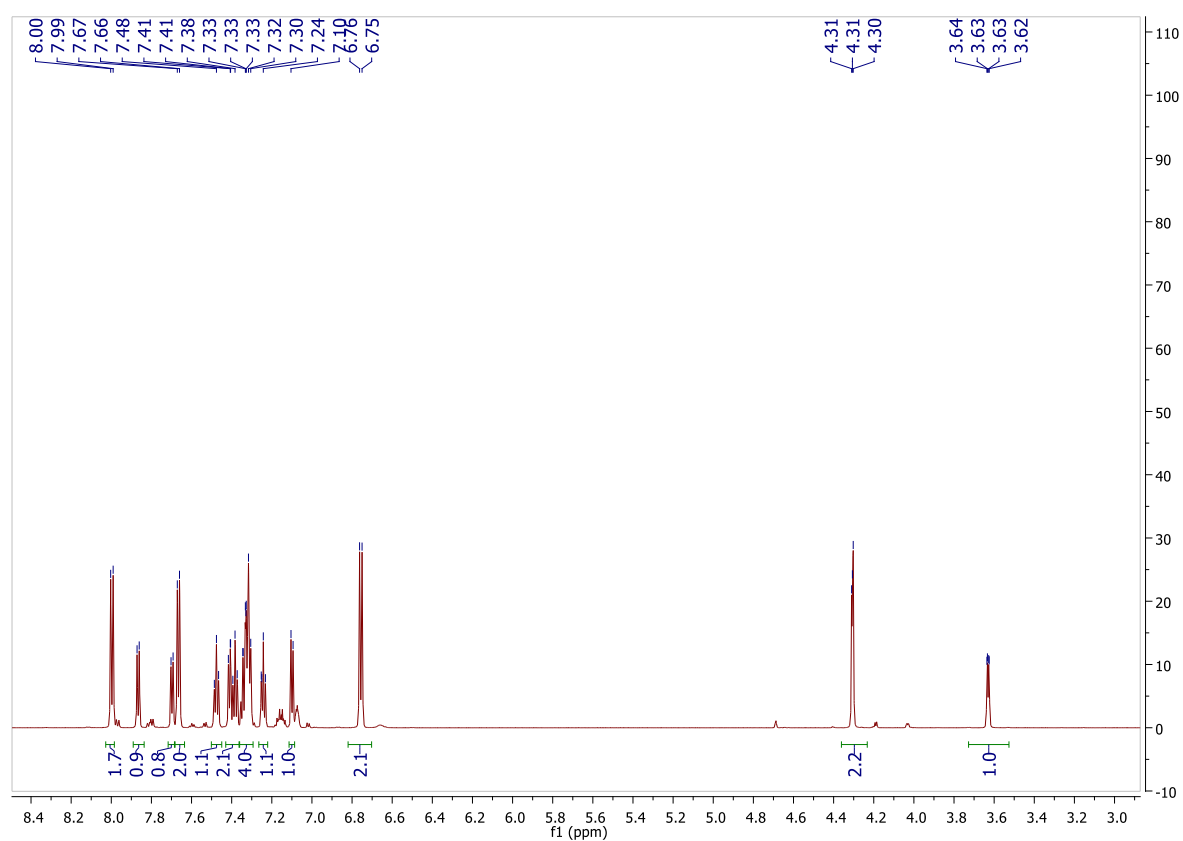
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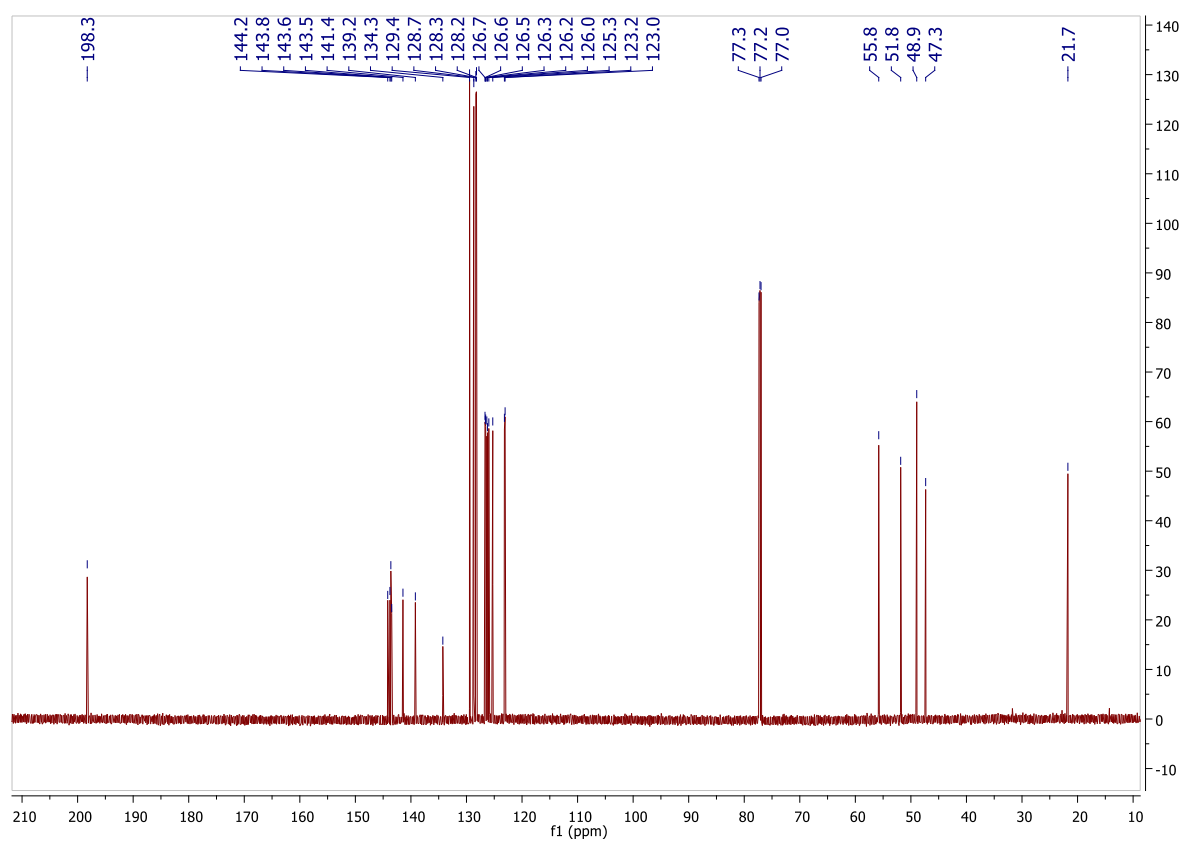
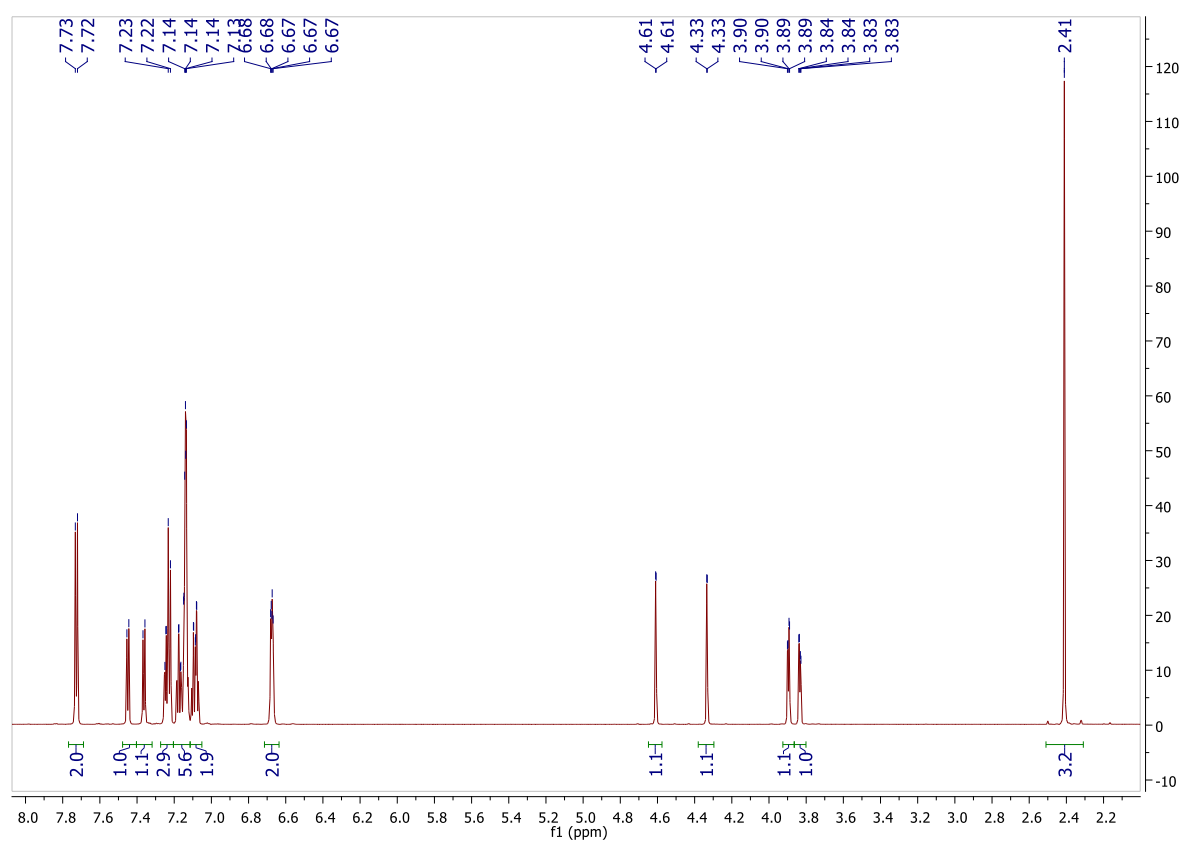
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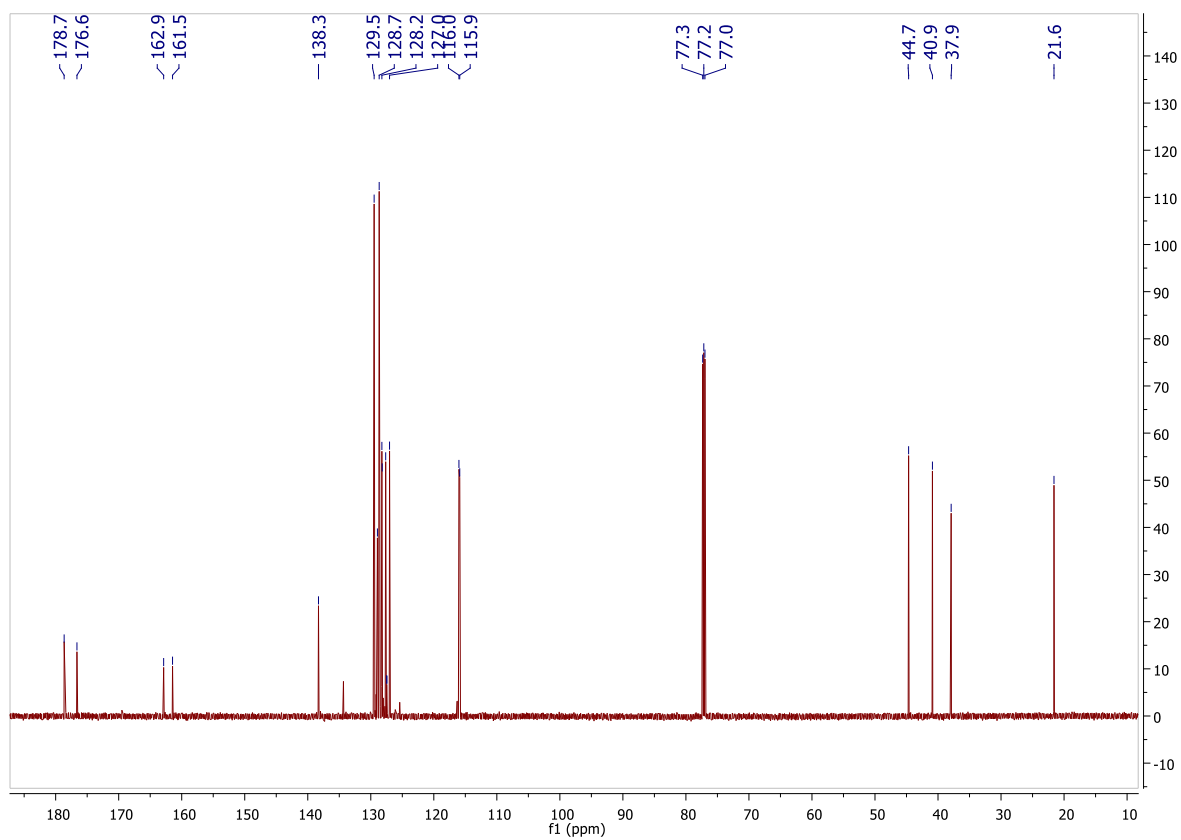
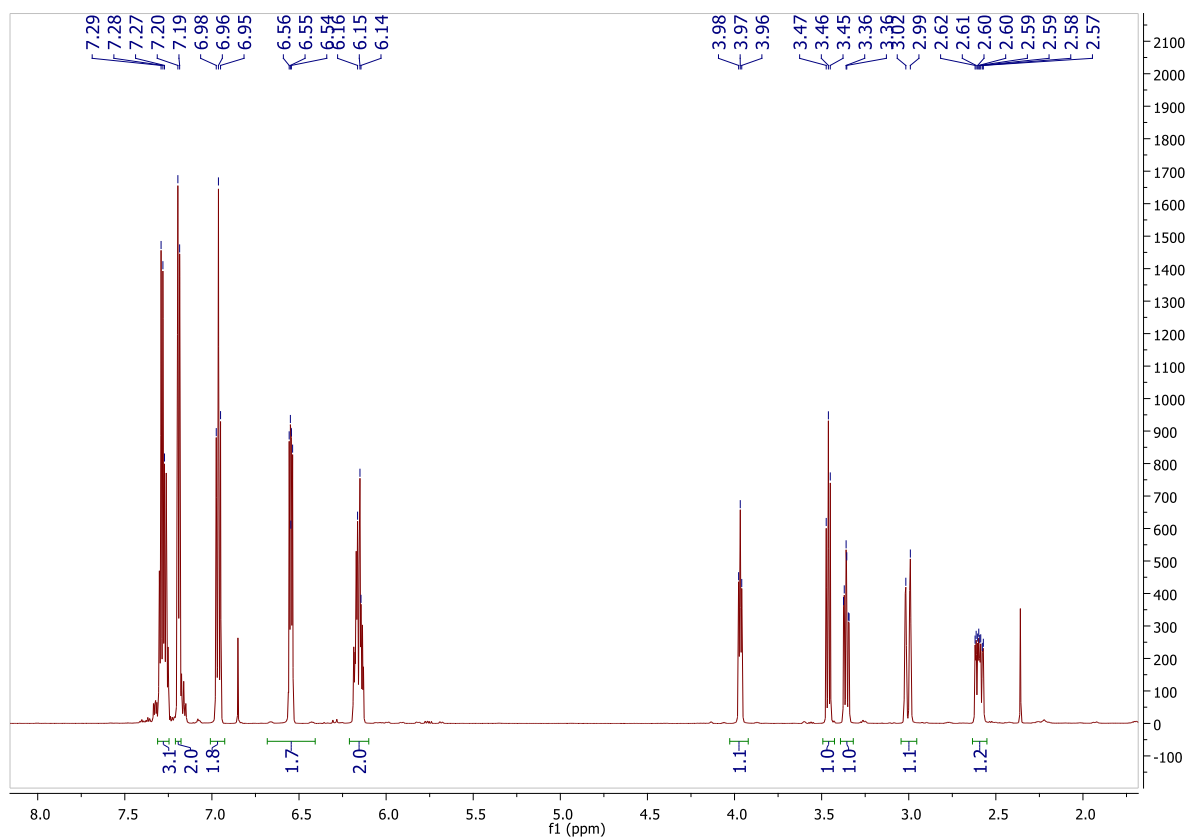
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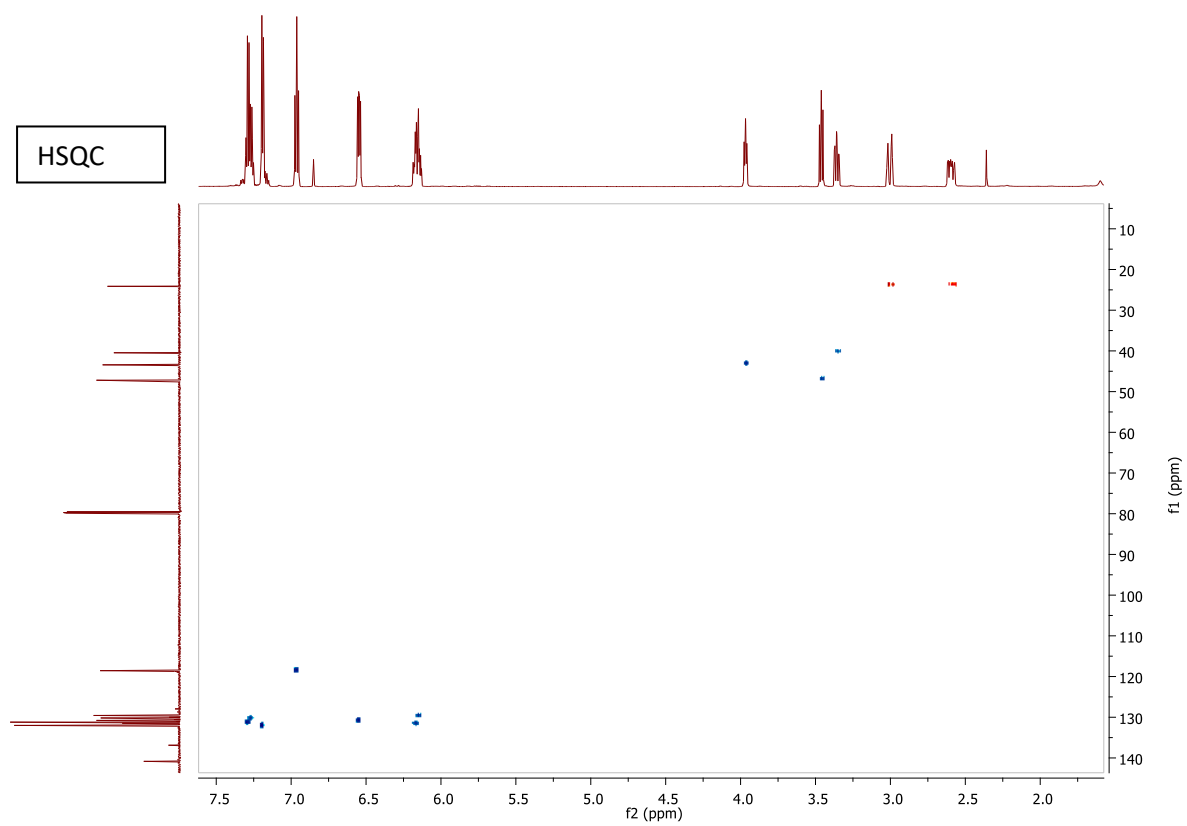
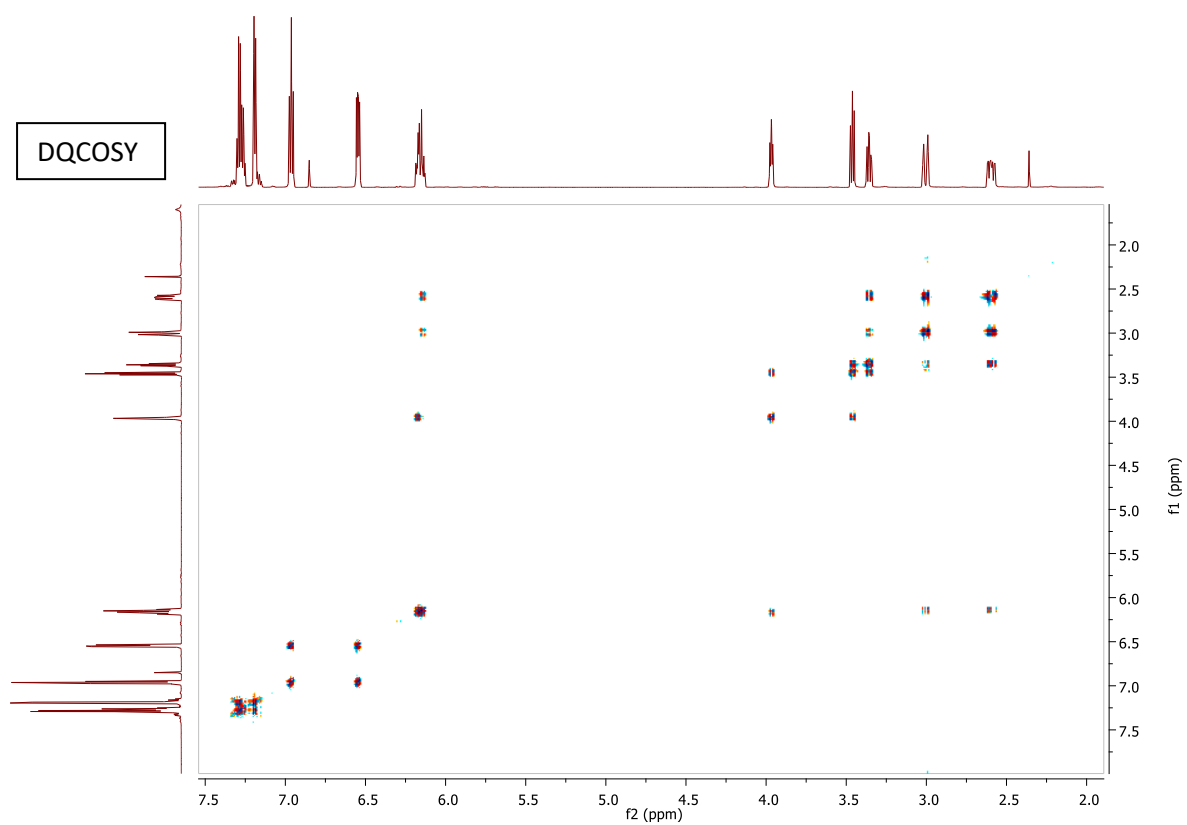


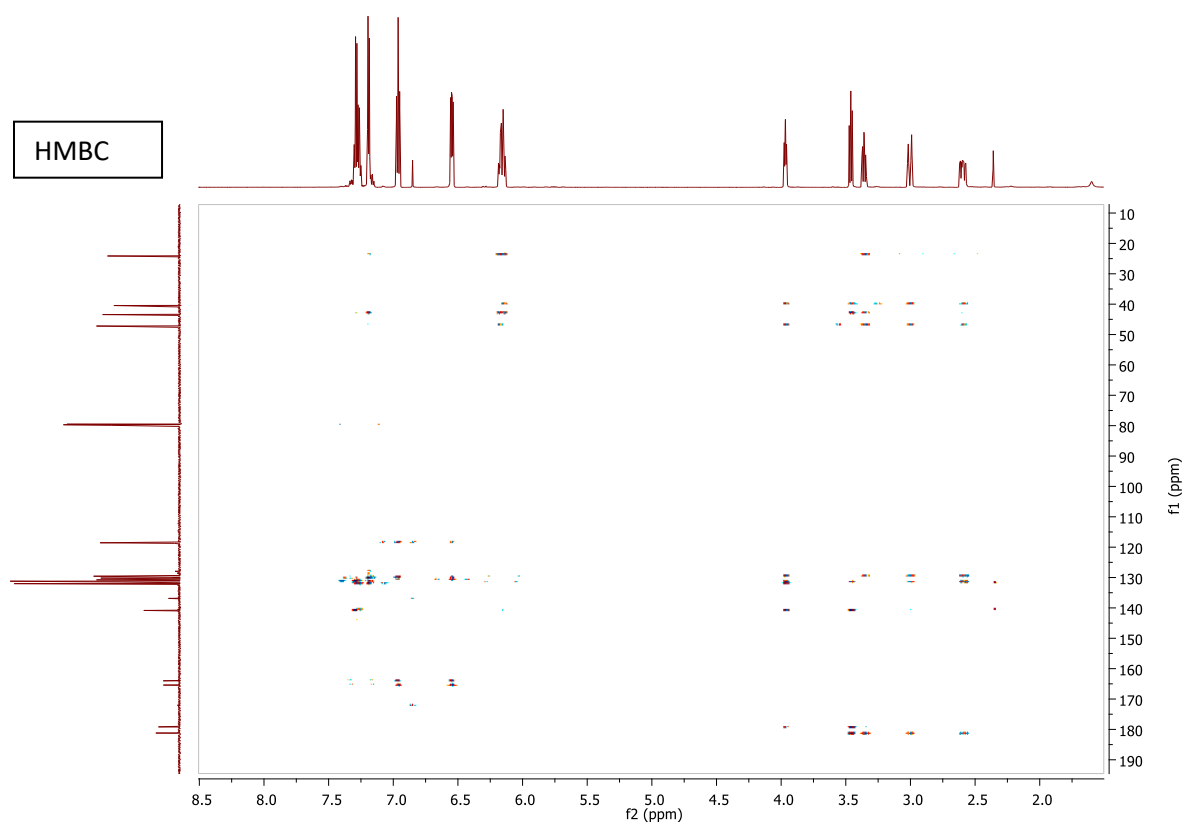
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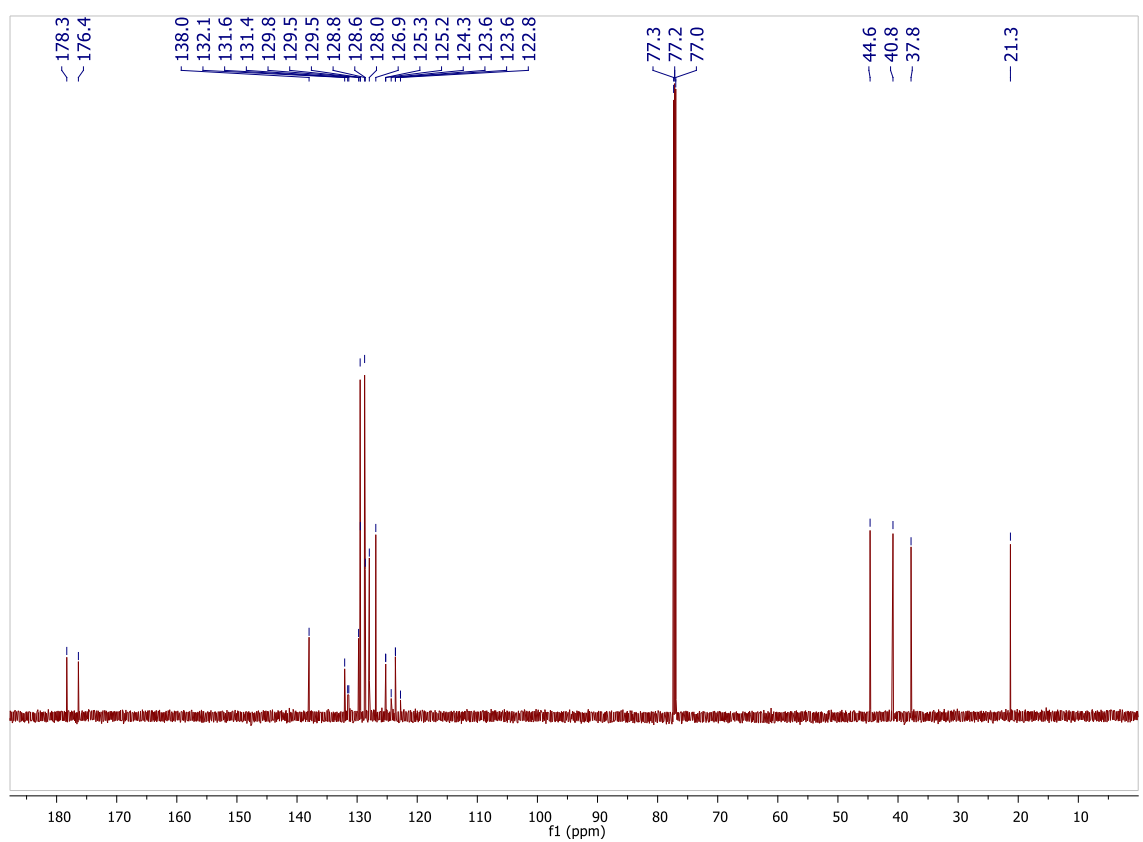
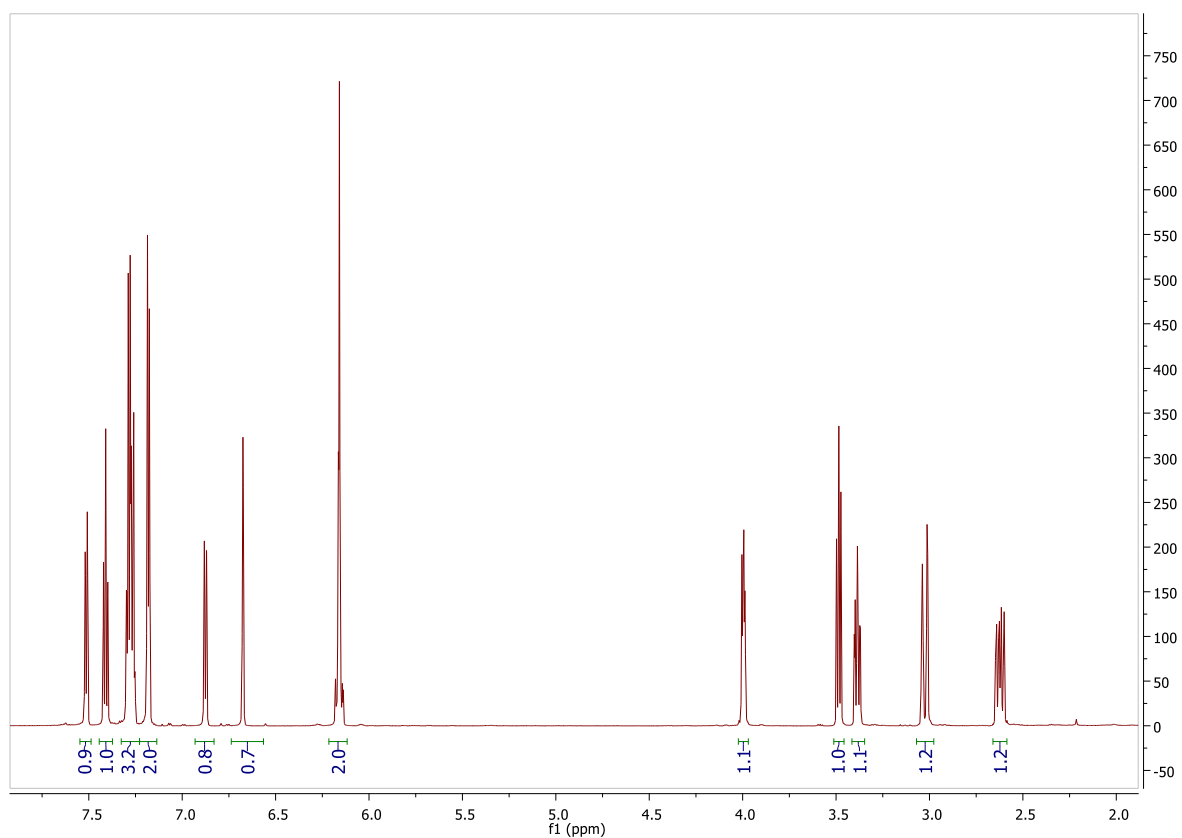
2a

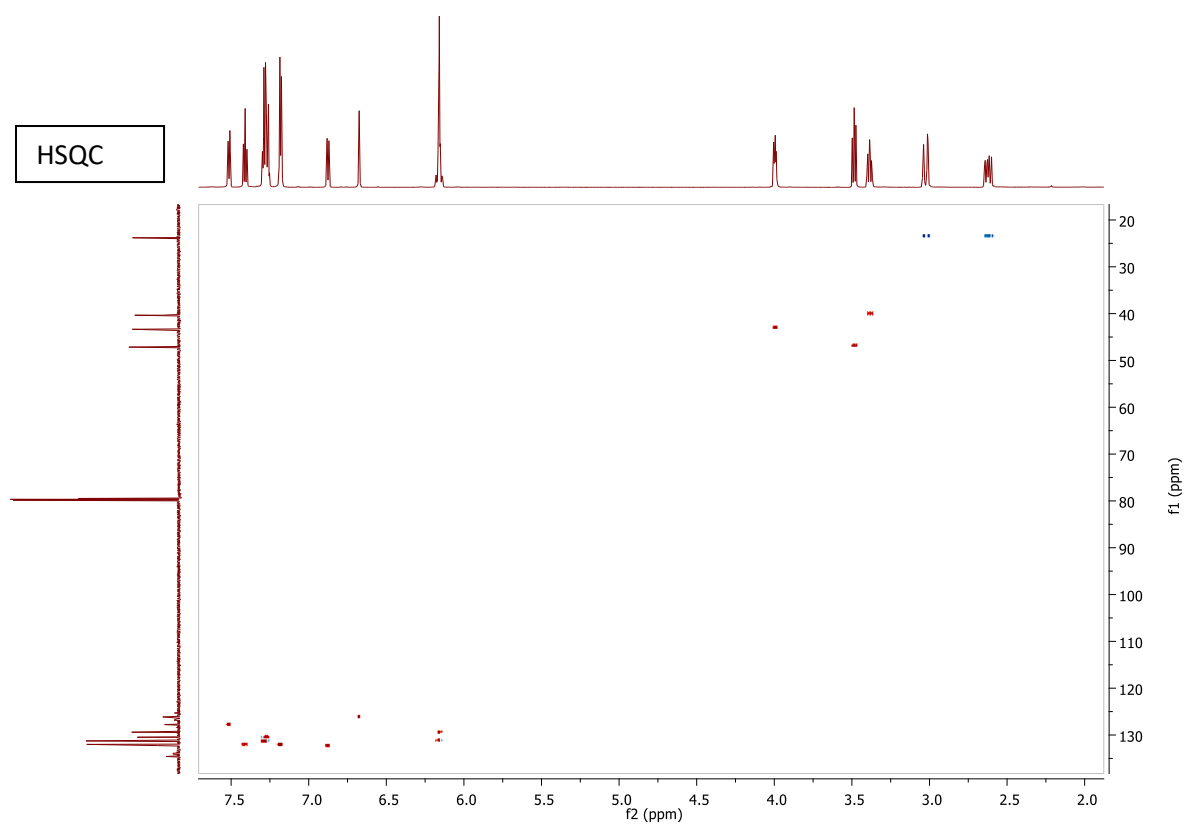
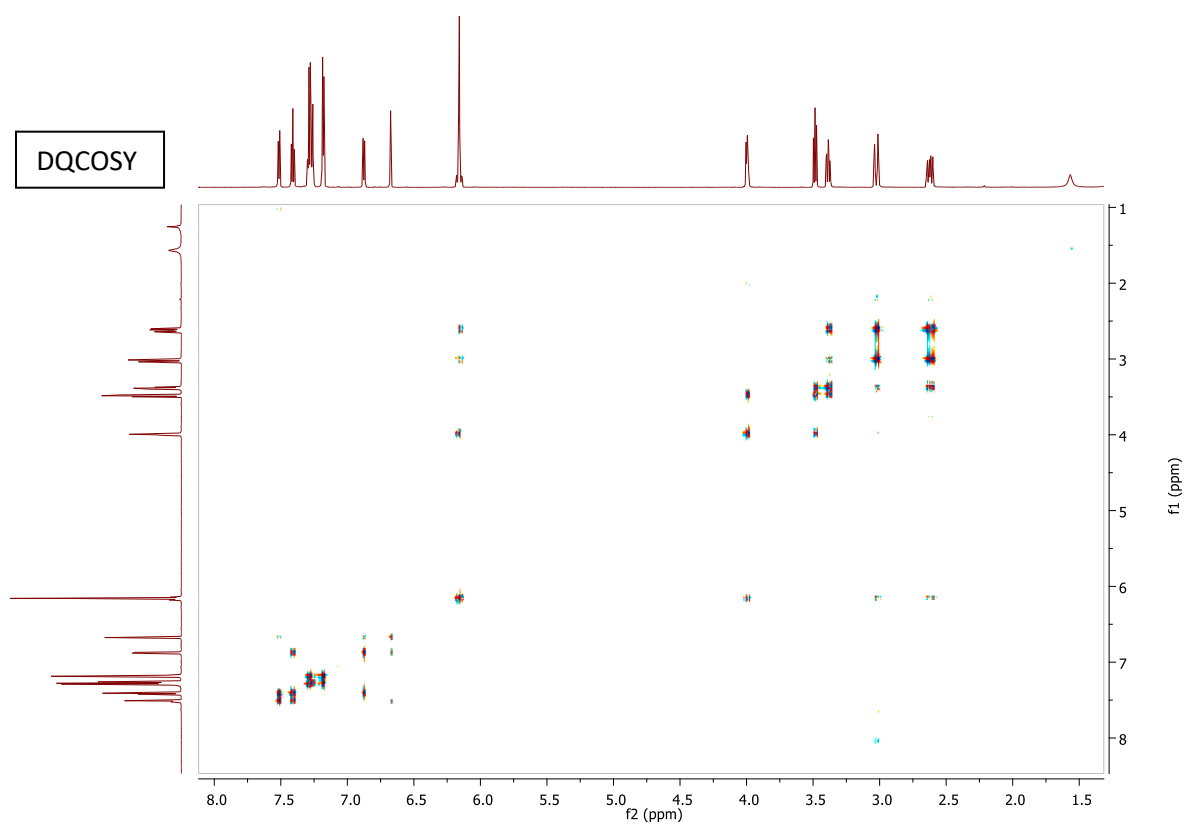


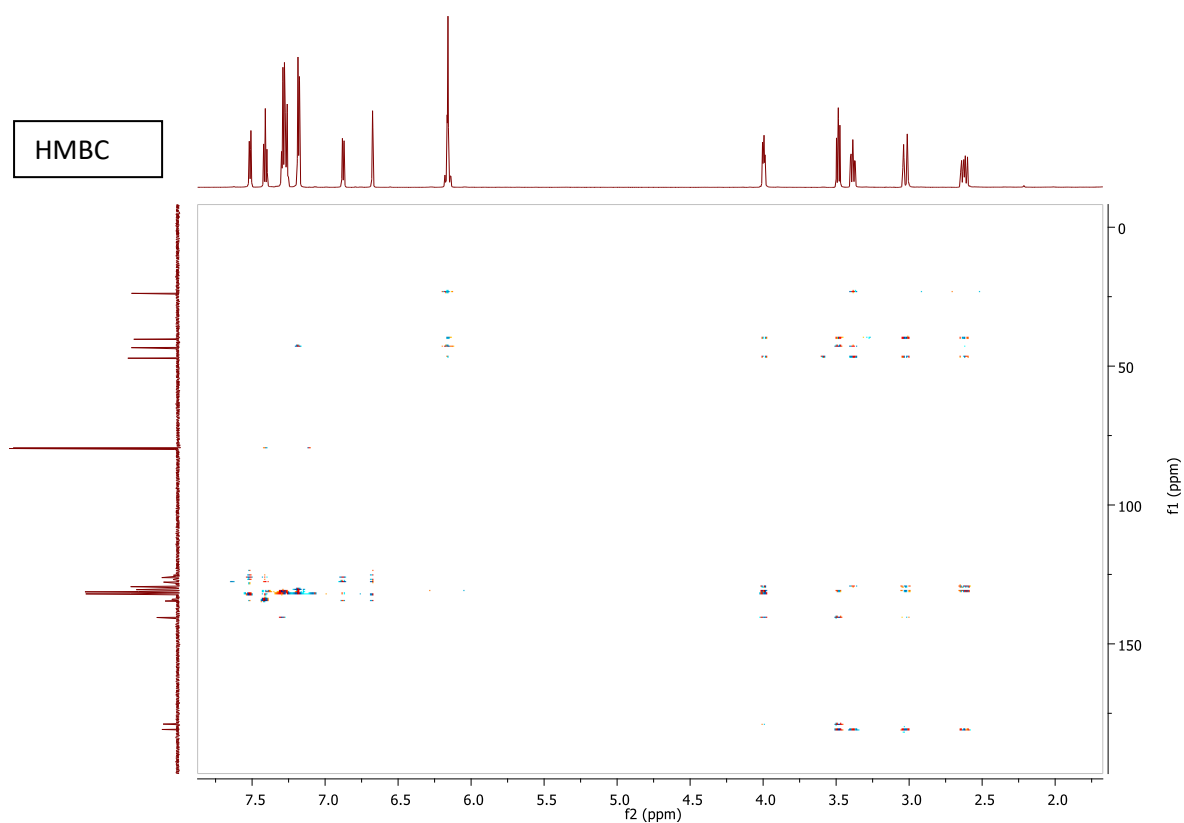




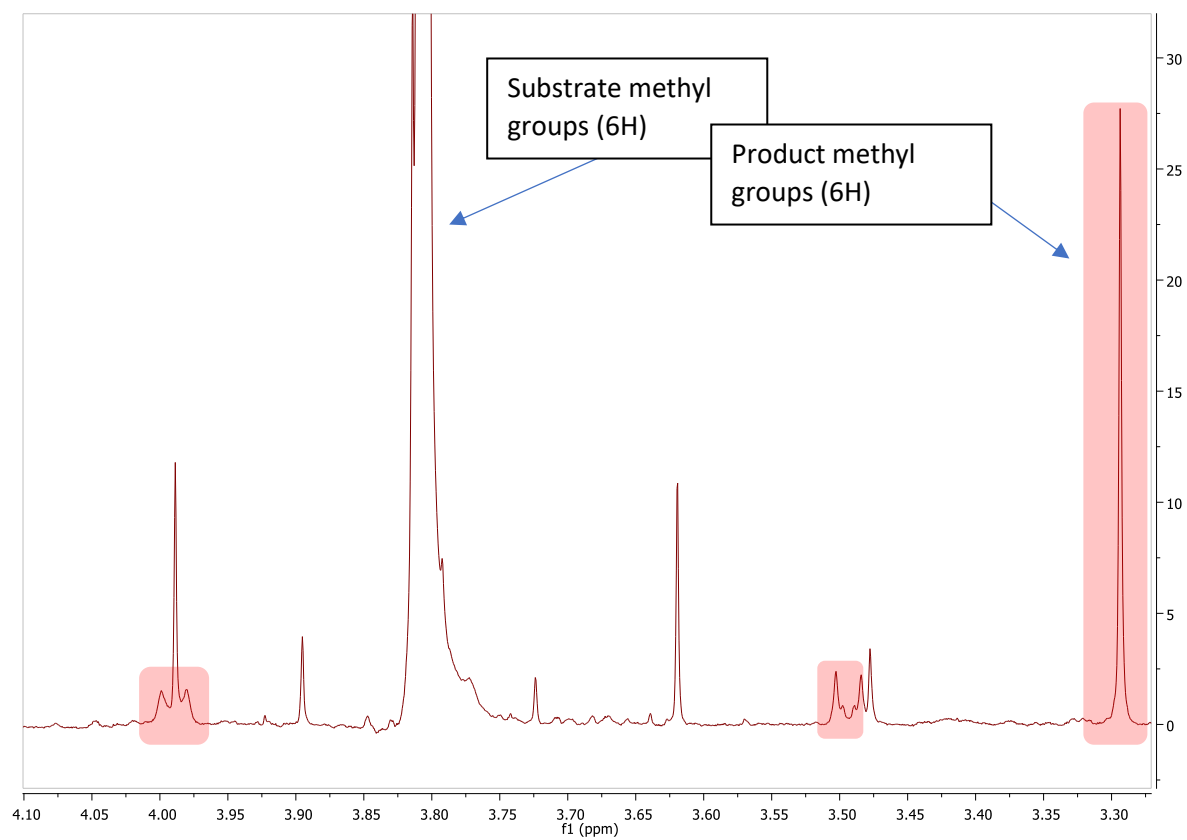
2b



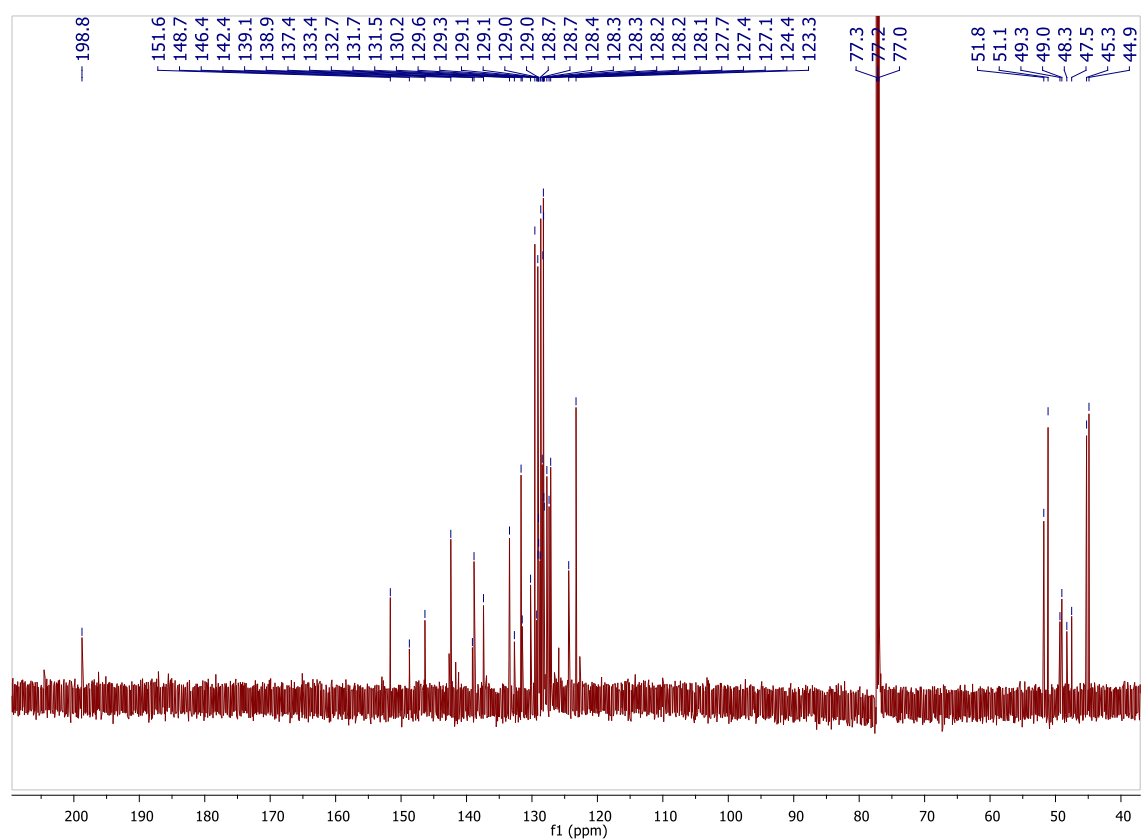
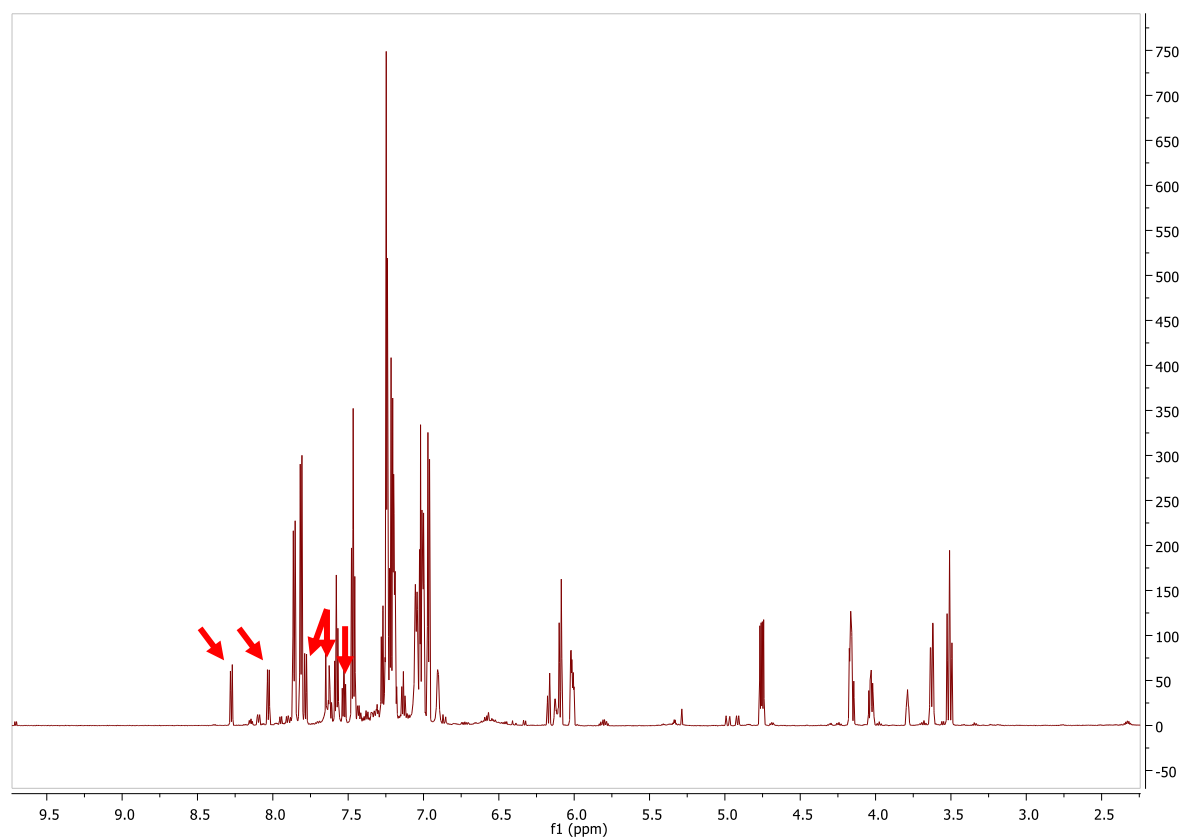




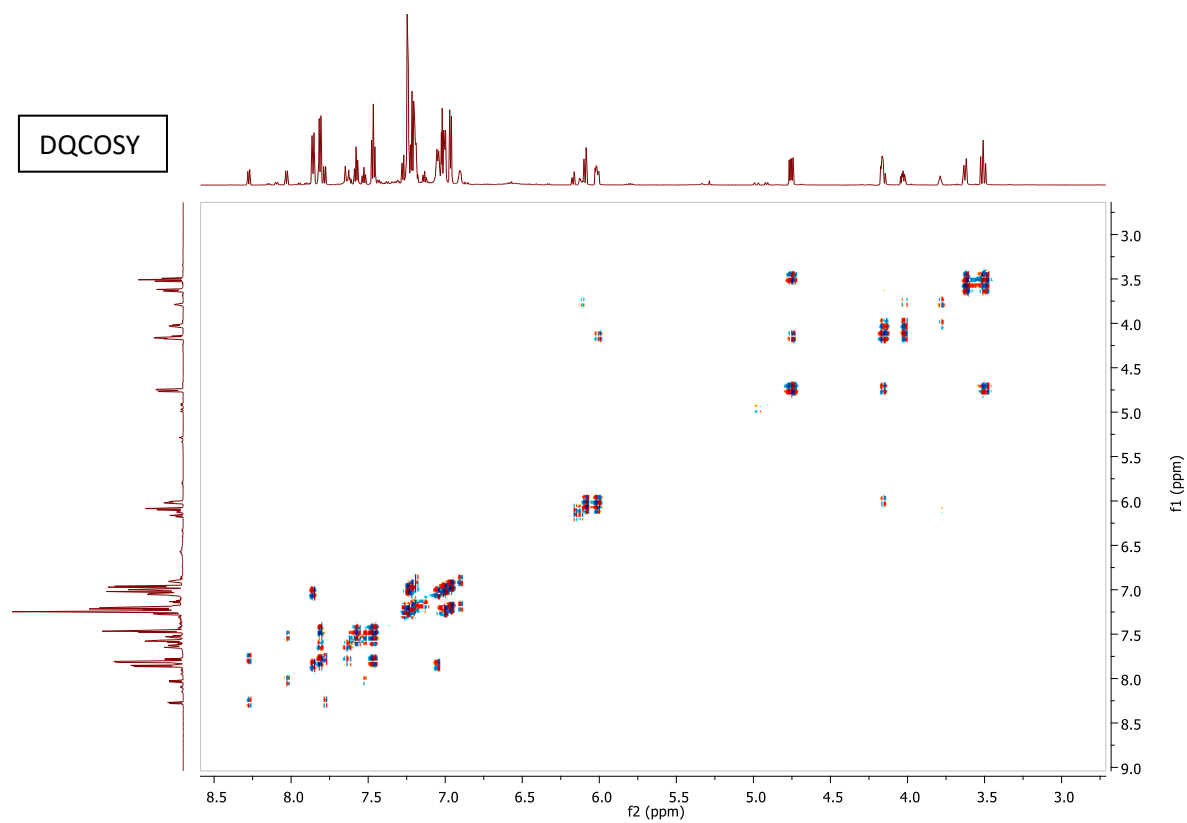
2c (highlighted signals in ^1H NMR spectrum of reaction mixture)



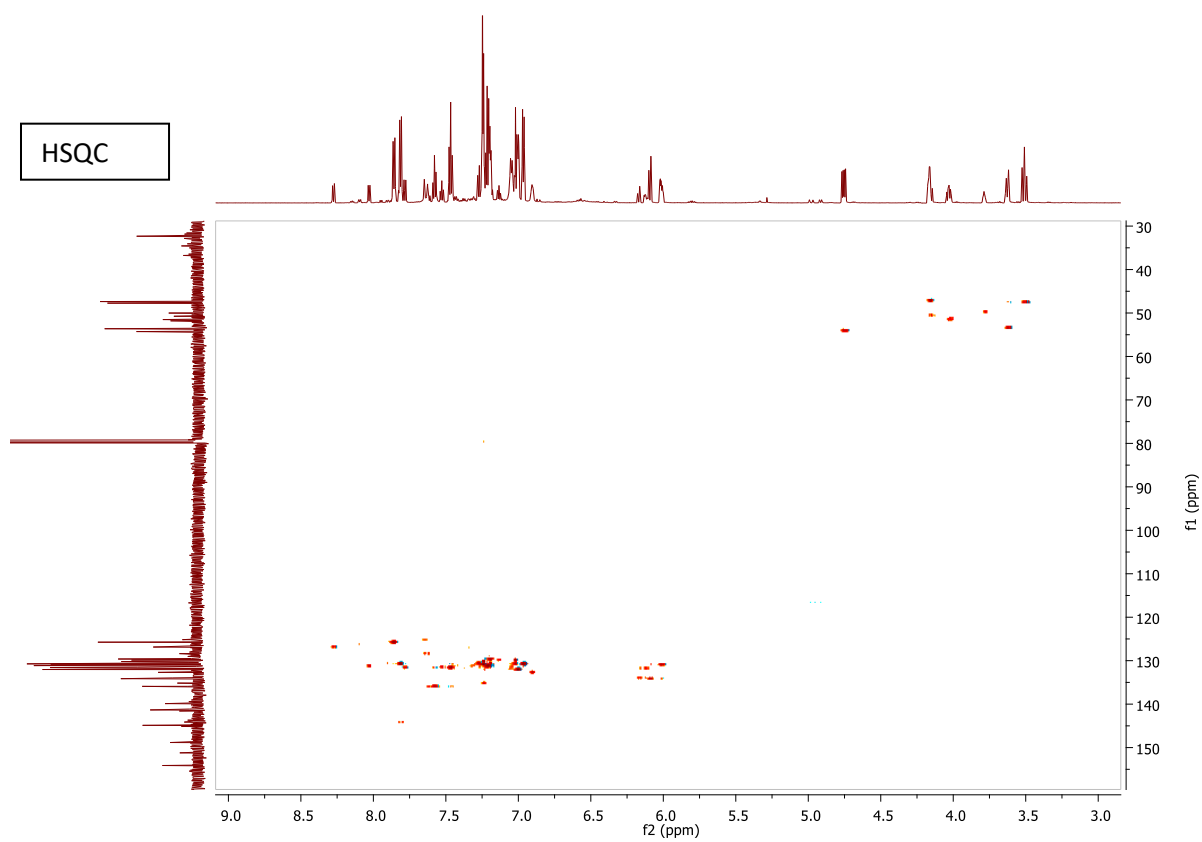
2d. (mixture of two stereoisomers with highlighted traces of unreacted 4-nitrochalcone)

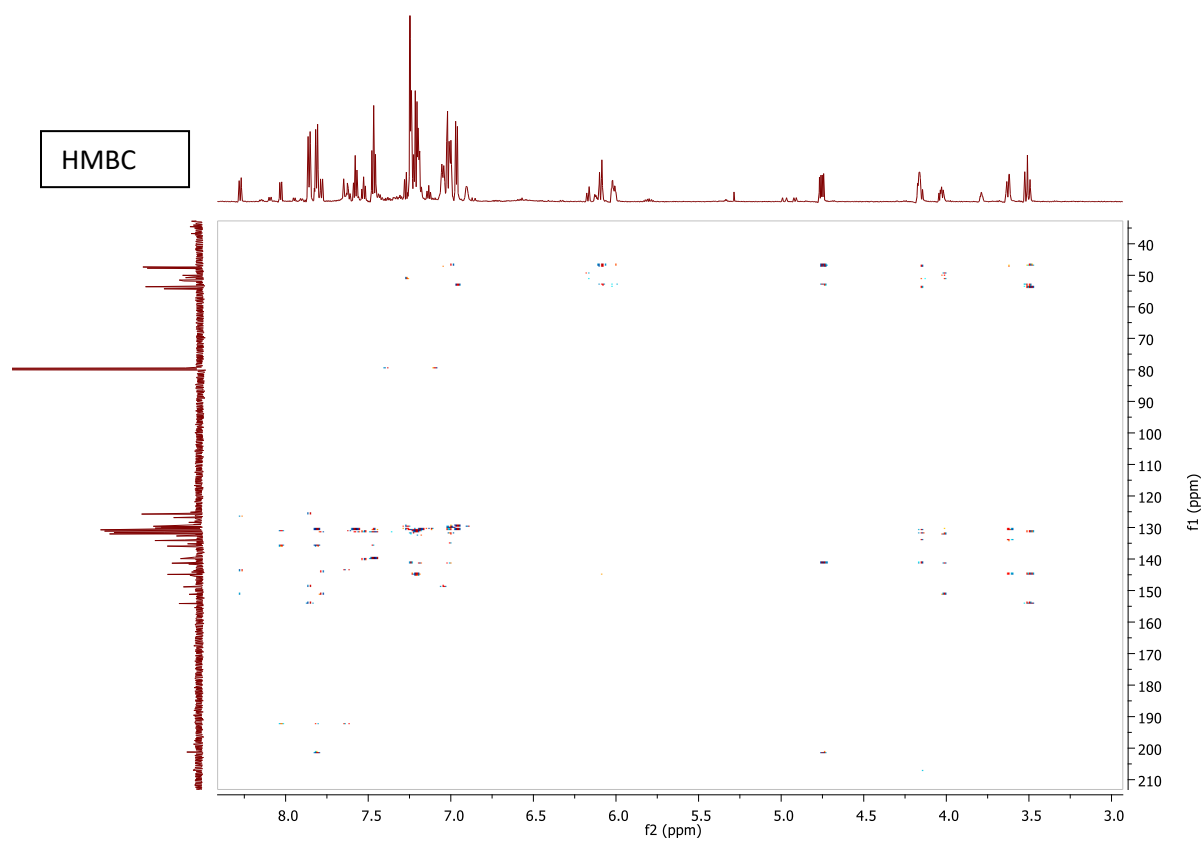
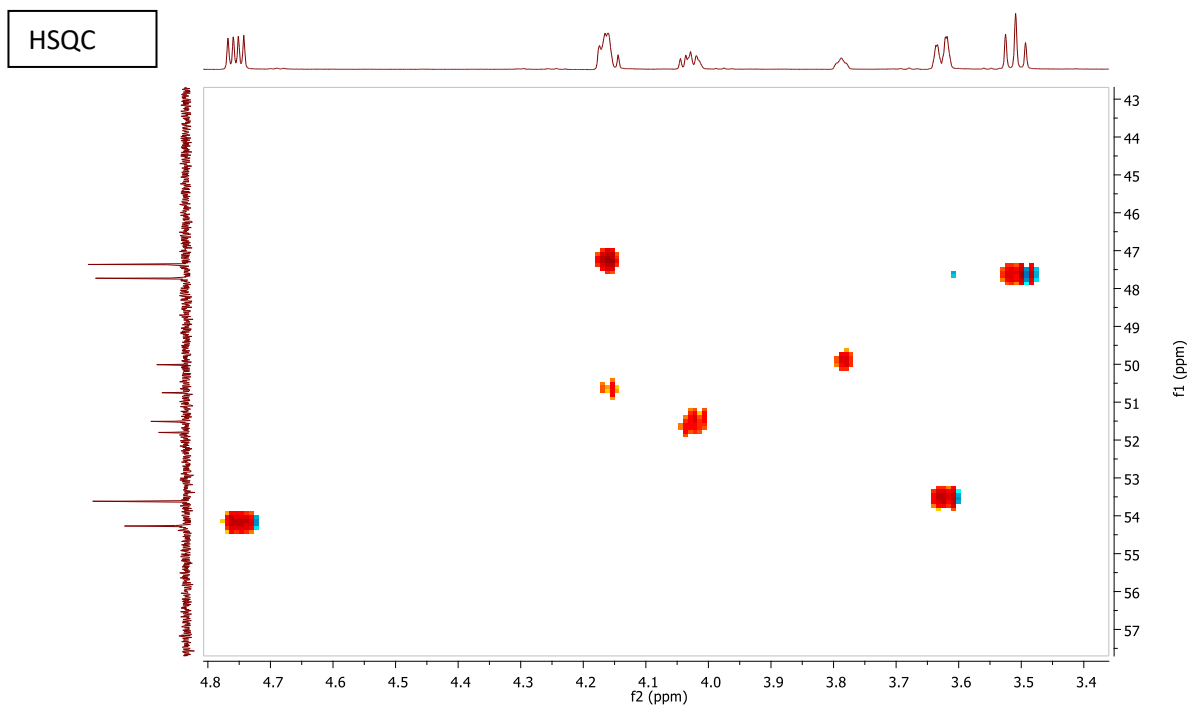


DQCOSY



HSQC





4. IR spectra

Recorded on Bruker Vertex 80v, range 400–4000 cm^{-1} , on AgCl windows (sample as powder)

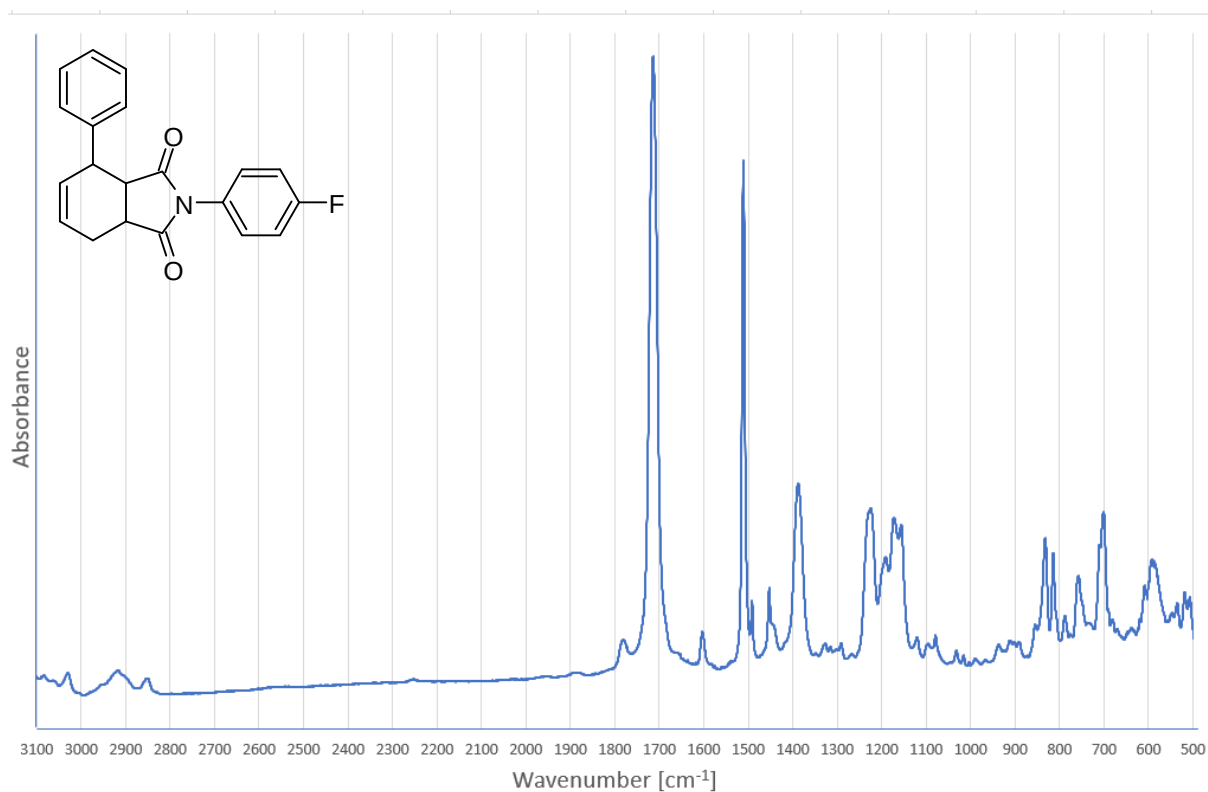


Figure S 1. IR spectrum of **2a**.

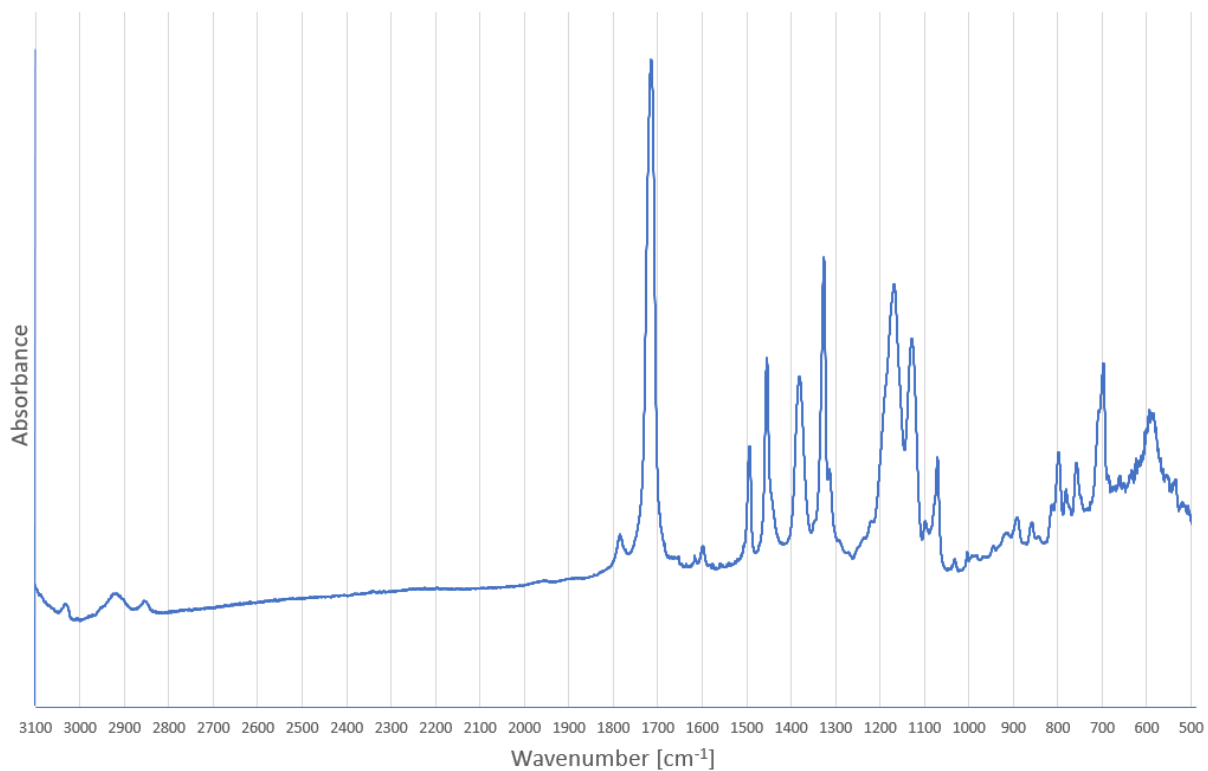


Figure S 2. IR spectrum of **2b**.

5. EPR spectra

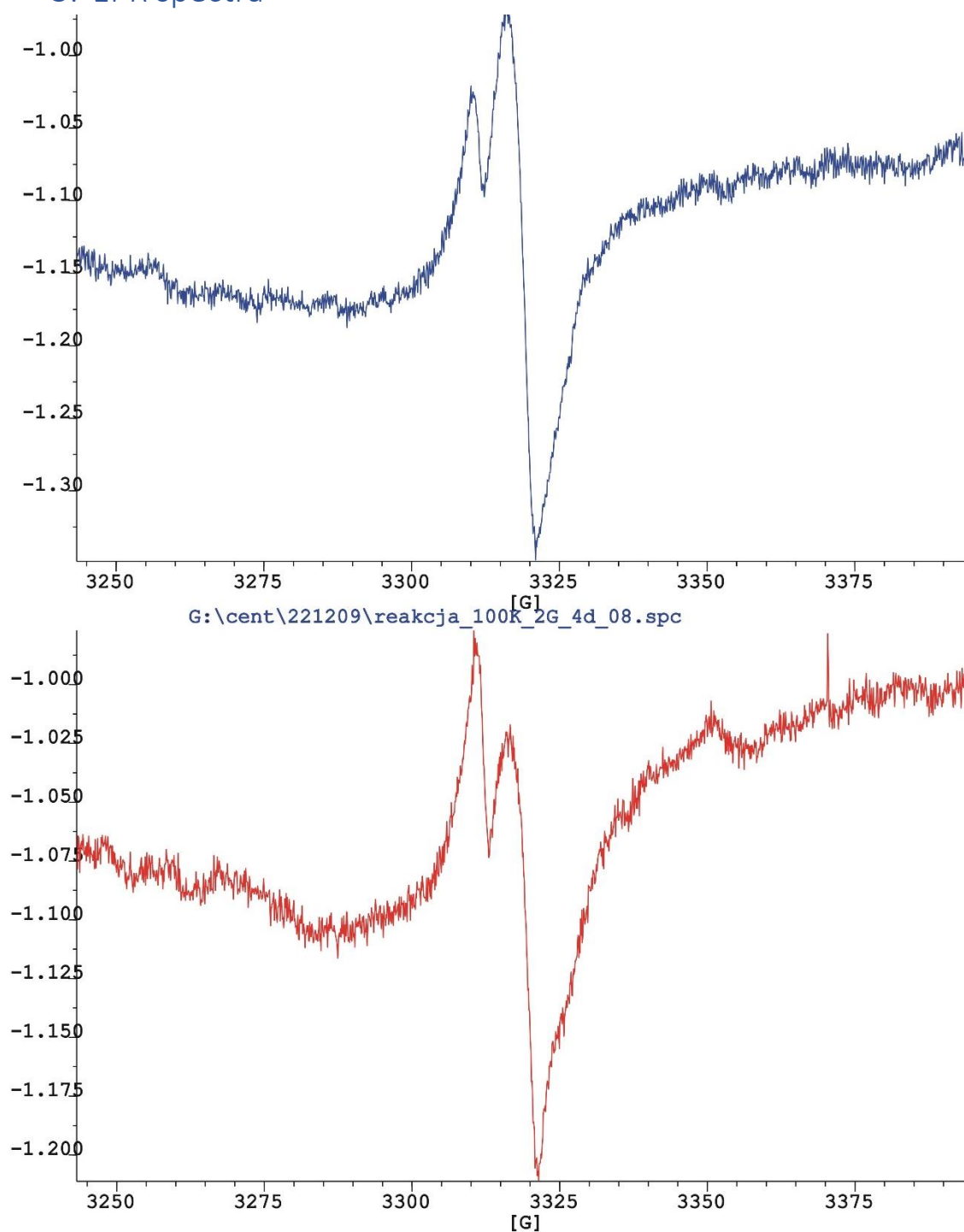


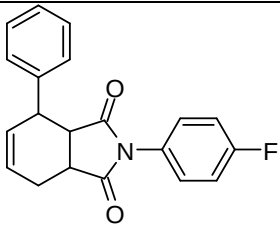
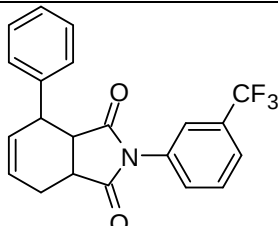
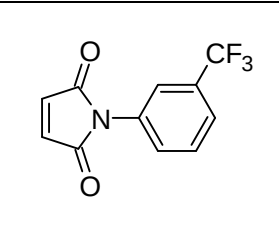
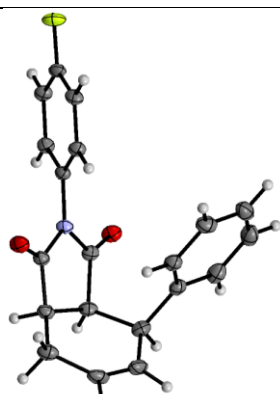
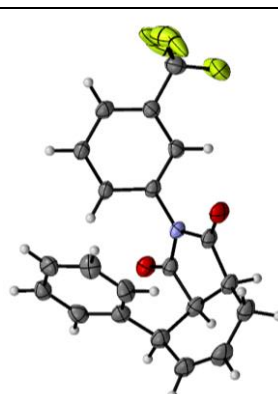
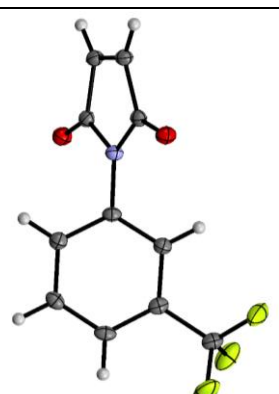
Figure S 3. EPR spectra (32 mW microwave power) of solution of chalcone and 9-methylanthracene in *o*-difluorobenzene, activated with AgSO_4 , which was filtered off later, then the solution was sealed in quartz tube. Lower spectrum recorded 4 days after the upper one in the same conditions. Intensities ratio of the two main signals change in time.

With pure chalcone in *o*-difluorobenzene mixed with AgSO_4 and then filtered, no signals in EPR spectrum were observed.

6. Crystal structure data

All crystals were measured on SuperNova diffractometer equipped with Cu(K α) microsource.

Table S 1 Crystallographic data for refined structures of cycloadducts to 1-phenylbuta-1,4-diene and substrate.

Compound			
	2a	2b	
Kα(Å)	1.54184 (Cu)	1.54184 (Cu)	1.54184 (Cu)
Temperature (K)	103(2)	100(2)	100(2)
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>I</i> a	<i>Pbca</i>
Z	4	8	8
<i>a</i> (Å)	5.94460(10)	8.0221(5)	10.6040(2)
<i>b</i> (Å)	24.1479(4)	19.1612(8)	11.7299(2)
<i>c</i> (Å)	10.6246(2)	22.4553(10)	15.5267(2)
α (°)	90	90	90
β (°)	100.951(2)	91.728(5)	90
γ (°)	90	90	90
<i>V</i> (Å³)	1497.38(5)	3450.1(3)	1931.27(6)
$\rho_{calc.}$ (g cm⁻³)	1.425	1.430	1.659
$\mu_{exp.}$ (mm⁻¹)	0.825	0.968	1.354
ϑ_{max} (°)	78.052	75.382	75.751
<i>R</i>₁	0.0405	0.0892	0.0313
<i>wR</i>₂	0.1097	0.2682	0.0801
<i>Goof</i>	1.059	1.231	1.069
Crystal size (mm×mm×mm)	0.390 x 0.200 x 0.080	0.166 x 0.261 x 0.372	0.210 x 0.170 x 0.160
Crystal colour	colorless	colorless	colorless
CCDC No.	2270169	2270167	2270168
			

7. Calculations

All calculations were performed using Orca 5 package.⁷ Geometry optimizations were done using r²SCAN-3c⁸ composite method, while single point calculations were obtained with more accurate ω B97X-V⁹ with def2-TZVP basis set^{10,11} and D4 dispersion correction.¹² All calculations were performed with CPCM solvent model¹³ with $\epsilon = 14$ corresponding to oDFB solvent. Defgrid2 was mainly used unless stated otherwise. Optimized structures of reactants and products have no imaginary modes while transition states have only one imaginary mode. GEDT¹⁴ was calculated on the basis of NPA (obtained from NBO programme¹⁵) for chalcone molecules.

Estimation of solvation reorganization energy, λ_{sol} , was done on the basis of 4-point approach proposed by Nelsen.¹⁶ According to this method in the internal reorganization energy, λ_{int} , is the sum of reorganization energies of isolated reagents. Thus, reorganization energy of diene is the difference between E_{SCF} calculated in optimized geometry and geometry of (diene)^{•+}. Accordingly, reorganization energy of (cycloadduct)^{•+} takes the difference in energies calculated for optimized geometry and geometry of neutral species.

Solvent reorganization energy was estimated using equation derived by Marcus:¹⁷

$$\lambda_{sol} = k_e e^2 \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{r} \right) \left(\frac{1}{n^2} - \frac{1}{\epsilon} \right)$$

where k_e is Coulomb constant, e is charge transferred, a_1 and a_2 are ionic radii of reagents (including their solvation spheres), $r = a_1 + a_2$, n is refractive index and ϵ is dielectric constant. For o-DFB the $\left(\frac{1}{n^2} - \frac{1}{\epsilon} \right)$ term is 0.410. Assuming that reagents are spheres (what is fairly close for cycloadducts), their radii are in the range between 7 Å (anthracene) to 9 Å (large cycloadducts) (these values are without solvation spheres) and such a case λ is around 30 kJ mol⁻¹.

The values obtained are presented in Table S 2 and Table S 3 below. To eliminate the influence of solvation energy, CPCM energy term was subtracted from E_{SCF} .

It can be seen that while reorganization energy of dienes are small and similar, for cycloadducts there are large differences. In the case of butadiene-derived species, reorganization is very small, much smaller than for the cycloadduct derived from anthracene.

UNLESS STATED OTHERWISE, ALL ENERGIES ARE IN HARTREES.

Table S 2. Reorganization energies of dienes.

Anthracene	E_{SCF}	CPCM	E_{SCF} @ CatGeom	CPCM of cation
	-539.9796407	-0.009141936	-539.9750708	-0.068490822
Without CPCM	-539.9704988		-539.9659289	
Reorganization energy [kJ mol⁻¹]	12.0			
Ph-C ₄ H ₄ -Ph	-618.6320938	-0.01210823	-618.6232547	-0.06943529
Without CPCM	-618.6199856		-618.6111465	
Reorganization energy [kJ mol⁻¹]	23.2			
Ph-C ₄ H ₅	-387.3781914	-0.007967809	-387.3695347	-0.07396902
Without CPCM	-387.3702236		-387.3615669	
Reorganization energy [kJ mol⁻¹]	22.7			

Table S 3. Reorganization energies of cycloadducts.

Chalcone-Anthracene	E _{SCF}	CPCM of cation	E _{SCF} @ NeutrGeom	CPCM
	-1194.35712	-0.07074143	-1194.325727	-0.020751422
Without CPCM	-1194.286378		-1194.254985	
Reorganization energy [kJ mol⁻¹]	82.4			
(Ph-C₄H₄-Ph) – (DMM)	-1153.178076	-0.084844487	-1153.16768	-0.023910827
Without CPCM	-1153.093231		-1153.082836	
Reorganization energy [kJ mol⁻¹]	27.3			
(Ph-C₄H₅) – (PhF-MIM)	-1077.414457	-0.09108285	-1077.411608	-0.026732359
Without CPCM	-1077.323374		-1077.320525	
Reorganization energy [kJ mol⁻¹]	7.5			

	ΔG_{el}^0 for diene + (cycloadduct) ^{•+} → (diene) ^{•+} + cycloadduct				
	r ² SCAN-3c			wB97X-V/D4	
diene/dienophile	E _{SCF}	H	G	E _{SCF}	Final ΔG_{el}
Anthracene /chalcone	111.9	114.1	115.1	-86.2	-83.1
Ph-C₄H₄-Ph / DMM	-103.8	-91.3	-99.9	-114.1	-110.2
Ph-C₄H₅ / PhF-MIM	-66.4	-60.7	-61.4	-119.6	-114.6

C ₁₄ H ₈ + Chalcone	r ² SCAN-3c			wB97X-V/D4		
	E _{SCF}	H	G	E _{SCF}	Final ΔG	GEDT
Reactants	-1193.317289	-1192.875818	-1192.951431	-1194.562416		-0.003
TS	-1193.280189	-1192.838414	-1192.911382	-1194.523507		-0.147
TS-reactants [kJ mol⁻¹]	97.4	98.2	105.1	102.1	109.9	
Product	-1193.334305	-1192.888726	-1192.960748	-1194.600575		
Product-Reactants [kJ mol⁻¹]	-44.7	-33.9	-24.5	-100.2	-80.0	
(C₁₄H₈)^{•+} + Chalcone						
Reactants	-1193.12222	-1192.680091	-1192.755772	-1194.356018		0.002
TS1	-1193.098464	-1192.656228	-1192.730893	-1194.328495		0.376
TS1-reactants [kJ mol⁻¹]	62.4	62.6	65.3	72.2	75.2	
Local minimum	-1193.104448	-1192.660727	-1192.735339	-1194.338824		
LocMin-reactants [kJ mol⁻¹]	46.7	50.8	53.6	45.1	52.1	
TS2	-1193.098924	-1192.655752	-1192.728622	-1194.339659		
TS1-reactants [kJ mol⁻¹]	61.2	63.9	71.3	42.9	53.1	
Product	-1193.110412	-1192.665284	-1192.738693	-1194.35712		
Product-Reactants [kJ mol⁻¹]	31.0	38.9	44.8	-2.9	10.9	

9-ClC ₁₄ H ₇ + Chalcone	r ² SCAN-3c			wB97X-V/D4		
	E _{SCF}	H	G	E _{SCF}	Final ΔG	GEDT
Reactants	-1652.899445	-1652.466139	-1652.543946	-1654.180806		-0.007
TS	-1652.861071	-1652.427506	-1652.503103	-1654.136003		-0.180
TS-reactants [kJ mol⁻¹]	100.7	101.4	107.2	117.6	124.1	
Product	-1652.914144	-1652.476882	-1652.551592	-1654.216495		

Product-Reactants [kJ mol⁻¹]	-38.6	-28.2	-20.1	-93.7	-75.2	
(9-ClC₁₄H₇)^{•+} + Chalcone						
Reactants	-1652.699582	-1652.265848	-1652.344043	-1653.969802		0.001
TS	-1652.66418	-1652.230456	-1652.305837	-1653.934626		0.212
TS-reactants [kJ mol⁻¹]	92.9	92.9	100.3	92.3	99.7	
Product	-1652.685887	-1652.249514	-1652.325475	-1653.96832		
Product-Reactants [kJ mol⁻¹]	35.9	42.9	48.7	3.9	16.7	

9-BrC₁₄H₇ + Chalcone	r²SCAN-3c			wB97X-V/D4		
	E_{SCF}	H	G	E_{SCF}	Final ΔG	GEDT
Reactants	-3766.85849	-3766.425654	-3766.504416	-3768.031189		-0.007
TS	-3766.819396	-3766.386218	-3766.462816	-3767.985186		-0.175
TS-reactants [kJ mol⁻¹]	102.6	103.5	109.2	120.8	127.3	
Product	-3766.873538	-3766.436643	-3766.512463	-3768.067126		
Product-Reactants [kJ mol⁻¹]	-39.5	-28.8	-21.1	-94.3	-76.0	
(9-BrC₁₄H₇)^{•+} + Chalcone						
Reactants	-3766.658071	-3766.223924	-3766.30583	-3767.819684		0.002
TS	-3766.623129	-3766.189791	-3766.266398	-3767.785077		0.167
TS-reactants [kJ mol⁻¹]	91.7	89.6	103.5	90.8	102.6	
Product	-3766.645306	-3766.209355	-3766.28644	-3767.819129		
Product-Reactants [kJ mol⁻¹]	33.5	38.2	50.9	1.5	18.8	

Ph-C₄H₄-Ph + DMM	r²SCAN-3c			wB97X-V/D4		
	E_{SCF}	H	G	E_{SCF}	Final ΔG	GEDT
Reactants	-1152.233244	-1151.822098	-1151.902067	-1153.368519		-0.003
TS	-1152.213185	-1151.801474	-1151.878146	-1153.339784		-0.148
TS-reactants [kJ mol⁻¹]	52.7	54.1	62.8	75.4	85.6	
Product	-1152.277087	-1151.861537	-1151.936354	-1153.429362		
Product-Reactants [kJ mol⁻¹]	-115.1	-103.5	-90.0	-159.7	-134.6	
(Ph-C₄H₄-Ph)^{•+} + DMM						
Reactants	-1152.038771	-1151.627931	-1151.706721	-1153.161318		0.002
TS	-1152.012454	-1151.600514	-1151.678831	-1153.126336		0.120
TS-reactants [kJ mol⁻¹]	69.1	72.0	73.2	91.8	96.0	
Product	-1152.042631	-1151.630067	-1151.704154	-1153.178076		
Product-Reactants [kJ mol⁻¹]	-10.1	-5.6	6.7	-44.0	-27.1	

Ph-C₄H₅ + PhF-MIM	r²SCAN-3c			wB97X-V/D4		
	E_{SCF}	H	G	E_{SCF}	Final ΔG	GEDT
Reactants	-1076.58929	-1076.260371	-1076.332681	-1077.608595		-0.011
TS	-1076.576306	-1076.247847	-1076.315189	-1077.582572		-0.204
TS-reactants [kJ mol⁻¹]	34.1	32.9	45.9	68.3	80.1	
Product	-1076.64829	-1076.315464	-1076.381928	-1077.679728		
Product-Reactants [kJ mol⁻¹]	-154.9	-144.6	-129.3	-186.7	-161.1	

(Ph-C ₄ H ₅) ^{•+} + PhF-MIM						
Reactants	-1076.381014	-1076.052656	-1076.123645	-1077.387642		0.002
TS	-1076.367084	-1076.038621	-1076.108982	-1077.365957		0.079
TS-reactants [kJ mol⁻¹]	36.6	36.8	38.5	56.9	58.8	
Product	-1076.414936	-1076.083828	-1076.150325	-1077.41446		
Product-Reactants [kJ mol⁻¹]	-89.0	-81.8	-70.0	-70.4	-51.4	

Ph-C ₄ H ₄ -Ph + NO ₂ -Chalc	r ² SCAN-3c			wB97X-V/D4		
	E _{SCF}	H	G	E _{SCF}	Final ΔG	
Reactants	-1476.376396	-1475.871023	-1475.961845	-1477.843561		-0.004
TS	-1476.348702	-1475.844042	-1475.93086	-1477.805273		-0.161
TS-reactants [kJ mol⁻¹]	72.7	70.8	81.3	100.5	109.1	
Product	-1476.397254	-1475.888465	-1475.974094	-1477.884485		
Product-Reactants [kJ mol⁻¹]	-54.8	-45.8	-32.2	-107.4	-84.8	
(Ph-C ₄ H ₄ -Ph) ^{•+} + NO ₂ -Chalc						
Reactants	-1476.181282	-1475.674888	-1475.767108	-1477.635561		0.014
TS	-1476.158597	-1475.652334	-1475.737678	-1477.616961		0.363
TS-reactants [kJ mol⁻¹]	59.5	59.2	77.3	48.8	66.5	
Product	-1476.162742	-1475.656205	-1475.742239	-1477.622199		
Product-Reactants [kJ mol⁻¹]	48.7	49.0	65.3	35.1	51.7	

	r ² SCAN-3c			wB97X-V/D4
	E _{SCF}	H	G	E _{SCF}
(Anthracene) ^{•+}	-539.1392281	-538.9357616	-538.9820005	-539.7690375
(Ph-C ₄ H ₄ -Ph) ^{•+}	-617.7636494	-617.5015802	-617.5568752	-618.4242921
(Ph-C ₄ H ₅) ^{•+}	-386.7397147	-386.5635866	-386.6082124	-387.1584906

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Coordinates

C₁₄H₈ + Chalcone

Reactants	TS	Product
H 1.62533459929060 5.09494512056877 3.96832279316917	H 5.51609065207811 1.41341343943119 -1.12732289194458	H 1.26068607667114 -1.40872322985853 5.48183899128278
H 1.89630381559777 3.07706033732206 2.54640938915120	H 5.66409634839338 -0.80566764436413 -2.23331191226328	H -0.35578013379831 -3.11016440128460 6.29309583532478
C 1.01831665119249 4.21314341234952 4.15353318032833	C 4.79778181950709 0.63510748762538 -0.88491745609697	C 0.30756791611890 -1.09770858753358 5.89998692528833
C 1.16771042043831 3.08080530288104 3.35242076291327	C 4.88031400329657 -0.61052735262459 -1.50656329970837	C -0.60266525519633 -2.05371787683854 6.35261545169768
C 0.09303210610970 4.21497016378722 5.18838526229252	C 3.80268312432263 0.88054196290992 0.05242916244393	C -0.00403390155578 0.25199731257037 5.98444506753413
H -0.02879200490045 5.09091295611490 5.81884518624728	H 3.74510740011363 1.84123753692948 0.55373528910435	H 0.69864451102970 1.00521412754613 5.64054246430790
C 0.38893111716063 1.95174325779293 3.59360863511626	C 3.96697694185445 -1.60991661203607 -1.18029628476488	C -1.82555461330872 -1.65328892031870 6.88435880563828
H 0.51753062195776 1.06092861327416 2.98541090471826	H 4.04598183916380 -2.59221796196189 -1.63737601525006	H -2.53145324238781 -2.39416624610889 7.24865099253780
C -0.71413445116561 3.09448180740048 5.41907983175149	C 2.84960843765252 -0.10054193988189 0.34887297652117	C -1.24098317215378 0.66269528870550 6.50008990135585
C -0.55411852854715 1.95830105145850 4.61741049120531	C 2.94926505998379 -1.35521941535219 -0.26552383595692	C -2.15156554224818 -0.30209552146647 6.94677900033732
O -1.36266515485801 3.74777459891221 7.59445887361922	O 2.22311333325377 0.73888408019332 2.45338159438589	O -0.60351065708138 2.92602342026088 6.66900170119769
C -1.67284291862504 3.13621165320840 6.56430337410885	C 1.83641749611611 0.18826260552965 1.41465148109670	C -1.52396021020345 2.12594154052457 6.57373871254957
H -1.14435448414676 1.06785922654085 4.81228492456271	H 2.25730925532195 -2.14885197172773 0.00089451003342	H -3.10852215224262 -0.00843523002304 7.36462784470105
C -2.97928618608801 2.48444853107839 6.48118421134646	C 0.42861944841730 -0.18747413184116 1.24972612016243	C -2.97087530267341 2.58475578725364 6.49273579471340
H -3.09231256392316 2.36722701261528 4.38691134923824	H 0.57360646606681 -0.96388299243668 -0.73543169837412	H -2.81495727119074 1.89565850873933 4.42799498325544
C -3.61049429191639 2.18317590491394 5.32702195635739	C -0.09596896588354 -0.85312694924379 0.11144587046152	C -3.61685954805357 2.14999337608712 5.13254864926248
H -3.47583314153867 2.36590932898205 7.44219230717525	H -0.07601811922599 -0.30814360551003 2.20421627330436	H -3.51410387438570 2.10238816543637 7.31492293739211
H -4.70271992427963 1.35462517561949 3.06878317429711	H -0.51065488029493 -2.78088981616369 -1.67321739192118	H -3.66661787445887 0.03278683221513 3.47890135602629
C -4.95658543938568 1.65053814414858 5.18694232621046	C -1.06408891131843 -1.95776979825883 0.23805392826919	C -4.54532199641803 0.96190228080564 5.20722701730252
C -5.38287615850558 1.24828426364787 3.91087743702714	C -1.15609679320806 -2.89304552858874 -0.80439791949062	C -4.43819120556466 -0.04344386631227 4.24231439150011
H -5.56102502261173 1.85778153795909 7.25649428155382	H -1.88116884379558 -1.39597431394584 2.16173091386666	H -5.64608382220673 1.60939826483045 6.95046449141013
C -5.85144159896806 1.52625390409361 6.26424055310995	C -1.90954405775015 -2.11244517081114 1.34549968472518	C -5.53726998258943 0.84348402050384 6.18680728047982
C -6.65267521519321 0.71904113392778 3.71702786611109	C -2.04978119874620 -3.95514743971197 -0.73734576320147	C -5.28878287934819 -1.14545443150231 4.25702128810177
H -6.96434764852628 0.40992407413074 2.72332031091597	H -2.09845359244049 -4.67121498332848 -1.55326377370160	H -5.18054535539483 -1.92137025159419 3.50390823490097
C -7.11987481708736 1.00419610302090 6.06703875648728	C -2.80328096462975 -3.17624143179487 1.41185214700750	C -6.39146099324878 -0.25567790879368 6.20179813736592
C -7.52547035312343 0.59626668452630 4.79472781658613	C -2.87822771627633 -4.10310976795003 0.37442523796596	C -6.26938770335980 -1.25629145738966 5.23964204010020
H -7.80617408051862 0.92569415690560 6.90553843312308	H -3.44996014817220 -3.27780127932593 2.27934546378651	H -7.15369346236988 -0.33149886248105 6.97273004116693
H -8.52299249845277 0.19205391877786 4.64613336534354	H -3.57696028161293 -4.93304713097776 0.43068439517105	H -6.93235882615983 -2.11685234507855 5.25803551050046

H -5.23209998231709	4.38997981968164	1.12897515425247	H 0.06874763238055	1.08924532161296	-3.33001627718289	H -3.40881260000448	4.66194203008525	2.13906152578656
H -7.26307568026473	4.14099213635826	2.50441365361094	H -1.58626412835711	-0.06232500384194	-1.81929933291944	H -4.85779803095519	3.12209766177562	3.59088303876545
H -9.27829634886291	3.84105704195755	3.88817439939877	H -3.88214817073251	-0.22195021315924	-0.80082799315002	H -7.15962928596451	3.76469416335626	4.54339766153435
C -4.67480407082312	4.71427665316449	2.00486054475591	C 0.40725507426551	1.67856961018924	-2.48124479011943	C -2.89492204293469	4.97157249277246	3.04624476162261
C -6.70749746235895	4.46462372092449	3.38266090476753	C -1.25327543793708	0.54969517637483	-0.98247316161718	C -4.34087488352961	3.40898933197902	4.51126618723000
C -8.72336222031039	4.15279889100294	4.77006462662109	C -3.52145858046238	0.34120074771812	0.05647770147536	C -6.65290138708197	4.08046225731794	5.45239809624277
H -2.83198930894347	4.94664590964257	0.95618542618996	H 1.88786700529734	2.75021700811810	-3.59909696426563	H -1.58298078210568	6.35203969012982	2.03964131907101
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C -3.34404653792325	5.02263344612391	1.91142149289296	C 1.42489718353750	2.60393103171271	-2.62717557202798	C -1.87053549324679	5.91893676889305	2.99385026995166
C -5.35732425510162	4.80047857627918	3.25228108074859	C -0.22035076357247	1.51493662041682	-1.23447397496121	C -3.25921751639219	4.43345199544795	4.27428140218010
C -7.35332489335037	4.51276070147425	4.61970142615104	C -2.20691356565236	0.83952263305928	0.04832304012150	C -5.27333547032935	3.96703292326655	5.55616677944574
C -9.32701312279548	4.18967573649137	5.99757806296623	C -4.34510988241941	0.57988910447804	1.14039236140052	C -7.38005679098901	4.59051109593731	6.53062000061560
C -2.61919777315797	5.44301412500430	3.05956193271345	C 1.86550888033015	3.35892858941325	-1.52613373826743	C -1.21998261416110	6.31500938111378	4.16182104558253
C -4.62080993274214	5.22452428702335	4.41720143987923	C 0.24368314301615	2.25617074032096	-0.11907772243703	C -2.59660652117832	4.81861779220454	5.44461990156927
C -6.61266797703992	4.92544564001707	5.78736680838590	C -1.72289491562825	1.54756140094293	1.17806531782453	C -4.61529804614118	4.35956402873017	6.72917207266663
C -8.59509198062295	4.58828232948213	7.14957385371055	C -3.86241365543133	1.27451791506420	2.26437207323915	C -6.72665078459323	4.97562221331277	7.69952169704253
C -3.24035124098037	5.54425786971652	4.27474854503276	C 1.29930527582806	3.17220430925135	-0.28002820149047	C -1.57935651522077	5.76207592312438	5.39237665071886
C -5.26860361448315	5.27927992568958	5.65386675503484	C -0.35517130470952	1.95528055321009	1.14532209511259	C -3.12144426037170	4.12658897630866	6.68310200156125
H -1.56179028806193	5.67525288808991	2.96863976921088	H 2.66672939491794	4.08125078392285	-1.65500516828739	H -0.42631324391396	7.05572216649965	4.11437333573925
C -7.27826880630543	4.94708817555453	7.04718118704189	C -2.56019225493618	1.73382854498069	2.29497963483648	C -5.33788820628657	4.85818899194932	7.80448484377462
H -9.09125476265826	4.60686545638975	8.11607312065110	H -4.51769924914725	1.44445794961098	3.11401599875847	H -7.29898857402848	5.37044672412277	8.53455457785950
H -2.68515818476260	5.85424197979204	5.15717173038127	H 1.65358846411319	3.73310024500235	0.58138558898356	H -1.06302376594580	6.05790710401160	6.30217721917577
H -4.70605069980187	5.58172253243702	6.53536794996353	H 0.07429950583999	2.40033874093202	2.04060493037831	H -2.61489556116704	4.45629046127830	7.59366333229913
H -6.71595321074996	5.25240823497315	7.92660335452918	H -2.17618133890740	2.25881884433087	3.16613265628963	H -4.82679342656506	5.15427750302933	8.71770181243654

(C₁₄H₈)^{•+} + Chalcone

Reactants	TS1	Product
H 1.555416 4.870280 3.824635	H 5.91945500600098 1.01034933495819 -1.00766965708218	H 1.994511 -0.996132 6.386873
H 1.951432 2.613471 2.869193	H 6.00667972159633 -1.37629644379567 -1.68571948995185	H 0.500509 -2.876385 7.011375
C 0.915629 4.039553 4.108565	C 5.14292801554888 0.32368671084933 -0.68376832326843	C 0.923047 -0.836875 6.461925
C 1.136311 2.771650 3.569887	C 5.18950469460092 -1.01704553630079 -1.06661703059844	C 0.081551 -1.893669 6.814145
C -0.118841 4.239682 5.011789	C 4.10706788012868 0.78130028159678 0.11763016239603	C 0.391112 0.416086 6.204637

H	-0.291900	5.219729	5.446110	H	4.06875071855012	1.81955343035808	0.43279640960083	H	1.034686	1.244031	5.924991
C	0.318043	1.706237	3.938045	C	4.19593932421175	-1.89846479967020	-0.64746395749644	C	-1.293316	-1.693231	6.914415
H	0.501341	0.714048	3.535975	H	4.24481967574047	-2.94780627452913	-0.92243304033184	H	-1.947060	-2.517018	7.184054
C	-0.964726	3.179853	5.365304	C	3.08274875496438	-0.09186467553200	0.50989332559475	C	-0.992824	0.627863	6.316192
C	-0.734268	1.908161	4.825298	C	3.13794048083058	-1.43805192160528	0.12840448207818	C	-1.833404	-0.435641	6.676221
O	-1.891717	4.297429	7.233555	O	2.28412130038825	1.27248478168352	2.25455943399415	O	-0.825247	2.824919	5.479523
C	-2.042421	3.434217	6.362304	C	2.01886526864716	0.43968892853301	1.39881036873021	C	-1.529912	1.965491	6.010570
H	-1.354947	1.069132	5.124683	H	2.38184861330569	-2.13906832813049	0.47107849716898	H	-2.907307	-0.299171	6.755989
C	-3.309450	2.693693	6.310405	C	0.58656498559606	-0.04763610016601	1.26845383160900	C	-2.986294	2.291948	6.273354
H	-3.264872	2.265596	4.253834	H	0.73302982793968	-0.84174618583876	-0.72059687520231	H	-3.080940	1.613360	4.196009
C	-3.837968	2.183417	5.176964	C	0.21696570899137	-0.93506250707020	0.23299538493536	C	-3.779300	1.969090	4.963501
H	-3.874205	2.713149	7.239894	H	0.16102128443362	-0.23050788690251	2.25436226308612	H	-3.373003	1.711283	7.112010
H	-4.942113	1.441248	2.893055	H	-0.58069527043486	-2.40538068087244	-1.79986617875099	H	-4.362636	-0.018371	3.250910
C	-5.155362	1.590557	5.034668	C	-0.84910704392080	-1.87020921375709	0.27974178922967	C	-4.852306	0.917000	5.125656
C	-5.601492	1.263515	3.739527	C	-1.17675348504639	-2.57593851929496	-0.90688381479316	C	-5.025525	-0.030678	4.113219
H	-5.695752	1.587470	7.134587	H	-1.38585900221072	-1.59857652997581	2.37237475638930	H	-5.596239	1.605994	7.037815
C	-6.013408	1.352090	6.123379	C	-1.62620489283815	-2.09971820631628	1.44083464295300	C	-5.708661	0.885098	6.231982
C	-6.867432	0.730282	3.535683	C	-2.24920591509032	-3.44468895432245	-0.93570482631138	C	-6.028629	-0.991736	4.201923
H	-7.198164	0.489786	2.529518	H	-2.49625081589279	-3.97430369849255	-1.85078350381844	H	-6.142336	-1.726686	3.409958
C	-7.273739	0.817382	5.915513	C	-2.70375195782346	-2.96469364554116	1.39753813697692	C	-6.713835	-0.073996	6.319800
C	-7.708716	0.509449	4.622267	C	-3.02222520015716	-3.63684980778770	0.21433355077846	C	-6.877323	-1.015090	5.306248
H	-7.930531	0.641666	6.762616	H	-3.30384462014464	-3.12314639435174	2.28852697800457	H	-7.369608	-0.086101	7.185864
H	-8.701501	0.095904	4.468917	H	-3.87010684701139	-4.31524408469940	0.18937001022053	H	-7.658175	-1.766742	5.379423
H	-5.066752	4.448384	1.197697	H	-0.67771852212258	1.68371873343620	-3.64823375722400	H	-3.394196	4.764288	2.158837
H	-6.994451	3.967012	2.645293	H	-2.39353589076797	0.69999818786865	-2.20537788062776	H	-4.902436	3.131886	3.467233
H	-8.916874	3.486773	4.094186	H	-4.34278525413502	0.13905522697114	-0.82630479552866	H	-7.131833	3.999903	4.421053
C	-4.533180	4.868946	2.045750	C	-0.12294825203761	2.01106617671524	-2.77310664817792	C	-2.905973	4.986012	3.103144
C	-6.452870	4.370685	3.497876	C	-1.85450872821734	1.03526666602787	-1.32102854572881	C	-4.372989	3.312537	4.405826
C	-8.369360	3.870709	4.950301	C	-3.80205659248142	0.44183975139747	0.06634524472097	C	-6.607919	4.203414	5.350850
H	-2.781058	5.360305	0.915897	H	1.40921453368947	3.00409847828281	-3.89003113134207	H	-1.636825	6.516125	2.281541
H	-9.946283	3.477666	6.347418	H	-5.42976301734453	0.05935216295251	1.40161541663343	H	-8.338287	4.964399	6.373457
C	-3.256887	5.379315	1.891468	C	1.03346911003312	2.74966361517152	-2.90378227072930	C	-1.925658	5.978753	3.180226

C -5.158692 4.884075 3.310826	C -0.62071765676124 1.69223894780941 -1.48613299291781	C -3.257752 4.309366 4.253214
C -7.065841 4.372047 4.762355	C -2.47006044214557 0.90266391298662 -0.06092378578181	C -5.253614 3.917065 5.468071
C -8.941696 3.866983 6.212710	C -4.40417940654759 0.40244421063114 1.30589636414508	C -7.277486 4.743066 6.445098
C -2.571807 5.927837 2.987908	C 1.72010178547990 3.19065872675574 -1.76109154955899	C -1.314433 6.319552 4.410017
C -4.452542 5.433493 4.433351	C 0.10769204871968 2.10361325321674 -0.33093199886466	C -2.589384 4.604417 5.487038
C -6.341705 4.881979 5.892943	C -1.74517083201557 1.27806341204275 1.10757229822921	C -4.571358 4.176751 6.674812
C -8.230676 4.353147 7.319741	C -3.69520394069666 0.80464226656732 2.44957105046936	C -6.596249 5.004847 7.640845
C -3.159078 5.959049 4.240839	C 1.26649824968474 2.86464611223282 -0.48927897088468	C -1.653425 5.653535 5.564625
C -5.053764 5.406142 5.704789	C -0.34698330903130 1.63933150380756 0.97059680812670	C -3.102443 3.799845 6.634941
H -1.571232 6.326853 2.852400	H 2.61796652231179 3.79159764252345 -1.87161728733150	H -0.571907 7.111043 4.431548
C -6.949252 4.853168 7.166910	C -2.37440249280955 1.21755113613645 2.35397772814669	C -5.233996 4.735097 7.758031
H -8.690966 4.337198 8.302797	H -4.18206554319835 0.78059086770973 3.41996766027652	H -7.136909 5.419124 8.486731
H -2.627448 6.378686 5.090563	H 1.81071080633706 3.20294165432128 0.38796799766865	H -1.189889 5.892278 6.517085
H -4.507769 5.800005 6.559443	H 0.10287704755529 2.12846026679530 1.83457787607758	H -2.588834 4.024628 7.572788
H -6.398095 5.233053 8.022961	H -1.82067643440298 1.50173401461398 3.24555584406318	H -4.703882 4.936435 8.684587
Local minimum	TS2	
H 6.30898780945735 -0.84028542132882 -0.27864799381267	H 5.96150763471607 -1.17390392634001 -0.86555109678978	
H 5.67647137750471 -3.19473946127157 0.18739084778039	H 5.28120668484384 -3.45336945587686 -0.15732741153583	
C 5.30530200769008 -1.07652812933479 0.06239482631683	C 5.00498609540875 -1.32800371078032 -0.37486367963806	
C 4.94772554705780 -2.40012933153660 0.32076027009101	C 4.62029782245869 -2.60967613390454 0.02040761070710	
C 4.37891680029953 -0.05929952089559 0.24099645169437	C 4.16578275617802 -0.24851306819328 -0.14143241287890	
H 4.64663403168396 0.97456580743989 0.04601280715521	H 4.45509619873302 0.75392581420027 -0.44185819554560	
C 3.65895865917264 -2.70440790388775 0.75378635250177	C 3.39202073446756 -2.80880557089328 0.64682621000469	
H 3.38467851999147 -3.73225707100192 0.97158108077720	H 3.09891457591020 -3.80320590892404 0.97000199655589	
C 3.07374215809250 -0.36077130014890 0.65456494451432	C 2.91855328488199 -0.44453973044637 0.46890255776805	
C 2.71877688538056 -1.69266329729974 0.91040451968339	C 2.53718343532889 -1.73436740091171 0.86226097932815	
O 2.51691879617299 1.89369874736894 1.06019713992168	O 2.53447201305407 1.85892881989358 0.79914779699158	
C 2.12238819613764 0.76434641495301 0.83635506894748	C 2.05774485447367 0.74316141004056 0.69452680806831	
H 1.72458803800287 -1.94698672175654 1.26247152444039	H 1.59113290585477 -1.90563470271132 1.36465172327114	
C 0.61099576295088 0.44045048650863 0.76436040583872	C 0.52962748643122 0.53131916629981 0.78736338325511	
H 0.70238792312759 -0.12359672234242 -1.35014737342330	H 0.57404711385690 -0.04663164495621 -1.34103943482395	
C 0.27125440979263 -0.40664507758497 -0.39093604031694	C 0.04437426883041 -0.24615295396181 -0.41110193016218	

H 0.37949699579258 -0.06795008184878 1.70936558117485	H 0.35400777370547 -0.04364659189220 1.70521427391152	
H -0.21463180009025 -1.94180266116453 -2.47685266079807	H -0.04755816882311 -1.99270066189645 -2.38976200949815	
C -0.53695405027910 -1.56102606011379 -0.36833629729712	C -0.55852773276968 -1.54328526542338 -0.33635964744898	
C -0.71976114051152 -2.28716243659778 -1.57844640229801	C -0.53331378221572 -2.36422081699089 -1.49117103652631	
H -1.08626976964356 -1.49706645884269 1.74215878394099	H -1.26039327190979 -1.40228731256223 1.71885633870029	
C -1.20327483682854 -2.02130817131510 0.79862490086600	C -1.20508139014220 -2.02069783293755 0.82758813984218	
C -1.52762245564417 -3.40510776525483 -1.61505279572561	C -1.10326100425458 -3.62270981859299 -1.47039631730448	
H -1.65727082429718 -3.95044360506081 -2.54517743360888	H -1.06629526390366 -4.25139655971148 -2.35461534233171	
C -2.01512363548694 -3.13897293166730 0.74501197633305	C -1.77913852286137 -3.27676091411743 0.83536763754348	
C -2.18215659480631 -3.83681987783289 -0.45509712405883	C -1.72860565782491 -4.08358486355640 -0.30848478231949	
H -2.52404528197423 -3.47668698407610 1.64302989362977	H -2.27298705712581 -3.63983728209452 1.73150365003087	
H -2.81905049602263 -4.71594477108541 -0.48684644764969	H -2.18167535691204 -5.07055410645735 -0.29260235776680	
H -1.72676642138326 2.27556239139438 -3.57012471748312	H -1.27696138142397 2.05192255074960 -3.49802895043614	
H -2.85983598387636 0.90349670984321 -1.91916923455239	H -2.13865649777893 0.35391582961463 -1.83652086032714	
H -4.43771299312129 0.09521958989288 -0.23551091403211	H -4.12613155576048 -0.12794604166166 -0.34259786532798	
C -1.01730678429625 2.61122839372175 -2.81866437974969	C -0.75348431776803 2.55162504377734 -2.68771534475928	
C -2.19221308141638 1.26397477658830 -1.13755958814289	C -1.69304989528480 0.93447975184294 -1.03025389651603	
C -3.76091214260705 0.40869099031203 0.55466153624877	C -3.60095134965791 0.35387689556015 0.47769519102564	
H 0.02962430441727 3.94718452800128 -4.12703773060819	H 0.06503264099667 4.10822148574691 -3.91657353783155	
H -5.05185266629554 -0.18588655241432 2.15777324032724	H -5.14529059266097 -0.00234232204423 1.92611849878845	
C -0.04695845669858 3.54375513893972 -3.12211128368195	C -0.00826787626050 3.69661289411526 -2.91470696308250	
C -1.12185682149818 2.10755540515142 -1.50068449677615	C -0.86639287869517 2.05909881214990 -1.37507532618257	
C -2.52711841733162 1.00811790725804 0.20646618749601	C -2.34550073419097 0.93714391579738 0.25427812837013	
C -4.09959068286102 0.25706216778989 1.88322943009901	C -4.16336886513364 0.42358806051286 1.74403919590138	
C 0.82895224147201 3.98416140664294 -2.12217958606256	C 0.65015833578829 4.32552761634046 -1.85265381508841	
C -0.19294519467885 2.51620405029713 -0.50333941980240	C -0.16077666358828 2.66684734147133 -0.31429737429376	
C -1.61662052587464 1.39750306151681 1.22519365122127	C -1.63284588370299 1.53197047703739 1.31450001957935	
C -3.21223783509010 0.67983915146043 2.88260264491899	C -3.46419613454474 1.03307470155716 2.78879421679808	
C 0.76427702628221 3.46601581429013 -0.82776596646821	C 0.59164011686199 3.80084827479421 -0.55651293422339	
C -0.24642900640383 1.82086944804342 0.81752765165267	C -0.21912899536312 1.91598105584596 0.98413237296527	
H 1.57534734647660 4.73792666379468 -2.35609343655348	H 1.23034395332989 5.22484075875336 -2.03820493548437	
C -1.97284107720544 1.22642756611951 2.55606898616379	C -2.18986639631241 1.57022493092441 2.58175666672935	

H -3.48947761387679 0.57127787320604 3.92724228588081	H -3.90997806732580 1.08011738728536 3.77819870023747	
H 1.46683596522911 3.80107421109391 -0.07321545130908	H 1.14295085358343 4.27165785927716 0.25117774290784	
H 0.24573154252907 2.41040942419681 1.59694253424485	H 0.26827887932761 2.45665847711531 1.79792351955086	
H -1.28016075461448 1.51786918983873 3.34182425035052	H -1.63767612482589 2.00920126713521 3.40847409929122	

9-CIC₁₄H₇ + Chalcone

Reactants	TS	Product
H 1.59458894882969 5.22876016342940 4.12428037526027	H 5.34557412766276 1.81026001893125 -0.88755509418309	H 0.96346861119318 -1.75760443484083 5.49992143342372
H 1.73192650569334 3.43373690997675 2.41340046644379	H 5.66775132156708 -0.29359144381095 -2.16863865329997	H -0.60909945304056 -3.21238517358588 6.75639210128692
C 0.98170419917950 4.33687148376129 4.22083502797987	C 4.69285461153907 0.95960158095773 -0.71142829787938	C 0.08981240446620 -1.32699183362066 5.98066976765789
C 1.05659602183451 3.32985827355508 3.25821272348180	C 4.87252047191656 -0.22045948518212 -1.43186044098262	C -0.79571374698169 -2.14449068005895 6.68395471478301
C 0.12353599416658 4.20063388827942 5.30329593465501	C 3.68203823382892 1.04934925260078 0.23703030299812	C -0.14709967505721 0.03695296839055 5.89164516646351
H 0.06031856735868 4.97712182471290 6.06021671012395	H 3.54852433616679 1.95973614916580 0.81331107679262	H 0.53338512868161 0.68247482084029 5.34482578134528
C 0.27314407454666 2.18582008488834 3.38779420104786	C 4.04258501346587 -1.31244613563372 -1.18919989090454	C -1.91778365685655 -1.59086067378253 7.29476322379371
H 0.34570551019783 1.38939224633926 2.65262764911981	H 4.19886510603493 -2.24575919490687 -1.72284411646808	H -2.60337283579942 -2.22252677379231 7.85201078505435
C -0.68977727530604 3.06724620918606 5.42478888295797	C 2.81252731286694 -0.02542707120570 0.45334331739705	C -1.28295163153038 0.60168608447206 6.48989315874241
C -0.60195456097131 2.05489270636051 4.46243525933306	C 3.01244518703229 -1.21521363168023 -0.25776812790952	C -2.16835133607177 -0.22645042418729 7.19192516246567
O -1.18202540960584 3.41780270438374 7.70619507286035	O 2.14402954332846 0.54705432696203 2.63898498660372	O -0.55901570075026 2.80801126425704 6.05755684066367
C -1.57353656142597 2.96166307962698 6.62463023437115	C 1.77929268877242 0.10422859686341 1.53387965702746	C -1.49309705042100 2.06937868436944 6.33088498297224
H -1.19172965486329 1.14946424435617 4.56923663345906	H 2.39315172343553 -2.08390549480055 -0.05319252123531	H -3.04653485390019 0.17998902655531 7.68134803640246
C -2.90010353097035 2.35167618290668 6.54351734664366	C 0.40258229821321 -0.27347736002463 1.31882157624918	C -2.92585826692255 2.57853498743290 6.39190395114945
H -3.14048906768065 2.42537450866390 4.45466483879202	H 0.59527684476576 -1.10454254526462 -0.62901350397050	H -2.80816144947150 2.01167736499529 4.28940345459594
C -3.60312511420629 2.16763754933851 5.40611608728406	C -0.12250550620371 -0.92434521230345 0.16697570820682	C -3.59941861940835 2.20979868921939 5.02278736391623
H -3.34342110071182 2.13978591939346 7.51450276775491	H -0.18456715274229 -0.26264708587263 2.23284067391714	H -3.46602769165030 2.08080793179420 7.20092233187604
H -4.81409687641926 1.42984340857521 3.17355907809421	H -0.48348554791076 -2.91853618656153 -1.55879051363708	H -3.53454291215713 0.09531131716320 3.36641235923964
C -4.96583019822300 1.66774465130692 5.30880012258643	C -1.07614764213110 -2.05711707861085 0.32252031139307	C -4.47906320289689 0.98472110711791 5.08193065541286
C -5.45790483277001 1.31269954924131 4.04229783799306	C -1.13811044624447 -3.01807442956799 -0.69525183289485	C -4.30780318774553 -0.01755079326066 4.12336499268857
H -5.47414141805697 1.83752605628002 7.40696708657421	H -1.91551009160084 -1.46094305616095 2.22458513738312	H -5.62356434291425 1.57748633942078 6.81806277129751
C -5.81525984096962 1.53507192596328 6.42136032163927	C -1.92885684031387 -2.19426698766749 1.42385029121498	C -5.47051405035683 0.81881269886387 6.05472760768708
C -6.74604804149127 0.81441716973678 3.89205202196538	C -2.01866343104969 -4.09101936979417 -0.61308495791065	C -5.10041445711412 -1.16221730576641 4.13592328080532
H -7.10886713522985 0.54107160125607 2.90520618125019	H -2.04645838137422 -4.82811666996513 -1.41092141148366	H -4.94439810697526 -1.93473976717000 3.38787564677593
C -7.10396373879443 1.04907002690844 6.26676745528296	C -2.81062651614259 -3.26784670368693 1.50546569587567	C -6.26637349013017 -0.32289671906102 6.06670042257618

C -7.57353701292899 0.68273015602998 5.00358314239188	C -2.86045307724419 -4.22019027373463 0.49015266818505	C -6.08334310477161 -1.31901251902618 5.10955987467555
H -7.75542521313758 0.96543476906035 7.13217301162624	H -3.46528728544562 -3.35770473950139 2.36811698835967	H -7.02929139939346 -0.43680357263650 6.83209843289310
H -8.58612590948097 0.30592592173627 4.88886921652478	H -3.54958314344623 -5.05726867323992 0.55816928187244	H -6.70037740828338 -2.21309549150926 5.12611048301474
H -5.16141333145357 4.33065363192906 1.10199274366144	H 0.09298073836579 0.52864106947448 -3.28097134412498	H -3.52014942043386 4.85250871864266 2.16689679036049
H -7.18505200968165 4.12196905379605 2.42503502688550	H -1.55425311825619 -0.32319535412459 -1.67192919300809	H -4.88924293969257 3.24542604944155 3.57013242919308
H -9.22119758425015 3.87406993060285 3.71552849271543	H -3.78532717443335 -0.42799058705571 -0.63746283642817	H -7.15117959419175 3.80773714958645 4.59228488095743
C -4.59735993443748 4.63821005538701 1.97905762945765	C 0.42426877253342 1.26483178844526 -2.55290177820337	C -2.97799571019000 5.13630149782920 3.06563733142631
C -6.64428802331469 4.42947261587412 3.31730168516436	C -1.18698903555674 0.33813618674200 -0.88833793827963	C -4.35030535603175 3.48644683645036 4.49048612474202
C -8.70337937552997 4.16804271150293 4.62519203282434	C -3.46122403039913 0.26446989543195 0.13505560125871	C -6.63735097124127 4.09095976955678 5.50751552699212
H -2.74466184176592 4.83368951451091 0.93937864048298	H 1.86423365573310 2.16637654285098 -3.85935931601091	H -1.73427408895179 6.58662880016715 2.07257795150485
H -10.41939247276433 3.97191581182462 5.87645149677378	H -5.33202260658869 0.25318873703512 1.18011363979957	H -8.43353496835178 4.64220554572321 6.56036056360336
C -3.26145920132076 4.91653242916284 1.89114041865026	C 1.41374189555705 2.17609163186147 -2.87106944735233	C -1.97773148350868 6.10733427215175 3.01666961532585
C -5.28731148958512 4.73440051334017 3.22111788034699	C -0.18539755528855 1.29494847933358 -1.29045822272135	C -3.28868047051517 4.53659005270786 4.27909827376724
C -7.31987239320267 4.49148443053453 4.53468668892656	C -2.15855722801585 0.78079420382586 0.07930653047796	C -5.25590562817518 3.98509596186854 5.58307079639082
C -9.36380530794374 4.22181727335204 5.82075372005750	C -4.31673382920279 0.63813543971048 1.15389095876061	C -7.35213187397916 4.55283269137183 6.61315422795625
C -2.54293029692045 5.31591161858778 3.04729269985198	C 1.83435928208710 3.11955368759370 -1.92008682228695	C -1.29651775342253 6.46731283052279 4.17720901518164
C -4.55344323114124 5.13400981932858 4.39858938765851	C 0.26388606571354 2.22486457774814 -0.31773339393287	C -2.58900043305329 4.88765668143824 5.44085766193656
C -6.61362765608310 4.87972131653252 5.73292335505102	C -1.71028321715631 1.66729358360060 1.09416222107761	C -4.58065370022980 4.33675918741155 6.76083418102966
C -8.66877257403759 4.60030762908308 6.99787014394117	C -3.87080555854173 1.50543769221744 2.16456233795188	C -6.68123033462653 4.89669021926955 7.78307109838378
C -3.16600751829166 5.42484787583974 4.26097390984366	C 1.28569078470761 3.13543769130453 -0.65457227310508	C -1.59720484029939 5.85629758344919 5.39509913469008
C -5.24928981948567 5.18478434608993 5.61638371094104	C -0.36384974812067 2.13862297370530 0.96746525380848	C -3.07887831015226 4.10970431090403 6.64745775573961
H -1.48009761380607 5.52740945835471 2.97113213071894	H 2.60847256902734 3.83661651475250 -2.17736073737648	H -0.52116745813706 7.22715863920994 4.13745121873843
C -7.33758418438721 4.91847118951004 6.95875175641913	C -2.58368340433656 2.00402237824706 2.14883087166402	C -5.29087358169846 4.78626892974924 7.86502717383852
H -9.20132735623917 4.63730312951909 7.94404907290251	H -4.54581586130675 1.79105381256300 2.96609737773247	H -7.23894878169410 5.25617305674288 8.64315040596717
H -2.59499468875194 5.71908578984478 5.13429083487516	H 1.63243742010740 3.85533681541168 0.07859008216822	H -1.05134553340818 6.12869473735112 6.29247965683951
Cl -4.36231514516964 5.63148668619022 7.06895509591441	Cl 0.29596817675283 3.09659157587009 2.26133011806269	Cl -2.21513179695254 4.55022981624993 8.18311473704126
H -6.82490495349907 5.20289925714901 7.87064608763795	H -2.25086075212885 2.67340956715050 2.93433999935113	H -4.77759912860343 5.05283163611043 8.78288960623482

(9-ClC₁₄H₇)^{•+} + Chalcone

Reactants	TS	Product
H 1.44666473747067 5.15531099625561 4.04562333165091	H 5.52438983753373 0.17310270632402 -1.76820851692410	H 2.03703009639738 -0.93799057791585 6.45528858359469
H 1.70369000834750 3.18670730603518 2.55386624363509	H 5.37758004369285 -2.30353951922704 -1.71223773214264	H 0.57368797325590 -2.82833393612798 7.11909354841288

C	0.83291854298073	4.27216123358799	4.19898361987391	C	4.77316896912264	-0.31397034561166	-1.15345905449774	C	0.96282100424569	-0.79549998829304	6.52313737964612
C	0.97471520830277	3.16748012945448	3.35921765994716	C	4.68705778770618	-1.70551843263935	-1.12443798724690	C	0.13819258806016	-1.85807642158256	6.89766442999238
C	-0.09284020656639	4.24395191071148	5.23271915314821	C	3.90185064259259	0.45286264208494	-0.39032117174792	C	0.41060759231769	0.44125339953729	6.23522999327636
H	-0.20787877338628	5.09659517351508	5.89572363981766	H	3.96458766825786	1.53741549603365	-0.39610151719534	H	1.04034495598484	1.27430864558538	5.93988426544127
C	0.19049317916536	2.03427718066516	3.56207898193364	C	3.72377922190574	-2.33152144362601	-0.33604683130105	C	-1.24048049011402	-1.68042658191004	6.98980351252454
H	0.31664731695890	1.16330088767213	2.92549739394510	H	3.67367932776254	-3.41537385284125	-0.29187727998981	H	-1.88008209463944	-2.50929452225240	7.27679909080049
C	-0.90781266400348	3.12048458951542	5.42374835820064	C	2.90879791994586	-0.17272902380963	0.37133698099443	C	-0.97778582759253	0.63015073866124	6.33973008398384
C	-0.75295107687444	2.01029156536124	4.58470269021406	C	2.82335528165729	-1.56965494722975	0.40058849075357	C	-1.80203693852531	-0.43892671072073	6.72168313557508
O	-1.56989970503642	3.72611700291181	7.60970386549964	O	2.47398528692495	1.60691598088581	1.83073835928604	O	-0.85547176610623	2.80398972522608	5.43694037397992
C	-1.86686812545983	3.13441019801278	6.56662929718381	C	2.01198154393636	0.68700793905658	1.18878356098088	C	-1.53511735860901	1.94630238309993	6.00341289946870
H	-1.34162585979335	1.11331976991576	4.75202432132005	H	2.08753900840377	-2.06457485993867	1.02830619853330	H	-2.87871399195228	-0.32097461119301	6.79409447674182
C	-3.17806877372263	2.48351203981293	6.46891541849581	C	0.48136004864186	0.38152211068357	1.21015114085548	C	-2.99562604249119	2.26128563682774	6.26876658670965
H	-3.27974101821053	2.36211480810140	4.37166434038819	H	0.56075445055067	-0.58016924204105	-0.76338304896228	H	-3.07846975387984	1.59023974744720	4.19426529944730
C	-3.79988614306957	2.17454674536549	5.31029674053533	C	0.10629388331038	-0.64334336576939	0.22131184769621	C	-3.78081126289338	1.95579717412482	4.95276062055997
H	-3.67558134178482	2.35557051378580	7.42804501606193	H	0.22136919818015	0.07818223065041	2.23011798053400	H	-3.38990361986002	1.68087624748567	7.10346938678927
H	-4.90113415143250	1.39581750109536	3.03775787332419	H	-0.54538052345805	-2.42060417028456	-1.59552244650165	H	-4.41138139329053	0.01431968601877	3.21104042613228
C	-5.13830814888284	1.62723430185339	5.16917055519692	C	-0.75402960363977	-1.73894070175779	0.44888772825812	C	-4.87436706076816	0.92397235370357	5.10562676660190
C	-5.57578899896493	1.26439861344070	3.88069257571019	C	-1.02528647696868	-2.61223585046386	-0.63912763702972	C	-5.07184101682583	0.00096196039883	4.07507541269225
H	-5.72008764381011	1.74828108120747	7.25407508468662	H	-1.18608958760958	-1.36143014926382	2.55160304461755	H	-5.59679237597197	1.59317381134876	7.03463689387384
C	-6.02053441678809	1.46037395058148	6.25143064781886	C	-1.38432642414289	-1.99412973786202	1.69328607135504	C	-5.72768668523693	0.89200755172083	6.21433079236509
C	-6.84596186876394	0.73823306720947	3.68041998827231	C	-1.89386863305737	-3.67342871346749	-0.49123602019724	C	-6.09762308726919	-0.93645657594023	4.14867123319092
H	-7.16512306048319	0.45938590725096	2.68044164814822	H	-2.09733622913228	-4.33123481520705	-1.33068014868654	H	-6.23123809363760	-1.65333417311440	3.34347753571453
C	-7.28916713673865	0.94356355917771	6.04565388152067	C	-2.25541661188349	-3.05911714138316	1.82739758916646	C	-6.75567677226529	-0.04391417690120	6.28641941636578
C	-7.70745468588330	0.57993248303319	4.76142942752045	C	-2.51592120853892	-3.89957634437223	0.74185080202102	C	-6.94409074963577	-0.96030295366338	5.25528450350992
H	-7.96609212142496	0.82791220163419	6.88723388234165	H	-2.73609498528542	-3.24484523447710	2.78309562670334	H	-7.40877756930803	-0.05720113130691	7.15433202804588
H	-8.70523658371227	0.17786799693618	4.61024559516409	H	-3.20130879332783	-4.73426094601780	0.85696694167051	H	-7.74253515406749	-1.69428495840841	5.31612197995133
H	-4.99289736913282	4.14164610841184	1.22881727483876	H	-0.23669061909684	1.82423505281032	-3.62932920860533	H	-3.34030021768863	4.75315787065471	2.18301001926336
H	-6.94300642742221	3.84253962023686	2.62115234657011	H	-1.87341865797169	0.57138107386376	-2.36802652755889	H	-4.85931953986759	3.14462675352486	3.44762089821434
H	-8.90733230202065	3.50907779420508	3.97831162489531	H	-3.93213010158212	-0.12080506334343	-1.31823030022980	H	-7.08131715447387	4.00490826552131	4.34588659671265
C	-4.45105608746853	4.59617200710354	2.05344798888962	C	0.15928299476916	2.25869712188855	-2.71575362966335	C	-2.85795757769704	4.97712224697398	3.12957763811354
C	-6.41676959636088	4.27493640211720	3.46844784530987	C	-1.52942537081411	1.02353400699709	-1.43919823604745	C	-4.34543236262028	3.30943960920243	4.39725924454067
C	-8.40147584237961	3.92442013449488	4.84509522970151	C	-3.59533834435433	0.26762634718528	-0.36121241300926	C	-6.58961169115174	4.19944423922333	5.29473693385819

H -2.65812113707552 4.92679023294003 0.92771520679658	H 1.61461570829058 3.48591382367688 -3.70070300487354	H -1.58020314094355 6.50468000616680 2.31913291359971
H -10.06784854409898 3.65610442860635 6.16641649403382	H -5.38366123840372 -0.25486045539591 0.70062301216120	H -8.35067471374806 4.95128100001067 6.26989486276101
C -3.15188558793616 5.03382602451326 1.88834957985096	C 1.18221810271035 3.18397526164167 -2.75202324132871	C -1.87885897290539 5.96665768700224 3.21403833955641
C -5.10027583551263 4.72630344868249 3.29955062370454	C -0.41143865364781 1.88209829367532 -1.47911474168511	C -3.22431061408718 4.29949806100766 4.27520102100368
C -7.07425216648898 4.37755606841496 4.70195400663953	C -2.32358499477221 0.87630408945420 -0.28328648965849	C -5.24029636071169 3.90779628955853 5.44823351184212
C -9.04572744672622 4.00770223149995 6.06628515302438	C -4.39852968887279 0.19705467241934 0.76015684484882	C -7.29302611287799 4.72756474748473 6.37165628777469
C -2.47066345672174 5.62413716921638 2.96260632114710	C 1.65202788485236 3.73970575224382 -1.55841760711130	C -1.28090187637151 6.30214631459914 4.45083759864760
C -4.39629058921045 5.31600051415611 4.40433187365876	C 0.10194820184175 2.41861718585898 -0.26699018734325	C -2.56432391176808 4.59136270940820 5.51691531595603
C -6.38949163817308 4.93060917217099 5.83784527690499	C -1.84191550097146 1.36352633352135 0.96121676936779	C -4.59247011538549 4.15351974042219 6.67801742397802
C -8.37607883785307 4.53813788396950 7.17631578400356	C -3.93549429190713 0.71333013939485 1.97175868570962	C -6.64660148058710 4.97150811780544 7.58770353313986
C -3.07716161209814 5.76711510356637 4.19793566218750	C 1.12624575779965 3.35152130453117 -0.32515156673242	C -1.62831037457980 5.63558194092526 5.60326643324153
C -5.06370119533516 5.39287987831801 5.65452601074050	C -0.39506440707966 1.78532813018191 1.00222092682588	C -3.11926574652307 3.76629251472888 6.64414508498373
H -1.45058475705988 5.97010302647357 2.82919417995157	H 2.44569827362544 4.48051888857773 -1.58357573480069	H -0.53724489363605 7.09198683220715 4.48417566736987
C -7.07289359557407 4.99208991809466 7.07059490730672	C -2.65898338158141 1.27173479939457 2.07650365804736	C -5.28898835637891 4.69559253090847 7.74619436254709
H -8.88351650847954 4.59627003115603 8.13415509683665	H -4.56491125232520 0.66747353910557 2.85540609311576	H -7.20797304145621 5.37722630391738 8.42389614498239
H -2.52551287766877 6.22355208885261 5.01175695385756	H 1.52815456365003 3.78014945213697 0.58510268453599	H -1.16515022597903 5.87712119609850 6.55323466153215
Cl -4.22624176590937 6.07668338040155 7.00021308573226	Cl -0.12045312391106 2.85974792542924 2.43483678428585	Cl -2.27791527279427 4.04597995932069 8.21422214364670
H -6.57863198622658 5.39996392139764 7.94487057106210	H -2.31562290332894 1.62638205632249 3.04140445874576	H -4.79826099488880 4.88574541797129 8.69420364884609

9-BrC₁₄H₇ + Chalcone

Reactants	TS	Product
H 1.58334317765205 5.23733371055048 4.11758223252771	H 5.31563179706948 1.83797447763539 -0.84325075412090	H 0.95230589680563 -1.77239491545715 5.50055621597228
H 1.70113025252412 3.47437868849287 2.37228360453673	H 5.65053199119680 -0.24903178602490 -2.14817379842973	H -0.61395775671685 -3.21429787355538 6.77941479068939
C 0.97498880951534 4.34157853920709 4.20687591596346	C 4.67007823727058 0.98039935181863 -0.67462956655028	C 0.08234821652975 -1.33648998883871 5.98323250960825
C 1.03862374399183 3.35277590071565 3.22484486450118	C 4.85677584243012 -0.19011784521468 -1.40859710992137	C -0.79967218912250 -2.14680849203325 6.69911310699524
C 0.13343593657550 4.18260597812458 5.29936852320063	C 3.66097093440453 1.05214022371680 0.27738524611737	C -0.15336656106057 0.02688640394786 5.88401032505706
H 0.07935633026414 4.94483569283267 6.07138267962776	H 3.52131206421365 1.95530280805400 0.86392066608270	H 0.52426319175633 0.66679914749438 5.32715501180414
C 0.26000292481810 2.20432097204006 3.34442646420015	C 4.03582452713008 -1.29119824145964 -1.17623687166992	C -1.91700780110330 -1.58651093487076 7.31248951342853
H 0.32374977513980 1.42193975993582 2.59352559178388	H 4.19741495265251 -2.21720855724655 -1.72092272263321	H -2.59982377281535 -2.21247341455678 7.87946079014976
C -0.67493948797442 3.04486743389752 5.41134791582972	C 2.80097547601843 -0.03188085639632 0.48372858778469	C -1.28450992311768 0.59838160099331 6.48485334050212
C -0.59932281948223 2.05116123659406 4.42884918198071	C 3.00790829974191 -1.21231126258354 -0.24084507311519	C -2.16627873373804 -0.22265068174034 7.19989808986828
O -1.12519191201155 3.33650187795874 7.70901462965389	O 2.13256012843155 0.48965103560999 2.68320185117955	O -0.56226952075632 2.79906289130680 6.02100075515018

C	-1.54020679125873	2.91486708129001	6.62231886073470	C	1.76771369774154	0.07793146810969	1.56594881880367	C	-1.49375351479860	2.06475745242414	6.31427847200183
H	-1.18576253254870	1.14253219073059	4.52714763743905	H	2.39527538606644	-2.08765046839339	-0.04417225523831	H	-3.04064520575912	0.18895580768347	7.69183946034537
C	-2.87503749694441	2.32339128586112	6.54604491720285	C	0.39027808196317	-0.28015803731260	1.33309220869169	C	-2.92435548721851	2.57803403867233	6.38674997356995
H	-3.13371110905806	2.41914223304655	4.45983852734281	H	0.59945908365213	-1.09766674368205	-0.61619167980284	H	-2.80918818172039	2.01483114744490	4.28142959836890
C	-3.59066459280141	2.15897259765572	5.41337954604694	C	-0.12610190386232	-0.92463809411388	0.17441700337723	C	-3.59984625218916	2.21166097568969	5.01575209789320
H	-3.31145139745157	2.10447305327654	7.51862153554723	H	-0.21212952536356	-0.25638525652119	2.23697233381033	H	-3.46379128119589	2.07717969147197	7.19369356937623
H	-4.82227285622759	1.42735680493252	3.19002107362924	H	-0.49338559039738	-2.88355695750537	-1.58870570075904	H	-3.53411280869831	0.09720819541509	3.35976133297098
C	-4.95879108589173	1.67264829326246	5.32536639594753	C	-1.07558072061843	-2.06373315979507	0.31439740871622	C	-4.47858068872571	0.98615165928962	5.07559109606018
C	-5.46180717242864	1.31834729589340	4.06294878615799	C	-1.14082488695395	-3.00390261558957	-0.72230608596644	C	-4.30687603718679	-0.01614738338523	4.11713526508459
H	-5.45252021707743	1.85456318174233	7.42580090512447	H	-1.90172500566038	-1.51091973144238	2.23523205259929	H	-5.62206435021048	1.57804003872920	6.81264606961874
C	-5.80263623287238	1.55159652114498	6.44347438768208	C	-1.91887557748418	-2.22692743211334	1.41917669644521	C	-5.46915226372935	0.81947420980617	6.04922748899751
C	-6.75484309162026	0.83016980136300	3.92227549458064	C	-2.01537796671678	-4.08260091037318	-0.65523623936068	C	-5.09890855461670	-1.16123313524219	4.13006606604635
H	-7.12610173053456	0.55707138358270	2.93850241978934	H	-2.04537785597586	-4.80381328183661	-1.46737443849303	H	-4.94283201826399	-1.93360415634531	3.38187798046694
C	-7.09664261028229	1.07697131710537	6.29815501462767	C	-2.79535065680811	-3.30607389926300	1.48527371117835	C	-6.26434014537346	-0.32265192675351	6.06151799074820
C	-7.57664738243837	0.70951273043441	5.03924183167378	C	-2.84821383688608	-4.23799847601543	0.45143788886368	C	-6.08133781504474	-1.31850444871679	5.10409053723820
H	-7.74391812099684	1.00290863835165	7.16755376149943	H	-3.44220588665135	-3.41710648062523	2.35130258567881	H	-7.02672379751418	-0.43712472201385	6.82735606141791
H	-8.59324967119752	0.34146478815225	4.93191440091088	H	-3.53232587899421	-5.07999986653520	0.50805466689485	H	-6.69789277640817	-2.21290838308730	5.12083565754058
H	-5.13498100954055	4.31122659061444	1.11136506571025	H	0.07223236255481	0.47632863971627	-3.27437081568351	H	-3.52395182594554	4.85615430066296	2.16765016826682
H	-7.16377755725245	4.10087457681857	2.41234558578282	H	-1.56371304479037	-0.33863978780053	-1.64790592168986	H	-4.88949161100610	3.25135406976405	3.56691792473719
H	-9.20887801986606	3.84830237560228	3.67353449835378	H	-3.77789476600560	-0.43809116315827	-0.59594147656122	H	-7.14582577801495	3.80876548926894	4.58366582682050
C	-4.57829220519871	4.62645402937298	1.99042816845880	C	0.41196602750849	1.22457644958107	-2.56263083129368	C	-2.98051728484984	5.14076604001249	3.06537825638034
C	-6.63464838970077	4.41566866927120	3.30905253053227	C	-1.18883046530783	0.33007294217053	-0.87449595912428	C	-4.34994364142646	3.48938930070512	4.48771309638808
C	-8.70760019654376	4.15136691254868	4.58948665048286	C	-3.45344906479871	0.26789431654272	0.16409972206093	C	-6.63615180424966	4.09031965644000	5.50173838438369
H	-2.71905378386741	4.82538656221987	0.96301920935115	H	1.84315608815214	2.09905933145925	-3.89703220644124	H	-1.74045753693266	6.59259252262266	2.06981035115270
H	-10.44200088517668	3.95328443843658	5.81497954496166	H	-5.32005447452591	0.26765637528063	1.21706592047085	H	-8.43726716670628	4.63669386046282	6.54895033473762
C	-3.24353352920842	4.91067461357104	1.91031405620201	C	1.40107530430726	2.12663534778414	-2.90532191341884	C	-1.98182323658508	6.11304388805396	3.01429546337999
C	-5.27880861825939	4.72677544258818	3.22618953175825	C	-0.18787535089228	1.27828003700801	-1.29624553186445	C	-3.28905326907746	4.54003603898511	4.27885164756325
C	-7.32483076621595	4.48231308478940	4.51726005351498	C	-2.15298287660649	0.78765017981080	0.09301026266234	C	-5.25488984928233	3.98525746914702	5.58135512426006
C	-9.38718315360207	4.20890513183019	5.77367390140901	C	-4.30618312618943	0.65529119485626	1.17973493407437	C	-7.35599464833999	4.54821316087085	6.60544236592872
C	-2.53718613760880	5.31911102266688	3.07058469275090	C	1.83066987440849	3.08541071577897	-1.97368692980875	C	-1.30003874718639	6.47355979512772	4.17404984600944
C	-4.55829643052207	5.13630354943210	4.41056002782706	C	0.27013941631258	2.22319770045929	-0.34004704907135	C	-2.58877525858626	4.89115375551417	5.44157400894205
C	-6.63478680195850	4.88239928208560	5.72276342006979	C	-1.69919850096524	1.69329433429442	1.09048670793788	C	-4.58116467366480	4.33443432355798	6.76226534737868

C -8.71061792382063 4.59886189458211 6.95755714982174	C -3.85813032245472 1.54274182691164 2.17163829515328	C -6.68887499058032 4.88888455337441 7.77814234131885
C -3.17051942171934 5.43028582756877 4.27845267610931	C 1.29212586586959 3.12377856933267 -0.70505133695976	C -1.59890655188645 5.86166214868010 5.39163803267009
C -5.27084904914870 5.19338832990640 5.61816929127969	C -0.35366273576343 2.16143877161414 0.94742116731177	C -3.07943609454391 4.10763755133613 6.64421749382115
H -1.47482670899033 5.53526499106255 3.00273444656608	H 2.60329721722709 3.79736978611738 -2.24885955129288	H -0.52565376051511 7.23434070090041 4.13427008623420
C -7.38101792081668 4.92359465783811 6.93545979391110	C -2.57300608780373 2.04460146411748 2.14090617198639	C -5.29893333567748 4.77957390842341 7.86359434178617
H -9.25630347014563 4.63953945235920 7.89609274913287	H -4.53009156914279 1.84218939414580 2.97067258336620	H -7.24885315505611 5.24520266795331 8.63803213767360
H -2.60747212015992 5.73073739985263 5.15490047181312	H 1.64450428357341 3.85609116607140 0.01283301128538	H -1.05335353409652 6.13380911658389 6.28932412463564
Br -4.32464250949035 5.70211427386965 7.21401422801351	Br 0.38083522957867 3.22427207068614 2.34467979407048	Br -2.13219339644608 4.57382536504059 8.32236119939323
H -6.88313670506872 5.21664720603723 7.85283548564417	H -2.24016449185631 2.73038093231838 2.91214152266725	H -4.78861836115168 5.04356960923949 8.78382987066687

(9-BrC₁₄H₇)^{•+} + Chalcone

Reactants	TS	Product
H 1.22805443456977 5.44376038047501 4.47616789467304	H 5.35132167802593 1.77810580794977 -0.82688323537855	H 2.046736 -0.926120 6.447069
H 1.50550610149956 3.75702970029059 2.67446696033941	H 5.64597919190647 -0.27089794528050 -2.20016525653632	H 0.593084 -2.818289 7.126680
C 0.65506444401731 4.52107790173702 4.50079246265895	C 4.69246209297574 0.92612665413069 -0.68290658789624	C 0.972255 -0.787323 6.518154
C 0.80851373254828 3.57481671093797 3.48779862971505	C 4.85666886019930 -0.22300064075959 -1.45501729653104	C 0.153068 -1.850908 6.901629
C -0.22991674843773 4.28389088048153 5.54374812506818	C 3.68902119872529 0.98338657610861 0.27598292892581	C 0.414248 0.445707 6.225503
H -0.35167488328838 5.01088223592955 6.34182013935946	H 3.56679647539770 1.86952529938771 0.89149319879484	H 1.039749 1.279532 5.923409
C 0.07696377739169 2.39015018113805 3.52592829227838	C 4.01860298028622 -1.31725603149682 -1.25390228653128	C -1.225934 -1.677992 6.998061
H 0.21393118175704 1.64030531050043 2.75207790049290	H 4.16262425457996 -2.22773682036594 -1.82884142990885	H -1.861252 -2.507746 7.291916
C -0.99288530000507 3.10923087955977 5.57244463365005	C 2.81144400246267 -0.09215733695671 0.45161217467191	C -0.974434 0.629833 6.334356
C -0.82605245588905 2.15787013108586 4.55897217655146	C 2.99567259193776 -1.25171127938266 -0.31177595630963	C -1.793254 -0.440136 6.725335
O -1.57177398937957 3.29116834179684 7.85470249870941	O 2.16575181295467 0.37336123121217 2.66929944566962	O -0.864656 2.797633 5.415638
C -1.90785569003527 2.89836535487787 6.73275325168860	C 1.78628411373406 0.00113131561776 1.54340382537988	C -1.537855 1.941974 5.993317
H -1.37094142137621 1.21921816243868 4.59539990903803	H 2.37008449913922 -2.12327043674983 -0.14093873518740	H -2.870129 -0.325922 6.800889
C -3.22273638022059 2.27146261979034 6.56567916534836	C 0.40024517104908 -0.33087573670418 1.31496718673679	C -2.996974 2.255863 6.265881
H -3.34525866049339 2.37411828070248 4.46708561132243	H 0.58003952573812 -1.09700307115570 -0.65913124156845	H -3.083003 1.582092 4.191049
C -3.85768775622157 2.09643234293569 5.38670460276729	C -0.13652126998335 -0.93109074915387 0.14119055015076	C -3.783784 1.951397 4.949156
H -3.70832538260504 2.02125070013767 7.50678313830857	H -0.18781773522122 -0.33834922582534 2.22838463487188	H -3.388697 1.671062 7.098141
H -4.92687981422558 1.38476100526017 3.07516275794699	H -0.53269500472382 -2.85404942862723 -1.65558599873519	H -4.430778 0.019109 3.204091
C -5.20037760958391 1.57034338286776 5.20648863360304	C -1.10796826549853 -2.05401594739580 0.25812484962925	C -4.881531 0.924463 5.103819
C -5.61896320138258 1.24402795925386 3.90228861181803	C -1.18670996572186 -2.97544862262481 -0.79433798844129	C -5.087760 0.006051 4.070787

H	-5.82235829920602	1.66879036105740	7.27993837637367	H	-1.93393982830237	-1.51588736631675	2.18333617916977	H	-5.593361	1.590669	7.037943
C	-6.10602049218330	1.39784802824950	6.26761716607785	C	-1.96026699742881	-2.21859114859548	1.35586708839989	C	-5.730559	0.892867	6.215801
C	-6.89233167058546	0.74008347524625	3.66735028065260	C	-2.08337279503087	-4.03723110008326	-0.74949453555114	C	-6.118042	-0.926316	4.145128
H	-7.19641924177761	0.48701625167490	2.65586392908550	H	-2.12422968905728	-4.74379744263989	-1.57395892445097	H	-6.258564	-1.639607	3.337927
C	-7.37944773133461	0.90715110298602	6.02665346843911	C	-2.85811980445335	-3.28109107558421	1.40015089798660	C	-6.763048	-0.038042	6.288632
C	-7.77732266826429	0.57400470912779	4.72807532736858	C	-2.92459864748232	-4.19433977112277	0.35051499591669	C	-6.960254	-0.949751	5.255018
H	-8.07589758565552	0.79025757418161	6.85200162336077	H	-3.51196928368183	-3.39294605529259	2.26081979827722	H	-7.412750	-0.051107	7.159096
H	-8.77843254331119	0.19216459936570	4.54917245876372	H	-3.62623193708692	-5.02283326682753	0.38953100564037	H	-7.762238	-1.679816	5.316448
H	-5.09303023780839	4.00124476311776	1.12010329268239	H	0.09604225796948	0.61492371759315	-3.25494001414526	H	-3.335755	4.746994	2.183967
H	-6.97592714044153	3.81221584587701	2.61066786722894	H	-1.55680075164152	-0.25188825690432	-1.67053162393652	H	-4.855350	3.145222	3.443504
H	-8.87559237846893	3.57494816452043	4.06438016076424	H	-3.78215267274193	-0.35655407279484	-0.64163521440309	H	-7.073179	4.004602	4.332234
C	-4.49133486244803	4.45239541221845	1.90429759933837	C	0.44080526735703	1.32782956362538	-2.51008299607644	C	-2.853744	4.972599	3.130349
C	-6.39220888844809	4.24131675446383	3.42127405267462	C	-1.17773746635176	0.37953582062425	-0.86811266362206	C	-4.342834	3.306769	4.394491
C	-8.31557761917765	3.98778780936013	4.89835979053649	C	-3.45141108371614	0.30921023518256	0.15130630753428	C	-6.587105	4.198204	5.284208
H	-2.74619038243812	4.67816308275764	0.68172177036683	H	1.88627695343667	2.24410132788189	-3.80034020661414	H	-1.577538	6.500828	2.319064
H	-9.92325286969586	3.79637076496281	6.30356033343961	H	-5.32466450980176	0.29173397331551	1.19227680348178	H	-8.353615	4.949776	6.250057
C	-3.18532101910898	4.83013195998682	1.66263262128599	C	1.44020753141269	2.23389598109917	-2.81008002944814	C	-1.876383	5.963088	3.214069
C	-5.07041500721260	4.63745207618357	3.17787751154066	C	-0.16356518792275	1.33291776652146	-1.24469940651897	C	-3.220685	4.295203	4.276220
C	-6.98255389082094	4.39303099334899	4.68282042771896	C	-2.14179968248201	0.80920056530490	0.11237460064760	C	-5.238835	3.905259	5.444203
C	-8.89660339331534	4.11229917481028	6.14699612445925	C	-4.30442345124178	0.66395289024627	1.17854112841115	C	-7.296651	4.725429	6.357356
C	-2.42841659449611	5.41850776442092	2.68576032422881	C	1.87575362959190	3.14667498552280	-1.83630590841108	C	-1.281303	6.300417	4.451591
C	-4.29015231635264	5.22411797013972	4.23371032608333	C	0.30054725285820	2.23032513942767	-0.24697826138477	C	-2.562273	4.587263	5.520832
C	-6.22171746721312	4.94438320105243	5.77225508854306	C	-1.68055875010767	1.66175778450898	1.15213493550050	C	-4.594764	4.148596	6.677759
C	-8.15535436456885	4.63896563236661	7.21218155276972	C	-3.84811326434466	1.49624203692119	2.21346796567292	C	-6.656074	4.967221	7.576490
C	-2.96703172840894	5.61725905866829	3.94418118013763	C	1.33252992540620	3.13554300284440	-0.56881874205461	C	-1.629262	5.634266	5.604022
C	-4.89128605376859	5.35498188669186	5.51239720366988	C	-0.32702936746147	2.11543553699452	1.03601451527111	C	-3.122534	3.759528	6.643257
H	-1.40373121255646	5.72051249406859	2.49375130137735	H	2.65726777674879	3.86136067945605	-2.07727367222495	H	-0.539372	7.091830	4.486104
C	-6.84538769273213	5.04752432215911	7.03389387149812	C	-2.55484347271587	1.97797890163959	2.21307034343174	C	-5.299687	4.689700	7.741081
H	-8.61106158662163	4.73026027117587	8.19316347340452	H	-4.51986051228472	1.76868383296438	3.02231797339054	H	-7.220496	5.372670	8.410739
H	-2.36054729196659	6.07621913350029	4.71559727157109	H	1.69032327176057	3.83217549057712	0.18118629147075	H	-1.167981	5.878103	6.554443
Br	-3.87518089917369	6.10687291735688	6.91740103960603	Br	0.41059126391603	3.11504802687061	2.47827506523760	Br	-2.203794	4.043008	8.361251
H	-6.29492992357790	5.45332928580502	7.87495811881409	H	-2.21594218308317	2.62185868511207	3.01709352159518	H	-4.813609	4.878110	8.691939

Ph-C₄H₄-Ph + DMM

Reactants	TS	Product
C 7.38316022837422 -3.00448381408642 -2.98869104907847	C 4.22439994980154 -2.00853711430542 -1.91612681668851	C 7.77536628029036 -2.38125725983522 -3.13644011319710
C 8.31793478304618 -2.16469257601461 -3.59003471277588	C 5.30280037280682 -1.13015789513909 -1.83582473927731	C 8.62326703932466 -1.37493041628889 -2.68185535768991
C 6.15930818509722 -2.49781333136830 -2.56801216589097	C 2.92912273885110 -1.54080499033191 -1.72653086975063	C 6.39821049311590 -2.27470234797776 -2.94814118168627
C 8.01224555250614 -0.81390641727262 -3.76926361215392	C 5.07530498031427 0.21876293560727 -1.56082859452675	C 8.08688855851180 -0.26029402857767 -2.03811308432093
C 5.83856503838460 -1.13842652655313 -2.73335873659605	C 2.68571836840695 -0.18366334972979 -1.46398415962261	C 5.85252627480038 -1.16312591948268 -2.30439237815198
C 6.79029657916421 -0.30570338321473 -3.35194329575897	C 3.78225092380981 0.68889829997402 -1.37286178693612	C 6.71214343969740 -0.15692085728612 -1.85113226123969
C 4.54395382109438 -0.66727014007545 -2.26240973082755	C 1.31093766465544 0.26620313057478 -1.25352089384563	C 4.35986861393737 -1.04386287218565 -2.08868224413984
C 4.12091034775315 0.61633653684844 -2.19757000952074	C 0.87258977700570 1.56080393971583 -1.54500468406492	C 3.78203369987516 0.24045665672511 -2.62191576659758
C 2.81356325383925 1.02757366564436 -1.73779974696197	C -0.41329287125573 1.99814897042223 -1.25815487058317	C 2.52813798058600 0.57644763368864 -2.32363524061581
C 1.70247756306466 0.25787907688368 -1.77362121323407	C -1.37669538584660 1.16421876452674 -0.68009027380509	C 1.73911048788348 -0.29410037730218 -1.38211141519523
C 0.39787807932668 0.58071670256811 -1.21557252618058	C -2.70107089976721 1.63960624255882 -0.26881933531024	C 0.43822663998050 0.32470307508992 -0.92438930114936
C -0.68034738240586 -0.28114876651390 -1.48534217317307	C -3.79895597158326 0.76822133512359 -0.33258149232073	C -0.75364965782327 -0.40059722271231 -0.97889605750655
C -1.94111174286873 -0.04590201088271 -0.95045716421496	C -5.06244796098132 1.18481624155357 0.07179845759333	C -1.94654922748857 0.15793342993330 -0.52430984492272
C -2.15687717811517 1.05933840084821 -0.13040382706315	C -5.25038875818155 2.47727253840931 0.55701314569991	C -1.96000831943934 1.45047509521695 -0.00669839343104
C 0.16392917138631 1.68981579782415 -0.38073324731532	C -2.90053778551321 2.93448981651052 0.23519589409264	C 0.41530053917044 1.62222457403234 -0.40304104410761
C -1.09730129552981 1.92494383671869 0.14818512659284	C -4.16383516984819 3.34845894122429 0.63870798469981	C -0.77461977238560 2.18173935796518 0.05215182130305
H 3.87540847714599 -1.44876263128720 -1.89996393434815	H 0.57553119930275 -0.53472770211284 -1.23199646219196	H 3.87525618335639 -1.86917095532352 -2.63075806560475
H 7.60800333768005 -4.05809382021843 -2.84712360792152	H 4.39279061814404 -3.06140681917808 -2.12506202163882	H 8.18482068054958 -3.25227236475842 -3.64101958566909
H 9.27499828486043 -2.55724532220086 -3.92160707060285	H 6.31635108715674 -1.49426363628178 -1.97817965199156	H 9.69672009153224 -1.45661000042680 -2.82862503693648
H 5.43441518385925 -3.15613779905884 -2.09486099382587	H 2.08850738156972 -2.22826260261404 -1.78714068540102	H 5.73807877164507 -3.06178544869674 -3.30380390754487
H 8.73270116036172 -0.15426251138838 -4.24553105913181	H 5.91376259832099 0.90542447023920 -1.48266405102937	H 8.74174837059513 0.53056087231887 -1.68230865983749
H 6.57052945951958 0.74518217435199 -3.51555245515118	H 3.62344956103994 1.73610187391817 -1.13060136922139	H 6.29954173681944 0.71646068317270 -1.34920792120564
H 4.80832122362692 1.42152319973895 -2.45383985852238	H 1.59824177330224 2.29605442585707 -1.88505982961137	H 4.38871218084563 0.84244352258342 -3.29412886651549
H 2.74885394236076 2.04218886059081 -1.34581901104379	H -0.63036612276384 3.05822683083128 -1.37005459110750	H 2.06275326741589 1.47135155273418 -2.72943188566869
H 1.76274743582181 -0.71501411561596 -2.26088007419449	H -1.33586836211603 0.10561308951209 -0.92151407673481	H 1.51491435225977 -1.25486361784088 -1.86895867374572
H -0.51589166496668 -1.14666451708015 -2.12337306422527	H -3.65416800282297 -0.24042572491267 -0.71204510869963	H -0.74547421508257 -1.41102452139429 -1.38111199486114
H 0.97632605092748 2.36665934679255 -0.13150798909304	H -2.05725320780136 3.61406340302879 0.32796112685081	H 1.33608651456308 2.19962844059215 -0.35229009345540
H -1.25582450774879 2.78445030601524 0.79396079606363	H -4.30174188784730 4.35309725198189 1.02904736169719	H -0.77714887121072 3.19136400069308 0.45396701989284
H -3.13956025141687 1.24418934446603 0.29396723841447	H -6.23582674900206 2.80280408626588 0.87794769630331	H -2.88919984791750 1.88767771737063 0.34814021501571

H -2.75699368733212 -0.72863359243697 -1.17168864581074	H -5.90237963984472 0.49844670279033 0.00879856457951	H -2.86649340634973 -0.41803327326520 -0.57683194628887
H 4.40536066530055 -4.72475944141300 1.08481463442190	H 2.72542312333012 -3.26102014761904 0.77842460400754	H 3.37633357299344 -4.79311260456458 1.25872816833195
H -0.16998798715320 -2.89274212909746 -0.12669167813100	H -3.55209889800608 -1.85790652515030 1.51407846887156	H -0.29429931632758 -2.69884541161936 1.65593512286521
C 4.32447536583191 -4.36506901275227 2.11407534771249	C 1.81107857874551 -3.19972421989154 1.37488207914103	C 4.31150467413370 -4.29182697516334 1.52154732397778
H 1.12019218278018 -3.94018253998165 -0.80856536545457	H -2.59329395049630 -3.11706208891153 0.66646878140430	H 0.28249729282949 -4.16497835124610 0.79368602411908
H 3.58509299471332 -4.94217993913166 2.66819765041536	H 1.13168456424876 -4.01354510242558 1.12093330288055	H 4.42707282169654 -4.23257525020109 2.60333296730477
O 5.67822049233359 -2.35504650997077 0.98862770299831	O 2.88610148531109 -0.80184664412345 1.72512658566994	O 3.96904530767182 -3.65706996057695 -1.04444933624867
C 0.80514343561026 -3.35231320317706 0.05295841329306	C -2.57047701662487 -2.33044816668276 1.42048623420763	C 0.58191780869016 -3.27535597519752 1.34711885743012
O 3.83261910377243 -3.00163867017227 2.12455876104335	O 1.08762251847110 -1.98751819411150 1.05830635732737	O 4.28774415069555 -2.91691362635211 1.06182477265030
C 4.59397884856482 -2.10370854316638 1.48275466157730	C 1.74108085599849 -0.84017761320090 1.29891254491568	C 4.07709866664773 -2.74331328619468 -0.25464435552579
O 1.81994874977873 -2.32879563842517 0.20996247706465	O -1.59638187363372 -1.37236873199781 0.94394614201336	O 1.38159474162402 -2.49803531556261 0.42204138578812
H 5.30074585363905 -4.41681493358028 2.60271079259399	H 2.06183152102527 -3.22547184011386 2.43867340873616	H 5.15450965398344 -4.82219409253534 1.07136875649430
C 4.00028825017166 -0.74786760583699 1.47138624021961	C 0.98400750351509 0.38533077484782 0.99022345514633	C 4.01165204810798 -1.25950807817687 -0.58570877600911
C 1.59833448002875 -1.43525738469212 1.18042154300696	C -1.39743519706794 -0.30331224365701 1.72477335342881	C 1.89424775698468 -1.35532464187672 0.90540210388781
C 2.70537476046381 -0.45630692933881 1.32693305851467	C -0.37837689529959 0.65076786284017 1.22088710947050	C 2.66042728140105 -0.59434420245582 -0.15764346280399
H 0.76422168221793 -3.97362079520732 0.95195709707516	H -2.26030810177536 -2.73345116200654 2.38832002666110	H 1.17520874091174 -3.54639520936201 2.22418928499206
H 4.72588344708112 0.05721152534721 1.55469089853763	H 1.63242426862571 1.25096137956752 1.08299365924281	H 4.78835021558782 -0.78289319408526 0.02180532579256
O 0.59052041137790 -1.38928212643243 1.86052529593963	O -2.03785691158422 -0.08738528680800 2.74138863109236	O 1.72625383788980 -0.96790048307533 2.04366641131842
H 2.37956625016999 0.58041156680599 1.35937561971737	H -0.58195579409577 1.64669449342427 1.60335138862560	H 2.90487030052009 0.36934519328362 0.29761602770879

(Ph-C₄H₄-Ph)^{•+} + DMM

Reactants	TS	Product
C 7.27068651791761 -3.02735363468138 -3.80347910332800	C 4.44645702324819 -1.81529814663913 -2.19092897403861	C 7.556172 -1.653138 -2.581950
C 8.38360588691616 -2.18511299848893 -3.74245135843486	C 5.47593517266878 -0.88460022571586 -2.34870770019299	C 7.840768 -0.287103 -2.342759
C 6.03327938788338 -2.55989753320597 -3.40307123791607	C 3.16244664810309 -1.37738499265524 -1.92701284434756	C 6.253177 -2.125324 -2.440306
C 8.25224296000604 -0.87068559010644 -3.27823513812326	C 5.21856097683370 0.48744466991044 -2.23970359319697	C 6.808867 0.603759 -1.964041
C 5.88028645797586 -1.23310257134756 -2.93004508345669	C 2.88277965614554 0.00719656116644 -1.81373964989682	C 5.206391 -1.242001 -2.049451
C 7.02124806156931 -0.39390731080037 -2.87486021692572	C 3.94080889489840 0.93614758038411 -1.97222396186472	C 5.503392 0.134670 -1.827357
C 4.57908274204500 -0.81864673180781 -2.52352412989719	C 1.54481495254809 0.39064866525726 -1.51597522197656	C 3.789111 -1.741140 -1.920205
C 4.24333839269607 0.42099322231212 -2.00675317124462	C 1.05849831135967 1.69006451196269 -1.39409541375711	C 2.936603 -1.055009 -2.960765
C 2.95525848285352 0.80448414642572 -1.59298181075639	C -0.19971288726320 1.98006190415164 -0.90422069091218	C 1.684708 -0.566660 -2.716236
C 1.80335175547473 0.05186856746522 -1.74572669714546	C -1.13213956961670 1.02221310919626 -0.37387521388191	C 0.974790 -0.706903 -1.404726

C	0.50607912931343	0.40601118703224	-1.27069204977083
C	-0.56287548775458	-0.48419017454205	-1.54044481022960
C	-1.83751213628402	-0.21795623227422	-1.07741399258612
C	-2.07807232719937	0.94049257921229	-0.33482570638968
C	0.24020389866738	1.57981429438548	-0.52114313106059
C	-1.03644602625092	1.83510961855995	-0.06228973590487
H	3.80051305464126	-1.57188730474345	-2.62159058261460
H	7.37776656149610	-4.04569928488367	-4.16393297572594
H	9.35695618372824	-2.55067012914770	-4.05670838354033
H	5.16172499015915	-3.20776077588411	-3.44514617185904
H	9.12315885630675	-0.22396789756269	-3.23503346876582
H	6.93767869303019	0.62683235933755	-2.51759399711399
H	5.02495341181737	1.16249244907140	-1.86535959876522
H	2.88479091050618	1.78047069487867	-1.12028031001215
H	1.86241039087983	-0.90206748244552	-2.26578807854729
H	-0.36568563305853	-1.38436633722217	-2.11672499947156
H	1.03555217792469	2.28222746370027	-0.29536422879890
H	-1.23305525249367	2.73256214476295	0.51603281714159
H	-3.07830871232874	1.14942590193271	0.03338882574647
H	-2.64845128692795	-0.90841347530913	-1.28742758401795
H	4.09177623186212	-4.51690079097645	1.06915823528038
H	-0.30038243262395	-2.79170729167273	0.20110434690858
C	4.56263803979264	-4.12465481606640	1.97430629809349
H	1.04153516276359	-3.93206824063518	-0.15421750861191
H	4.28776594922861	-4.72092136645744	2.84323153292165
O	4.94650176248889	-2.06457480681773	0.30155595326269
C	0.62818009820006	-3.23289042220393	0.57186813087542
O	4.05694727919926	-2.79059823837224	2.25134632271463
C	4.29655722755037	-1.87438229192950	1.31124728808841
O	1.63895684508931	-2.20679419653948	0.73443858495646
H	5.64779080033554	-4.09645877171684	1.85010979131505
C	3.73245396492499	-0.54090487043521	1.66148481222801
C	-2.53435842572124	1.42784799003770	-0.19342766445549
C	-3.54128238956738	0.48056358928129	-0.44158907350309
C	-4.87774871289187	0.81798130631616	-0.28089212033882
C	-5.22627643627087	2.09837234296478	0.14782322921601
C	-2.89554279627158	2.71268658421154	0.24621780228724
C	-4.23189002791140	3.04172394384311	0.41254167315782
H	0.84218780909077	-0.43318211852376	-1.41144360310107
H	4.65404308542027	-2.87733912499451	-2.27617084440255
H	6.48568909790299	-1.22674753548631	-2.55695075895461
H	2.35210406812784	-2.09129591530528	-1.80270263022773
H	6.02832268060918	1.19989287141547	-2.36299842894059
H	3.75497828611122	2.00128991875960	-1.88329253681766
H	1.69496388113377	2.53178925573207	-1.65156001968712
H	-0.47625577796854	3.02988573951673	-0.84677233880134
H	-1.02684976248227	-0.00649933399570	-0.71613868860283
H	-3.26494268173376	-0.51816994704168	-0.76993237543440
H	-2.13193606275151	3.44816200193703	0.48270733870541
H	-4.50350390532746	4.03503034570889	0.75721400964763
H	-6.27187688287242	2.36081844815264	0.28103815507360
H	-5.64952944349143	0.08245854989556	-0.48760035211370
H	1.24190467452821	-4.04034867830054	1.74169102258625
H	-3.98701117170107	-1.01814848059547	2.25015391573046
C	2.12622152202621	-3.46232329020122	1.46220929357014
H	-3.20211197109182	-2.63203329079926	2.14853387007543
H	2.97606001227606	-3.72527573305754	2.09034619355601
O	0.15652556809974	-2.10812644444030	0.25652183589425
C	-3.10822270695359	-1.61119726278858	2.51632717666801
O	1.89433660991205	-2.04931688290631	1.70685590827295
C	0.86294915816360	-1.50651759012830	1.04659795392063
O	-1.93442071420531	-1.07436246756854	1.84680766243510
H	2.35832837762273	-3.62258102161507	0.40624857167580
C	0.77121113109031	-0.06257345827506	1.32772790133880
C	0.730750	0.625312	-0.711633
C	-0.365708	0.749569	0.178719
C	-0.575372	1.939046	0.883734
C	0.295658	3.033590	0.696456
C	1.592495	1.731846	-0.900487
C	1.378551	2.925707	-0.198306
H	3.793317	-2.836467	-2.112252
H	8.365421	-2.338238	-2.875180
H	8.871644	0.083598	-2.450524
H	6.017288	-3.184609	-2.620407
H	7.038819	1.662937	-1.776142
H	4.700436	0.825588	-1.530148
H	3.370826	-0.953675	-3.968113
H	1.134867	-0.071506	-3.533585
H	-0.032359	-1.131986	-1.629332
H	-1.050991	-0.102016	0.314962
H	2.440719	1.649749	-1.596961
H	2.062649	3.775865	-0.341751
H	0.128536	3.970889	1.248969
H	-1.424727	2.023657	1.578571
H	4.140412	-4.097144	2.514673
H	1.674256	-5.587369	-1.881399
C	4.005442	-3.032123	2.785428
H	2.800563	-6.003562	-0.516701
H	3.337160	-2.936086	3.657886
O	5.099491	-2.759809	0.351569
C	1.899133	-5.438386	-0.807801
O	3.344284	-2.327248	1.709303
C	3.988780	-2.278030	0.537836
O	2.208901	-4.049453	-0.552236
H	4.991596	-2.575304	2.996196
C	3.206093	-1.495135	-0.507312

C 1.31844229745353 -1.19159225972863 1.55234494964166	C -1.62888387854169 0.18294752086506 2.14058429509860	C 1.257480 -3.149425 -0.854198
C 2.43463927730038 -0.24186165144035 1.74941508106124	C -0.40514024594122 0.70342203676228 1.42480012685303	C 1.685250 -1.726434 -0.485527
H 0.44655836369100 -3.72907996777808 1.52892835742355	H -2.95781166454880 -1.59810695187387 3.59819061779895	H 1.028336 -5.752109 -0.200311
H 4.47700792760689 0.23936441002626 1.80865859874600	H 1.72462042820859 0.45339114619068 1.41658743626740	H 3.357002 -0.425711 -0.235144
O 0.22526792434210 -1.04829843255794 2.06842320678051	O -2.23968974027983 0.88912726608940 2.91562882841897	O 0.171645 -3.436547 -1.331761
H 2.12619967478374 0.76589850447863 2.01390746482898	H -0.22761017072409 1.73026103319868 1.73859988119786	H 1.329978 -1.581458 0.558552

Ph-C₄H₅ + PhF-MIM

Reactants	TS	Product
C -4.48191445903203 0.83405789694636 1.03983534609167	C -1.35345995726092 -1.01092763380549 0.94058961211020	C -3.71803854314875 2.12162663302226 -0.33986541099118
C -4.13796946071985 -0.35797608454972 0.55054869275323	C -1.21713756031560 -2.30604699343819 0.46182193439802	C -3.65675907508770 0.62810168253050 -0.70656140614718
C -2.69363904879051 -0.33140103631362 0.18379190742583	C 0.24190505670577 -2.63362569767332 0.46398369774092	C -2.19956057337541 0.24573275836368 -0.57228340017204
C -3.28454203593476 1.71963046005534 1.03484293524079	C -0.03134522502851 -0.45496716382487 1.19501418819880	C -2.31297377723810 2.47269145262918 0.10575443869656
N -2.23773289275777 0.96521101959563 0.47388597897419	N 0.90780419116223 -1.45355852602369 0.80499851456261	N -1.49427763299171 1.35378186722852 -0.09534557636901
O -3.19025097529473 2.85166638967240 1.46240853929309	O 0.28263042419029 0.62142732201771 1.67647465492909	O -1.92154643717356 3.52727889262760 0.56099574534682
O -2.01825826144569 -1.23886616804793 -0.25803196115347	O 0.77410488427095 -3.69810653385902 0.20593599998887	O -1.69570193730514 -0.82707109061701 -0.83757894529377
C -0.90061882507461 1.41927432021244 0.32797961738882	C 2.31500827287858 -1.28142244932615 0.82150614874216	C -0.09474406658098 1.34419271391106 0.17847420453578
C -0.65756085447330 2.64980896217251 -0.28156234077476	C 2.88065428047923 -0.21360289740196 0.12452685809239	C 0.73570717153508 2.25680807090623 -0.46744845822220
C 0.64612976939213 3.11235633951757 -0.41641477697225	C 4.25753500680232 -0.02391277083837 0.14185692320683	C 2.09925594249820 2.25848886727594 -0.19699487865122
C 1.67840384329859 2.31605174816596 0.05011930065421	C 5.03633269207788 -0.92644334911638 0.84717659509357	C 2.59042873566325 1.33327324914179 0.70918260211058
C 0.15573759815101 0.64220546800711 0.80362233783963	C 3.12072786273933 -2.16848581006053 1.53477131390169	C 0.42028100471711 0.42612856291345 1.09026523032857
C 1.46405355355253 1.08866909018960 0.65446403964528	C 4.50109356268627 -1.99837933593441 1.54131947592961	C 1.78417248548813 0.41306727275539 1.35874830932877
H -1.48497820850077 3.24898559399496 -0.64528702497561	H 2.24387993235225 0.46664001494107 -0.43233116076247	H 0.31958709918855 2.96198175536061 -1.17981602331412
H 0.85844805529994 4.06897708996045 -0.88292697024069	H 4.72104190779791 0.80086977771039 -0.38965565233326	H 2.77062470507338 2.95851951726100 -0.68339756317351
F 2.95272427893588 2.75849236552082 -0.08757852196619	F 6.38142358128250 -0.75203989342826 0.85873433079928	F 3.91943995841586 1.32837022838588 0.97268602502045
H -0.04018461728916 -0.30632083024024 1.29147580705695	H 2.67142721939438 -2.98798849741972 2.08529744178616	H -0.24133126087937 -0.27344864532474 1.59085854425530
H 2.30327686741880 0.50109554462191 1.01228266769108	H 5.15028094399480 -2.67708635770698 2.08493144933187	H 2.21467508239362 -0.29096774955358 2.06326643207174
H -5.44200608612458 1.17356054620080 1.40722568350887	H -2.24832684978416 -0.53850021500476 1.31879950978839	H -4.38886040635443 2.29616181600988 0.50812293697961
H -4.74617368052609 -1.24238494887568 0.41042865197073	H -1.94314799996947 -3.09901938326822 0.58464492722937	H -4.21172095245298 0.04060517252158 0.03501478234250
H -5.54451766998369 0.39566732713758 -2.62224919996845	H -3.47743374307552 -2.23026151268577 -2.12690276821258	H -6.27595416570304 0.61794165044948 -2.88675397778454
H -5.61054229770075 2.45729079819795 -1.34816586904997	H -3.72076071124925 0.12002882005738 -1.67111478851148	H -6.26837708568175 3.03403573607903 -2.36216528769540
H -5.58366338433899 4.31156177494594 -0.26325796352215	H -3.93807766118004 1.82817147797118 -0.30397815097666	H -6.09205155556795 3.97601198864733 0.18672584540016

H -5.52746019731325 6.57748721621842 0.67643668496821	H -4.03917311552356 4.16908338825974 0.43887477665513	H -6.49208288282728 6.31282975397898 0.87978950169881
C -4.60631270569196 0.94109149274808 -2.51953718010635	C -2.57485185747110 -1.66637817340455 -1.89978135875776	C -5.41758928723802 1.09426308033780 -2.41970698740932
C -4.80346573742949 4.99797170455910 -0.57808735094211	C -3.02979908901130 2.42350732096790 -0.28963737871489	C -5.45769736137266 4.77030576246094 -0.20187578498620
C -4.71155886029663 2.26943918326411 -1.93360653892627	C -2.71960180868694 -0.30128256806464 -1.61558354706806	C -5.41590104041360 2.39702404068972 -2.13990692207269
C -4.77015609234162 6.27712544959070 -0.04259769204617	C -3.08695028634740 3.74209750346438 0.13665600038240	C -5.68552707701407 6.08641536555349 0.18764707364891
C -3.80582477621392 3.25524172503397 -2.10313071824158	C -1.68530155177551 0.48016324393964 -1.13706486015648	C -4.19074197731079 3.03019138619852 -1.51876859921276
C -3.83376182447156 4.58514945997762 -1.50995703988345	C -1.80434617559727 1.85257415895654 -0.68031485880369	C -4.42388626763201 4.45933126276146 -1.09029921854051
C -3.47093211082971 0.33194292976515 -2.88971789301324	C -1.39784636057393 -2.36509444629477 -1.68437188854920	C -4.19976166631325 0.27473547788837 -2.11030095114380
C -3.76740687785036 7.17570838848825 -0.41347820578071	C -1.92731227809871 4.51863567269433 0.18970759266718	C -4.88301106022023 7.11253559319746 -0.30980636974815
H -3.74465436937281 8.17452889018343 0.01297253362281	H -1.97804776007729 5.54996752547490 0.52728069031772	H -5.06036694637895 8.14056764272625 -0.00621921217232
H -2.95689743386121 3.06532171401719 -2.76140873020740	H -0.66331720196618 0.14152044539211 -1.29496414330140	H -3.38435165748630 3.02275694317771 -2.27011685608088
H -2.49695342659033 0.79756782116094 -2.75465664559478	H -0.43982377064158 -1.86161375312894 -1.78296229382430	H -3.41968612842736 0.49124390857827 -2.85615028396963
C -2.82961868507964 5.50086634504696 -1.87130995802777	C -0.64320384841374 2.64209914930765 -0.60673007000164	C -3.62893063209995 5.49271502122172 -1.58678918263145
C -2.79570008812740 6.78073037590973 -1.32961905369506	C -0.70529478499809 3.96335034674371 -0.18274051236092	C -3.85531616580536 6.81204394235103 -1.19991153645105
H -2.06951924268086 5.19521993376511 -2.58720653975041	H 0.31050365605577 2.20575091672726 -0.89193938844878	H -2.82251901919212 5.26105426409584 -2.27902031492091
H -2.00957778504838 7.47082465076547 -1.62319781009857	H 0.20154263617211 4.55974943407296 -0.13777834321424	H -3.22661463570133 7.60564454790804 -1.59462490393697
H -3.48842793756214 -0.66400876768272 -3.32128164938790	H -1.37333651399644 -3.43689255698984 -1.85705147185449	H -4.40229785289899 -0.79714821565072 -2.16777053057373

(Ph-C₄H₅)^{•+} + PhF-MIM

Reactants	TS	Product
C -3.93462473004105 2.78967745223593 1.90345685014937	C -1.04227703397182 -1.32507870798682 1.21053513366452	C -3.76527957888134 2.09595078253930 -0.35267761617639
C -4.37252305867336 1.58191924347860 1.54936946936325	C -0.98276757224416 -2.49110343554265 0.49078013443182	C -3.68274007420106 0.60653637003714 -0.68400003550612
C -3.29518250367389 0.87440529187396 0.80455116653389	C 0.47215104585741 -2.83817513771844 0.32342894488561	C -2.21211754346374 0.26443335313694 -0.58447681485222
C -2.53188363883868 2.95265858734992 1.43198627276596	C 0.32110083046498 -0.79707599454411 1.40127054887048	C -2.36567037966439 2.50580444287865 0.05564648968689
N -2.19654885150125 1.76161002910453 0.74660994812925	N 1.19483268284821 -1.75738478690451 0.84868021067343	N -1.51543874965978 1.40298589026762 -0.11245598937994
O -1.79942524776403 3.90193910257686 1.60080787866355	O 0.65895922716031 0.23821177269891 1.93898818441904	O -2.02383738656554 3.59606059822165 0.45213880841126
O -3.33877824996863 -0.23393306960308 0.31705896651535	O 0.94203536925970 -3.83304279826505 -0.17916949760518	O -1.68308747280461 -0.78209523600918 -0.86701790755866
C -0.93365256807547 1.47547634326652 0.17162965513582	C 2.60782098834547 -1.62719534532873 0.79437064885443	C -0.12933724067992 1.41869146329721 0.16774400669915
C -0.21758306461213 2.49035531348014 -0.47364321835227	C 3.16955016601080 -0.45807201884011 0.28004823699827	C 0.67287858000404 2.42273384793590 -0.38574077530482
C 1.02595896260402 2.21728422109244 -1.02575249028168	C 4.55067110203461 -0.32522452272738 0.22764198414670	C 2.03050575927472 2.43278051311513 -0.12015459027495
C 1.52539158772304 0.92780165250129 -0.93129541745946	C 5.33148009745347 -1.37564362308265 0.68423700033373	C 2.55070410221885 1.43260012978845 0.69668625198175
C -0.39841356743925 0.18519858137313 0.26685627359524	C 3.41278145518882 -2.66924028089503 1.25497308836401	C 0.41357156652084 0.42649230589360 0.99338250187363

C 0.83894462233074 -0.09432906393431 -0.29752406059220	C 4.79490655959608 -2.54699031373130 1.19459499886575	C 1.77134689325263 0.42781867156917 1.25927864286521
H -0.62319000807212 3.49241127040249 -0.54333315355749	H 2.53207149178338 0.33993730884101 -0.08572011106309	H 0.23638189880253 3.18115953211191 -1.02678949088994
H 1.59688970215595 2.98972279713002 -1.53053060390196	H 5.01681386551091 0.57080767404719 -0.16873778518083	H 2.68504640506002 3.19086359335092 -0.53710627464808
F 2.73193764390091 0.65993101360729 -1.47746720947522	F 6.67649078231821 -1.25128849848493 0.62952940128145	F 3.86753986449383 1.44147409075024 0.95542952536894
H -0.93831377359366 -0.59599326205043 0.78760657896657	H 2.96293074676604 -3.56685770310080 1.66525396379925	H -0.22683518910268 -0.33457012734185 1.42612836720075
H 1.27087229262330 -1.08777106114261 -0.23565169454805	H 5.44712493300562 -3.33972074198501 1.54589239615580	H 2.22649794866227 -0.32466998523040 1.89448068938415
H -4.44541222328021 3.57231538791293 2.45013030151543	H -1.91585742860823 -0.82758939237289 1.61353677783215	H -4.43371940501560 2.29313982651620 0.49151354480698
H -5.33821463680353 1.12433471930658 1.72342104675200	H -1.74839305283642 -3.25615952264251 0.44672221609934	H -4.18053208466887 0.02956418876404 0.10560372849841
H -3.92813867818991 -0.13829179243129 -2.73580052114490	H -3.40579946524844 -2.08082032188530 -1.87063775921745	H -6.30972048945455 0.59734807715807 -2.89655612177449
H -5.04701313718027 1.77033418045859 -1.88962448846994	H -3.91696762720494 0.21322417876412 -1.50028822669227	H -6.30267149525137 3.00178745909296 -2.36728863423965
H -6.01142275734875 3.43645923873785 -1.05250922967931	H -4.32978198446319 2.21592242736552 -0.92994675665705	H -6.14278363768213 3.98227198679865 0.07301677688280
H -6.91568401770925 5.45556109420632 0.01071960454378	H -4.60245973240667 4.55394744104269 -0.22907746161711	H -6.43539827372568 6.32287628036636 0.81557242114574
C -3.33509787433108 0.77099216180767 -2.67403989651627	C -2.56831304326679 -1.41278852268580 -1.68024824473143	C -5.46548744301073 1.04938219670201 -2.38163592433212
C -5.38094716443280 4.31193461111590 -0.94180520820221	C -3.45860690247967 2.79491849321653 -0.64331444758002	C -5.45233965078385 4.75270226000488 -0.26126875011235
C -4.00848335379120 1.91669052573190 -2.17633610305858	C -2.87072228265358 -0.07147540811424 -1.43985310635980	C -5.45376284768097 2.36674684814675 -2.13213893542086
C -5.89026995595282 5.44448288894632 -0.34486051879267	C -3.61348101808227 4.10723751883819 -0.25032001322608	C -5.61726335676180 6.05862609746731 0.15280089257556
C -3.42566938070704 3.16014650634792 -2.00005787071856	C -1.92039295153402 0.86876716780249 -1.06418057000567	C -4.20695471368977 2.99932524123038 -1.56566769126377
C -4.03830047848568 4.29807528816283 -1.40979444849488	C -2.16422322349718 2.21294705709043 -0.67508371508456	C -4.38447216296207 4.41114237222168 -1.11827030499300
C -2.02004710551669 0.70248797434898 -3.03800274965598	C -1.29275536960563 -1.98669257434010 -1.62079451881980	C -4.28950915382035 0.19479004819903 -2.03925803926782
C -5.08757063186080 6.58347473444760 -0.19237471781652	C -2.49774381261795 4.86801307685165 0.12414547797166	C -4.72220024351153 7.05020852220714 -0.28171111828737
H -5.49865935001598 7.46979318821870 0.28228279245257	H -2.63193404914122 5.90061298424609 0.43347704168388	H -4.85496085898946 8.07657562622096 0.04793755774679
H -2.39403157714463 3.29986250553937 -2.31717415059865	H -0.87255173198983 0.57419344955511 -1.05670270439392	H -3.40444578221900 2.94728052075232 -2.31655046081927
H -1.35263258277521 1.55801832816625 -3.01730216325915	H -0.40000610845841 -1.37111031953080 -1.68323315928903	H -3.53818293020318 0.31539455172441 -2.83709946142701
C -3.24362226995868 5.46523186243790 -1.25044350058764	C -1.04666969379783 2.99985602398205 -0.29242338032196	C -3.48960931682955 5.41567821346070 -1.54621700729674
C -3.76403966375545 6.59023763743605 -0.64585165367909	C -1.21552529651995 4.31148431964093 0.10337375366748	C -3.65977334652900 6.72313459035965 -1.13235449852854
H -2.21649760704019 5.45427735503560 -1.60542413678399	H -0.05624905434687 2.55303272877336 -0.31413373860614	H -2.66798440938310 5.14761811548327 -2.20472827467695
H -3.15090360895996 7.47700428344082 -0.52163092207296	H -0.35808554995423 4.90898272496168 0.39606277739305	H -2.97182036227936 7.49502926659765 -1.46265704212095
H -1.60122443654387 -0.24196494221795 -3.37020358758229	H -1.18015735867473 -3.02336637700881 -1.92367772394046	H -4.55054438171470 -0.86585034578687 -2.02548535587599

Ph-C₄H₄-Ph + NO₂-Chalc

Reactants	TS	Product
O 1.37097516931813 -1.02519564730174 2.42319333515169	O -2.54785650699839 -1.25190498908536 2.14327137961126	O 2.87543373895878 -1.76818928976792 1.84174291926333
C 2.76099972892006 -4.74475575553319 -0.17454608744802	C -0.55579486757744 -4.17433262980600 -1.04877171575309	C 3.04408783684419 -5.04899252072964 -1.59923224059532
C 2.97686398790220 -3.46574523609237 0.32605476103941	C -0.74912100829282 -2.89294851204151 -0.54394085809291	C 3.27033738736415 -3.75234603765025 -1.15005528955151
C 6.21230087912857 0.65878237975262 1.74698020651542	C 0.91315678573903 2.11255118600375 1.62540503885839	C 5.17649377407432 1.47096346667759 0.51618002679042
C 7.44140196734895 1.27293195957921 1.60761657712776	C 1.81392155453214 3.04561088222607 2.09581776973081	C 5.96308795356967 2.26714796434185 1.33180968137700
C 3.61240244178406 -0.86716705178366 1.80755019730584	C -0.95972197366544 -0.11919084492228 0.85992902362032	C 3.22215149973667 -0.77074588476216 -0.28240181073842
C 1.77865068697886 -5.55784283065972 0.38479759896331	C -1.00514266777068 -5.28155659755448 -0.33465887564701	C 2.28485203890151 -5.93176392067589 -0.83540869197280
C 2.20142034832483 -2.98423157421130 1.38868919771638	C -1.40788855582689 -2.69902514740336 0.67612520431791	C 2.75838950852769 -3.33207804706425 0.08439909279814
C 2.33682248787372 -1.59401275978222 1.90653599917502	C -1.69212717474249 -1.35734272027234 1.26636728906592	C 2.95338084489506 -1.95914689024423 0.63325261430695
C 6.10506154287574 -0.74320248629731 1.75599260549749	C 1.33972445999585 0.82684793895116 1.21917943067488	C 5.52844126056706 0.14112785018374 0.25013504850593
C 4.82920638033123 -1.44320313985259 1.81747085128037	C 0.44642133272215 -0.16863730833369 0.68417412187770	C 4.72286380202600 -0.71714042239696 -0.69617385266400
C 8.57923871270300 0.47907561497592 1.47392021111588	C 3.16697046744952 2.70516819729892 2.18573211558960	C 7.11242559867723 1.71819559620250 1.89423633043035
C 7.27887506526038 -1.51083063796080 1.65234185899511	C 2.71587364717919 0.52235461289527 1.32260704831188	C 6.68679274668510 -0.37882075590561 0.83679494911499
C 8.51659888597250 -0.91004651307537 1.50451331118815	C 3.62365534346341 1.44253077127718 1.80513171160530	C 7.48611940425085 0.39932063540406 1.66105422608901
C 0.99904932677855 -5.08355877112091 1.44054624902971	C -1.65870240427595 -5.10144992370312 0.88435305621177	C 1.76611122842561 -5.52040363738569 0.39229296417868
C 1.20210059934816 -3.80171808093465 1.93267653137918	C -1.86464244060770 -3.82263538605335 1.38120817782776	C 2.01073504273292 -4.23502773559875 0.85361363040310
C 8.60634794548106 0.13555220922874 -1.97415431888170	C 4.27723624786745 -0.54210727858401 -2.37709908015209	C 8.55578660146251 -0.74446649316271 -3.04294491694603
C 8.94024659281473 1.48724383875037 -1.97696306965636	C 5.02130968346864 0.62728596589683 -2.21555780653949	C 9.06149565385695 0.55040036282426 -2.94823284180312
C 7.27832303286662 -0.25492675970828 -1.84734054567305	C 2.90192633595342 -0.52179671449522 -2.19397642897860	C 7.20148296459083 -0.98106207456645 -2.82558644227462
C 7.92936909541805 2.44362619660114 -1.85829008545917	C 4.37734577394695 1.81158740858066 -1.85950756347983	C 8.20226334220981 1.60172374557389 -2.63734487348219
C 6.24953284491399 0.69393948771107 -1.71524235207793	C 2.23496432086186 0.66872815292051 -1.84917027095859	C 6.33143724001314 0.06600614439456 -2.50857331653602
C 6.60317642470363 2.05697066651031 -1.73321128122212	C 3.00234987585845 1.83413398995626 -1.66840689644870	C 6.84808436235832 1.36107435993978 -2.41752381242119
C 4.88504823865855 0.21928971980999 -1.54202635528364	C 0.80285561075849 0.63120104181362 -1.63891015288112	C 4.88747490959344 -0.25050781338228 -2.20117251607700
C 3.80400033945273 0.96966104566721 -1.22902113217212	C -0.01877709042199 1.74815204927686 -1.51014287274945	C 3.88426908012638 0.80998465632068 -2.55285420971803
C 2.45801771986527 0.47664098739905 -1.03772445017475	C -1.34874949804755 1.66893640824407 -1.13215448885168	C 2.60488137218299 0.60699622517529 -2.23399204839267
C 1.97280221459360 -0.70440350772045 -1.48685759412498	C -1.98490874663946 0.44847290928210 -0.80496468473054	C 2.22948444669356 -0.64305207101394 -1.48191223162709
C 0.64285551924053 -1.24631314555407 -1.25477289841285	C -3.40955282731887 0.42086908836327 -0.42437654881268	C 0.80335268520547 -0.65544894773843 -0.98124599831705
C 0.30967127428977 -2.47927971820997 -1.84451453016637	C -4.20528674853105 -0.66136102506972 -0.82134066639830	C -0.02835726159479 -1.74895119795265 -1.23152555787265
C -0.93154551915113 -3.06637505411584 -1.63309336648164	C -5.54869598347314 -0.72360480662726 -0.46627900523216	C -1.33376418287430 -1.77555769067289 -0.74509388366936
C -1.87572358049811 -2.43284635027050 -0.82756904105907	C -6.11515929488074 0.29047547578507 0.30267586533339	C -1.82325821714346 -0.70603688911224 -0.00009060635103
C -0.32324131387645 -0.61878189196195 -0.44634390877776	C -3.98568594255881 1.42888246703459 0.36039065162109	C 0.30274944190727 0.41445595819004 -0.23235364522909

C -1.56359180088019 -1.20539015760902 -0.23983888163439	C -5.32741856986659 1.36443616933387 0.71673883914587	C -1.00079899005440 0.39064968485678 0.25400886324951
H 3.35408677912163 -5.10352611139567 -1.01093646939522	H -0.05225311748547 -4.30535787680324 -2.00206113102593	H 3.45984723228633 -5.36851664493688 -2.55033397030094
H 3.71747554137091 -2.82427614323011 -0.14076591482230	H -0.39176033128486 -2.05224126514967 -1.12435435535717	H 3.86957941388351 -3.08826315086439 -1.76277744545122
H 5.32629656301250 1.27841314141517 1.83301249571919	H -0.13376927434623 2.38892766259254 1.55983198652357	H 4.28537636295938 1.89934869587288 0.06708298394252
H 7.52496019896736 2.35254003659433 1.58339198168827	H 1.48249399154438 4.03229082281213 2.39709586632518	H 5.69616392838202 3.29847155531356 1.52922653276855
H 3.49941054971539 0.21429223825361 1.81325914628571	H -1.32989815178907 0.70622289236071 1.46311767475122	H 3.01972086830238 0.09683736149545 0.35248479139858
H 1.61331085539732 -6.55823866719878 -0.00572829958007	H -0.84760603753257 -6.28264800282601 -0.72628742373754	H 2.09798206379320 -6.93976224764314 -1.19519478995933
N 9.87363519989688 1.12761902063120 1.27796452680448	N 4.11326792747406 3.68289304803031 2.67849671613866	N 7.94993385593049 2.55306290287235 2.75742383301397
H 4.89941076935490 -2.52859158677278 1.86431104191776	H 0.90814562658551 -1.12113302326008 0.43961699429126	H 5.15694263090037 -1.72220574926855 -0.65095213284799
H 7.20894094283261 -2.59506441728937 1.66815763088178	H 3.06403269021207 -0.45913316375044 1.01302505751474	H 6.97154060890747 -1.40849165419673 0.63841935469793
H 9.41807803882342 -1.50227966671342 1.40348251311615	H 4.67640480025222 1.19771716304357 1.88108144727518	H 8.38298266191884 -0.00541419332485 2.11463619539160
H 0.23064565200272 -5.71576243108490 1.87639754753523	H -2.00850491071747 -5.96243939237582 1.44673461238454	H 1.16931264918421 -6.20487902298995 0.98821936877601
H 0.59535659185721 -3.41864541647382 2.74769747559525	H -2.37659170146931 -3.67414241126100 2.32639666285063	H 1.60931846681688 -3.90409051352665 1.80644503736093
H 4.76154500765435 -0.86026468017125 -1.63377967811037	H 0.34081327209624 -0.32992031979967 -1.83677611519116	H 4.62511622864095 -1.14466321074567 -2.78883270161565
H 9.38396973914230 -0.61835287043660 -2.06398184928883	H 4.77343273707037 -1.47039181996008 -2.64624971883517	H 9.21615849673993 -1.57127655538864 -3.29010281438164
H 9.97748356457899 1.79655583115556 -2.07166461002546	H 6.09812841533034 0.61314169618326 -2.35804195388658	H 10.11786249023796 0.73916665153076 -3.11800990149629
H 7.02451048164653 -1.31256685017189 -1.83392787984237	H 2.32206389854105 -1.43443881427450 -2.31609733409739	H 6.80991129189860 -1.99415147492626 -2.89876890846827
H 8.18162240506333 3.50074426514998 -1.86522891170700	H 4.95392458637538 2.72145231274605 -1.71690362933434	H 8.58688695337956 2.61522605976384 -2.56143241973330
H 5.83567197069601 2.82069687597470 -1.64761187181977	H 2.52472187919993 2.76149108491671 -1.36639738627141	H 6.19595027074941 2.19097223124131 -2.15951011061512
H 3.93574958663254 2.03555575150322 -1.04844222285820	H 0.41849100796168 2.73981689481513 -1.59622555034518	H 4.19900441542632 1.69666274584086 -3.09675670100774
H 1.79554220268100 1.14573276020703 -0.49036446594539	H -1.88139651351576 2.59794552268838 -0.94342394964798	H 1.82872334727893 1.32409294434632 -2.49028412664038
H 2.62236450558191 -1.33611838292752 -2.09298763675682	H -1.68597353290708 -0.42142923633970 -1.38555698349506	H 2.36156067064171 -1.50749923140003 -2.14700077145570
H 1.04714249954972 -2.98259621151190 -2.46529054968102	H -3.76312055192783 -1.45733694954780 -1.41688871489852	H 0.35208982893120 -2.58723346788691 -1.81126022856217
H -0.10052813777769 0.32779340212927 0.03624704313949	H -3.37802550398836 2.25931979594392 0.71126694987442	H 0.93688111186993 1.27542479723090 -0.03031377625418
H -2.29322463345813 -0.70651184703080 0.39242817563117	H -5.76033047060175 2.15175139316841 1.32771870957173	H -1.37623949702688 1.23021122209534 0.83278552742100
H -2.84602598865502 -2.89015284298444 -0.65593447466020	H -7.16288876693738 0.24152180058783 0.58556154892224	H -2.84081622858464 -0.72486070886578 0.38029272595165
H -1.16190392334127 -4.02283499666018 -2.09469490692245	H -6.15350157156724 -1.56673675306798 -0.78842386097730	H -1.96860459207146 -2.63327790315356 -0.95024784905625
O 9.92185878601036 2.35519583951169 1.33126406413742	O 3.69007390766989 4.79182810370628 3.02053670939431	O 7.60641607495574 3.71807786432823 2.94740117267186
O 10.85280643280014 0.41519730309802 1.06227714678878	O 5.30714655745671 3.37069800363238 2.73335836358542	O 8.95787156409699 2.05079599918416 3.25005502028335

(Ph-C₄H₄-Ph)^{•+} + NO₂-Chalc

Reactants	TS	Product
O 1.00375401235104 -1.83738703967676 2.36386703756453	O -1.34082597379209 -0.68520187603236 2.53796720863860	O 2.62780892865477 -1.54804527509041 1.74518797659028
C 2.97500907484718 -5.23112285377592 -0.28329641384930	C -1.20755004755775 -4.29338871852192 -0.56613383184921	C 3.03000600099595 -5.06293043291214 -1.44534371680754
C 2.96645660663231 -3.93325670206015 0.21625738148645	C -0.91954089511947 -2.97716064659823 -0.22546043686688	C 3.20450893163225 -3.73169666581608 -1.08877146577198
C 5.47773616290462 0.68674207228928 1.83928868694183	C 1.20123634685565 2.11675695520396 1.38535173940254	C 5.23654571796930 1.41234587682359 0.53457114209029
C 6.57895935537704 1.51455618356489 1.73614593774428	C 2.10110180190634 2.85353759628103 2.13409307923141	C 6.06678252413501 2.14566286505696 1.36693878554016
C 3.17570094865556 -1.26762506623511 1.74452152746056	C -0.83397188467797 0.09075416852800 0.35863702076158	C 3.20556583679549 -0.69909061625844 -0.35663238552687
C 2.20892655108412 -6.22013947976183 0.32853918509653	C -2.05055174328118 -5.05589989602382 0.23839858192437	C 2.34468026410801 -5.93061816128424 -0.59872231120534
C 2.17308182747743 -3.61002802695340 1.32475831258691	C -1.45441471320605 -2.42112919931618 0.94362818843313	C 2.70440463278184 -3.26332933455543 0.13446384301280
C 2.05399634936883 -2.21839335006720 1.84161010302399	C -1.20359149021129 -1.02728321621492 1.37669071045503	C 2.84011330958632 -1.86388450423981 0.58500424415296
C 5.60745283199016 -0.70572802049600 1.67243654985521	C 1.53988610132815 0.83244147921766 0.92179856754188	C 5.53916351074363 0.08464397048476 0.20883908450458
C 4.47525230363283 -1.62021276615836 1.70083301938220	C 0.64134857911930 0.04128145942592 0.08511428573970	C 4.69390354247662 -0.70987809075124 -0.76153060522006
C 7.82450031537339 0.94655395957439 1.47119924799268	C 3.34623995312069 2.29863420298357 2.41544454502545	C 7.20898075482510 1.53483554582450 1.87538214333901
C 6.88361688697769 -1.24310486848551 1.43297940598972	C 2.81384036316900 0.30997664886014 1.21720598798915	C 6.69065181475046 -0.50082973386065 0.74402982646637
C 7.99629608536921 -0.42558310134333 1.32802755861492	C 3.71915996519356 1.03314851248794 1.97101768003979	C 7.53514456698751 0.21701681443290 1.57857027376873
C 1.41840476956130 -5.90576772934638 1.43451478668252	C -2.59072526085964 -4.50716645992170 1.40172850948033	C 1.84107341628452 -5.46982018398339 0.61823730983372
C 1.39049137372375 -4.60682761313326 1.92222091027179	C -2.28744087315202 -3.20285002079777 1.75951123639863	C 2.02253371223365 -4.14727316344793 0.98801860582660
C 8.78027250461731 -0.33227378780068 -2.32568451136184	C 4.49698522456784 0.15041102827203 -2.42817797392775	C 8.55787885295712 -0.60173226714478 -3.02985825571985
C 9.29661857677213 0.96145170895999 -2.21672704771761	C 5.00768093661287 1.43359401459890 -2.22010013036671	C 9.03300442085535 0.70234593904858 -2.85687997254977
C 7.42788458739199 -0.54966271532678 -2.14385078390728	C 3.13837165654406 -0.07706528707750 -2.29643543405421	C 7.20866033872354 -0.87393025673259 -2.86538789805806
C 8.45110531149684 2.03835007255377 -1.92574567363974	C 4.15097794486990 2.49150388867778 -1.88687114700749	C 8.14587741838307 1.72901003411682 -2.52464275539365
C 6.55600929237609 0.52526796508747 -1.84001526659415	C 2.26402347256576 0.98157336168795 -1.97063856745299	C 6.31005633567284 0.14860997067934 -2.52412462533546
C 7.09962296477362 1.83087272103374 -1.73281751418912	C 2.79237812581395 2.27129093857999 -1.76090188304521	C 6.79666181952139 1.45531911569008 -2.35645519327951
C 5.17604266268147 0.22823287451568 -1.64323523197605	C 0.85559311747389 0.68940159279748 -1.78427632082222	C 4.87290593871018 -0.20551131725598 -2.25974978050934
C 4.19452686451091 1.13218555242775 -1.27355610666763	C -0.17410358573229 1.69318819882007 -1.93743763232473	C 3.85640154471423 0.84721760101081 -2.60092516182815
C 2.83889295937616 0.82183370489403 -1.05965855988124	C -1.45244589993197 1.39554462154057 -1.61839083641524	C 2.57057711496248 0.65196304339458 -2.27402597358592
C 2.24519101961930 -0.40200699578676 -1.31857141409062	C -1.77054365327547 0.11376828842698 -0.89849124736707	C 2.18160731364888 -0.61777641458176 -1.57433491288213
C 0.89389980118966 -0.75809249316437 -1.03582859618004	C -3.22324788612408 -0.01644910465884 -0.50560510010853	C 0.77253887274532 -0.65816073547795 -1.08232217478712
C 0.46303166644198 -2.05918228714063 -1.39697335122493	C -3.97806128855069 -1.09958593324465 -0.96065297904131	C -0.02485094144467 -1.79289224847247 -1.31364411588031
C -0.81783748797959 -2.48478748502143 -1.10145108243821	C -5.31089855985600 -1.24085339645100 -0.58269563580482	C -1.31426821905448 -1.85398080062962 -0.81265877012668
C -1.70023675519451 -1.62393061456294 -0.44424490815040	C -5.90147901954554 -0.29926917900716 0.25565134812157	C -1.82667176062500 -0.78294513094212 -0.07181759011833
C -0.01884480429100 0.10300860213934 -0.37616501679968	C -3.82396390960581 0.92855780645047 0.33124152629275	C 0.24581472259908 0.41735873031647 -0.34062869498809

C -1.29692892903487 -0.33102184036322 -0.08922500707329	C -5.15552467851235 0.78789074475194 0.70934448146742	C -1.04130811396119 0.35260861308901 0.16191765284662
H 3.57830671588340 -5.46918728389596 -1.15452986606914	H -0.77575853575437 -4.72166348529970 -1.46557082113413	H 3.42751780213609 -5.42072264965449 -2.39003492457454
H 3.54758055972264 -3.16410458909957 -0.28301365525231	H -0.25603775842120 -2.41408751660615 -0.87156687584133	H 3.74567795510791 -3.08358584234915 -1.76648356089448
H 4.51018635302267 1.12918202313173 2.05210546335300	H 0.24214033426870 2.56051240181084 1.13827409417886	H 4.35503804378642 1.89519146361788 0.12218618593930
H 6.48255274114543 2.58713860956507 1.85504579470883	H 1.85154192967243 3.84686608423084 2.48718637029189	H 5.83994774419388 3.17594727190314 1.61374848459525
H 2.87232982940443 -0.22564132675211 1.81987330123007	H -1.05777040035193 1.00487033057725 0.91371565408628	H 3.00544453275518 0.19254600014882 0.24143282507544
H 2.22268387679305 -7.23525022481057 -0.05835273611080	H -2.28640556042779 -6.07906986687750 -0.04016998664462	H 2.20318217215162 -6.96851476468393 -0.88626910969403
N 8.98884859992817 1.82498390510441 1.33105231191009	N 4.31103185112528 3.08574517088537 3.20248826926516	N 8.09729038163064 2.30704888785650 2.75296273340802
H 4.73514370385890 -2.67680663031402 1.67506534612957	H 1.04471409126873 -0.94728865547708 -0.12828383864261	H 5.07809571801952 -1.73424645939006 -0.75355629017077
H 6.99537676256792 -2.31678137381621 1.31087315219738	H 3.08600527637624 -0.67618368058489 0.85211408963287	H 6.93441100118920 -1.53072195865506 0.49780155486346
H 8.97762402314166 -0.83829418848476 1.12740874798054	H 4.69719360351612 0.63266588889539 2.20910107166488	H 8.42869178721797 -0.23506770236553 1.99210065712522
H 0.82161657239571 -6.67690518813130 1.91309131826286	H -3.25032907966082 -5.09963749540307 2.02872059327617	H 1.30713710179013 -6.14613706665288 1.27888781070610
H 0.76958168984664 -4.34916326678466 2.77495356945500	H -2.70693252409557 -2.76492892963980 2.65962585134134	H 1.62769879118143 -3.77845148974116 1.92910763909904
H 4.90235371823408 -0.81737482873204 -1.77526689537786	H 0.57066398085372 -0.30168349470190 -2.14585533754023	H 4.63249517179566 -1.08140692305182 -2.88273302299767
H 9.44013716109794 -1.16421146287456 -2.55127804031111	H 5.16429622793332 -0.66608647841035 -2.68591286618441	H 9.24514707725675 -1.39945987160935 -3.29557950978978
H 10.35943984271587 1.13420005858833 -2.35879888778568	H 6.07516171705373 1.61283285803736 -2.31019522436956	H 10.08927201042552 0.91799790679715 -2.98915879913181
H 7.01759225871664 -1.55308792081870 -2.22232622196616	H 2.73140213806181 -1.07526751383029 -2.44014555427568	H 6.83672660579956 -1.88797223943274 -2.99473939148625
H 8.86048925009982 3.04062056286530 -1.84403126114382	H 4.55758573443340 3.48419723453383 -1.71937820478837	H 8.51140725444212 2.74406679659601 -2.40045051923235
H 6.46087603106301 2.67671277605300 -1.50183884216805	H 2.13714848666463 3.09121088254264 -1.48192489673053	H 6.11581156682849 2.26064168499256 -2.09646687679177
H 4.47463774709643 2.16587413586497 -1.08892464900417	H 0.08526149207458 2.68267463329142 -2.30378611435882	H 4.15442461046206 1.72109691429503 -3.17366139202430
H 2.22896180635535 1.62901977280627 -0.66235125966716	H -2.25489777907064 2.10483714839504 -1.80397319813497	H 1.80839462277561 1.39636902486043 -2.48502095984868
H 2.84306906402405 -1.18422024763035 -1.78268797507047	H -1.51886945860006 -0.72757584607063 -1.55849613449530	H 2.36351524324919 -1.48090123454708 -2.22650516997173
H 1.15784531783297 -2.72225474725053 -1.90502380687534	H -3.51670955206887 -1.84013858627622 -1.60996129082131	H 0.37873546592895 -2.62072491017733 -1.89075327382682
H 0.28158060532037 1.10288742111342 -0.08185539434096	H -3.25292154725619 1.78240563708192 0.68985046804923	H 0.85758370017747 1.29645379664575 -0.15340918323532
H -1.99043695002416 0.32959285590633 0.42175152707018	H -5.61248199654769 1.52874390403691 1.35932209910514	H -1.44224157194674 1.17943554878574 0.74008086814603
H -2.70607546906841 -1.95845811508616 -0.20716964226153	H -6.94059695606648 -0.40863493362175 0.55299733068553	H -2.83737942353704 -0.83203161330751 0.32280108688243
H -1.13625235557980 -3.48548264229765 -1.37658697751341	H -5.88662585930542 -2.08849064628380 -0.94349300322898	H -1.92821629481021 -2.73072314512104 -0.99465123634371
O 8.81015742246360 3.03731471464831 1.41356141307533	O 3.94894192890721 4.17807639364284 3.62512022790719	O 7.79346562810173 3.47025145099488 3.00188122790450
O 10.08235685166730 1.30521700055183 1.12502164119210	O 5.42330598926787 2.60514598739516 3.38964168721736	O 9.09973246372203 1.75108196901395 3.19235407397128

Dienes and their radical cations

Anthracene	(Anthracene)**	Ph-C ₄ H ₄ -Ph
C -4.62858179359904 1.84254052989424 -0.04059241069101	C -4.62447357031044 1.83300228902728 -0.04267966762753	H -2.79231157515838 -0.70526368840049 -1.10914196639703
C -4.17508473937880 3.12126986461706 -0.21963400257358	C -4.16519102183238 3.12870902343100 -0.22433282666360	H -0.51563599287396 -1.26046196565016 -1.88889952364560
C -2.90071334722953 3.36837356308747 -0.80825397258163	C -2.90300519843300 3.36175537813855 -0.80746237053507	C -1.97375331586414 -0.01714377799250 -0.91630023083479
C -3.83403421755755 0.73247367420416 -0.43957197703217	C -3.84165325220723 0.73897397397786 -0.43603189252755	C -0.69217385725197 -0.32994813789701 -1.35417916958667
C -2.60463014197386 0.92678153970264 -1.00840355958664	C -2.59611463050225 0.93564738376839 -1.01265287562231	H 5.48189574650191 -3.22948514157397 -2.23627975174010
C -2.09439886927201 2.24173274892992 -1.21328359853296	C -2.10098479800618 2.24070155080675 -1.21075446476769	H 7.66771332159090 -4.05340661139053 -3.03788994800131
H -5.60195248335157 1.66812779459279 0.40927930938096	H -5.59777904771181 1.66474106490791 0.40761163109120	H 1.76146346910633 -0.84527915617015 -2.03859592990203
H -4.78067961287036 3.97175899497132 0.08458060692477	H -4.77247492788269 3.97648675027148 0.08074013779249	H -3.20703908834570 1.42054711108644 0.11407976907779
H -4.21121063274303 -0.27517500612001 -0.28904269374892	H -4.21342611399697 -0.27006245570683 -0.28755539466585	C -2.20739714859010 1.17323510815044 -0.23163728172543
H -1.99553428111382 0.07936870405541 -1.31416040350376	H -1.98923719956263 0.08727580151860 -1.31680906552154	C 6.19893856811800 -2.53221902289894 -2.66371276917606
C 0.57867497156243 6.40036487630868 -2.35544638250574	C 0.58630674178413 6.39386122968035 -2.35898536150627	C 7.42950839223169 -2.99594626302836 -3.11397997985332
C 1.37325590561781 5.29031118254248 -2.75439646025134	C 1.36914636782607 5.29983804909505 -2.75231357047580	H 3.89943726774734 -1.55919618905991 -1.94222660179404
C -0.65072716181325 6.20605087436230 -1.78663663069526	C -0.65923415066143 6.19719014011934 -1.78238201199007	C 0.38945594357220 0.53971044585785 -1.12362639644617
C 0.91976457721786 4.01156970031392 -2.57535149681413	C 0.90986166468776 4.00412669629989 -2.57065778719760	C 1.70533511696511 0.15891602277887 -1.61795669455051
C -1.16095008762214 4.89110086851853 -1.58174049474140	C -1.15436677814246 4.89214242310833 -1.58426988279358	C 4.55807383984581 -0.74575249624193 -2.24730556125699
C -0.35462058513189 3.76446600489332 -1.98675703010519	C -0.35233744110589 3.77108873031441 -1.98754467875556	C 5.85939793156640 -1.16939640379389 -2.74526116449844
C -2.41235866997856 4.66297195866185 -1.00336799589255	C -2.41281954597682 4.66382238422459 -1.00296692586360	C 8.35329814690685 -2.10889149801107 -3.66162251053797
C -0.84297660588907 2.46985544627911 -1.79165370065090	C -0.84252495549505 2.46901684520279 -1.79205234468504	C -1.14329056474794 2.04369205721900 0.01358720340856
H -3.02023374162868 5.51271653425060 -0.69812924533328	H -3.02090055360363 5.51288158932887 -0.69806385031522	H 9.31536755952295 -2.46746299663294 -4.01626785540950
H -0.23510480318200 1.62011285355153 -2.09689528699266	H -0.23444590392098 1.61995723777868 -2.09695914744371	C 0.13772172134350 1.73328827426865 -0.42033401213472
H 1.52537830354709 3.16108737157070 -2.87954175046287	H 1.51715818683770 3.15635368096836 -2.87571752176322	C 2.81632081001768 0.93025989053985 -1.63201638004295
H 2.34663880837161 5.46472846097359 -3.20423851015778	H 2.34246111534155 5.46809949958409 -3.20258372231633	C 4.12391527390858 0.52722113918956 -2.10373921957612
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H -1.25984509521773 7.05345976602915 -1.48090697918576	H -1.26612615536657 7.04555738985181 -1.47824149517734	C 8.02924061453634 -0.75389793101089 -3.75744553284564
		H -1.31541058435753 2.96959606240417 0.55587947041877
		H 0.94986064961209 2.42061884280482 -0.20249195670032
		H 2.74699374208568 1.96312415024315 -1.29375087202251
		H 6.56865801781043 0.76791538821061 -3.41136172653156
		H 4.80570777306538 1.34709749685286 -2.32535992897103
		H 8.74056817398658 -0.05653227194803 -4.19187716004944

(Ph-C ₄ H ₄ -Ph)**	Ph-C ₄ H ₅	(Ph-C ₄ H ₅)**
H -2.59896127578193 -0.93800378211845 -0.51015462623727	H 5.49030186440566 -3.22802236421675 -2.22492394127574	H 5.35753803548672 -3.24998692378329 -2.45219686777215
H -0.29719956042316 -1.51245051663313 -1.21763695223604	H 7.67292095862273 -4.05209807758890 -3.03707593612050	H 7.57495565275662 -4.07223141724056 -3.19250767954077
C -1.84014963337512 -0.16471765112706 -0.57743710367670	H 1.68543332801807 -0.85849407026143 -2.08392442714023	H 1.92511842552405 -1.00557851884922 -1.39411118850642
C -0.55557544115577 -0.48588880514104 -0.97210131080034	C 6.20510980365053 -2.53085871355634 -2.65625285278828	C 6.12379950871323 -2.55281667760384 -2.77924133288500
H 5.18166627386511 -3.21880356532345 -2.92199764963353	C 7.43385355962198 -2.99482591829277 -3.11271785033925	C 7.35697654793546 -3.00917207516811 -3.19084668524457
H 7.39223510904408 -4.05006632029551 -3.66447815519577	H 3.91165050739110 -1.55548713435569 -1.90857128117736	H 3.87754026782086 -1.56454599070388 -2.04716979436035
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H -3.16877552019770 1.41336191330446 0.04585642210404	C 1.68974653690101 0.13947379239406 -1.65192326993601	C 1.80435594249831 0.07326028042764 -1.41230409606362
C -2.15954119008729 1.15910579181492 -0.26487318151566	C 4.56298737503910 -0.74450264628026 -2.23628396099627	C 4.54760536649813 -0.75837369889452 -2.33885566176656
C 6.01066423667175 -2.52905866212990 -3.05561970860888	C 5.86523323842589 -1.16929643956450 -2.73866927900697	C 5.83408001956048 -1.15971227580211 -2.77447969247177
C 7.24462566129464 -2.99243637272603 -3.46982767348513	C 8.35403658378381 -2.10779431166394 -3.66558222020748	C 8.33052051716198 -2.09334338694205 -3.60831661171995
H 3.77519017298451 -1.54103645112074 -2.28378169210550	H 9.31466016357736 -2.46615495357195 -4.02444040902974	H 9.30275233470712 -2.45263451698303 -3.93326461805257
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C 4.50729821273978 -0.74085061508754 -2.37248607009526	C 6.80295107636907 -0.28777962661528 -3.30768253547430	C 6.83837520241916 -0.24578591628251 -3.20282089510660
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C 8.30253575814595 -2.09501905378123 -3.63707424995143	H 2.71514604951894 1.91103332795528 -1.23214428919264	H 2.58662197344005 1.99263807413369 -1.80335415087443
C -1.18540715069295 2.16172026601163 -0.34905604479300	H 6.57078901284708 0.76876385070424 -3.40375112141157	H 6.64511719484267 0.82107937612872 -3.21056592855630
H 9.27336886392997 -2.45752208107888 -3.96235836135185	H 4.77538048658038 1.35156561594007 -2.36462593304148	H 4.74958490720340 1.36367717523234 -2.54052715323525
C 0.10036754402866 1.85269907832576 -0.74336334362134	H 8.73934867773987 -0.05526122192768 -4.19663748660353	H 8.83192163089295 -0.02038086086147 -3.93929394965654
C 2.83689209996225 0.95229738633948 -1.65575657965152		
C 4.12104420067458 0.55430257945217 -2.07216639359084		
C 6.89089645561364 -0.25522142433632 -2.97400832037759		
C 8.11899349172008 -0.72919434006337 -3.38786755124547		
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