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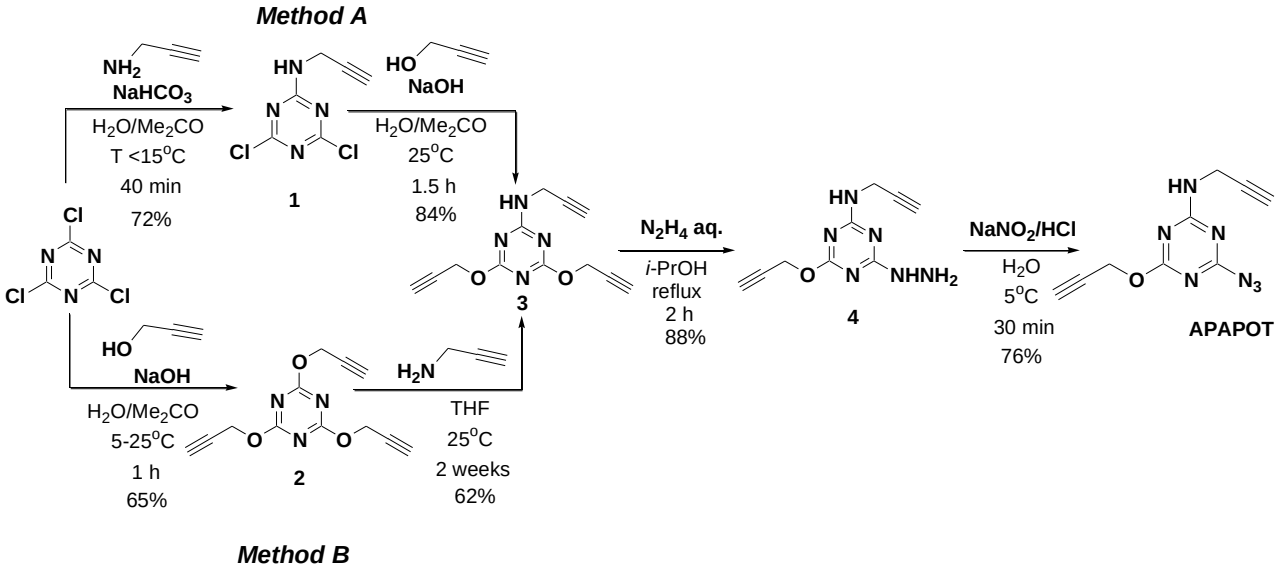
New non-symmetric azido-diacetylenic *s*-triazine monomer for polycycloaddition

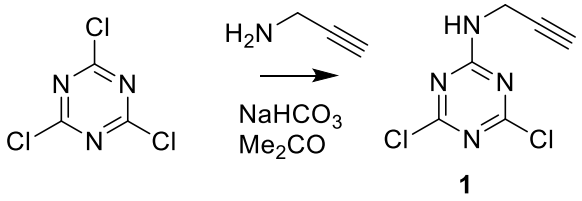
Artem O. Petrov, Sergei V. Karpov, Georgiy V. Malkov, Aleksey V. Shastin and Elmira R. Badamshina

General. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III spectrometer (500 and 126 MHz, respectively) in DMSO-d_6 or $CDCl_3$ with TMS as internal standard. IR spectra were registered on a Bruker Alpha spectrometer in KBr pellets. Elemental analysis was carried out using an Elementar vario MICRO cube CHN*S*-analyzer. Melting points were determined on a Kofler bench with a heating rate of 4 K min^{-1}. Monitoring of the reaction progress and assessment of the purity of synthesized compounds were done by TLC on ALUGRAM SIL G/UV254 plates with visualization under UV light.

General Scheme of synthesis of monomer APAPOT

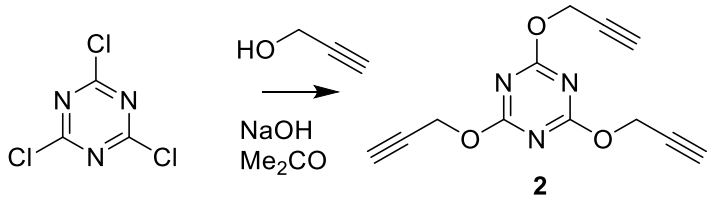


Synthesis of 4,6-dichloro-*N*-(prop-2-yn-1-yl)-1,3,5-triazin-2-amine (1)



A solution of $NaHCO_3$ (2.50 g, 30 mmol) in H_2O (7 ml) was added with stirring and cooling in an ice bath to a solution of cyanuric chloride (1.30 g, 24 mmol) in Me_2CO (7 ml). Then, a solution of propargylamine (2.50 g, 24 mmol) in Me_2CO (10 ml) was added dropwise to the resulting mixture at such a rate as to keep the temperature of the reaction mixture below 15°C. The resulting mixture was stirred for 40 min with cooling, then water (100 ml) was added. The formed precipitate was filtered off, air-dried and has been recrystallized from CCl_4. Yield 3.58 g (72%), colorless crystals, mp 156–157 °C (CCl_4) (mp 153–155 °C).[S1] IR spectrum, ν, cm^{-1}: 3233 (≡CH), 3266, 3178 sh (N–H), 2928, 2860 (CH2), 2123 (–C≡C–), 1625, 1556, 1518, 1349, 1324, 1262, 1243(C–N), 855 (C–Cl). According to the ^1H and ^{13}C NMR spectra, the compound is identical to that described in the literature.[S2] Found (%): C, 35.6; H, 1.8; N, 27.6; Cacl. for $C_6H_4Cl_2N_4$ (%):C, 35.5; H, 1.99; N, 27.6.

Synthesis of 2,4,6-tris(prop-2-yn-1-yloxy)-1,3,5-triazine (2)

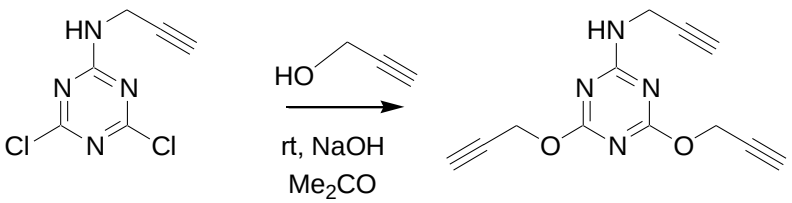


2

Propargyl alcohol (10.1 g, 180 mmol) was added with stirring to a solution of cyanuric chloride (10.0 g, 54 mmol) in Me_2CO (100 ml) at 20 °C. Then, 5 mol.% solution of NaOH was added dropwise to the mixture at such rate as to keep the temperature of the reaction mixture below 5 °C (TLC control). In the end of the reaction, water was added, the resulting white precipitate was filtered off, washed with water, air-dried and recrystallized from *i*-PrOH. Yield 8.57 g (65%), colorless crystals, mp 77–78 °C (*i*-PrOH) (mp 77–78 °C).[S2] IR spectrum, ν, cm^{-1}: 3267 (≡CH), 2965, 2938 (CH_2), 2135 (-C≡CH), 1571 (C-N of triazine), 1452 (CH_2), 1135, 1332 (C-O-C), 816 (C-N). According to the ^1H and ^{13}C NMR spectra, the compound is identical to that described in the literature.[S3] Found (%): C, 59.08; H, 3.86; N, 17.02; Cacl. for $C_{12}H_9Cl_3N_3$ (%):C, 59.26; H, 3.73; N, 17.28.

Synthesis of *N*-(prop-2-yn-1-yl)-4,6-bis(prop-2-yn-1-yloxy)-1,3,5-triazin-2-amine (3)

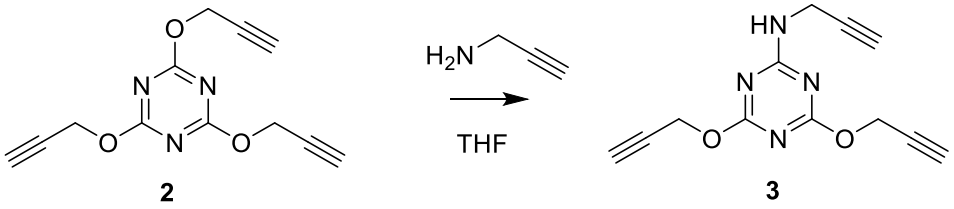
Method 1.



1 **3**

Propargyl alcohol (1.5 g, 26 mmol) and Me_2CO (25 ml) were added with stirring to a solution of NaOH (1.20 g, 30 mmol) in H_2O (10 ml). Compound **1** (2.4 g, 12 mmol) was then added. The resulting mixture was stirred at room temperature for 1.5 h, and then H_2O was added. The formed precipitate was filtered off, washed with H_2O, air-dried and recrystallized from *i*-PrOH. Yield 2.4 g (84%), colorless crystals, mp 168–170 °C (*i*-PrOH).

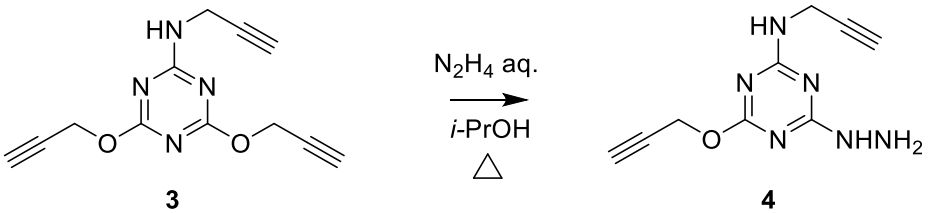
Method 2.



Propargylamine (1.45 g, 26 mmol) was added to a solution of compound **2** (6.2 g, 26 mmol) in THF (15 ml). The reaction vessel was closed and left for 2 weeks at room temperature (TLC control. At the end of the reaction, THF was evaporated *in vacuo*, and the residue was recrystallized from *i*-PrOH and air-dried. Yield 3.8 g (62%), colorless crystals, mp 169–170 °C (*i*-PrOH).

IR spectrum, ν, cm^{-1}: 3297 (≡CH), 3560 sh, 3178 sh (NH); 2955, 2860 (CH_2); 2123 (-C≡C-); 1450, 1465 (CH_2); 1740, 1620, 1518, 1415, 1341, 1324, 1262, 1243 (C-N of triazine); 1340 (C-O-C). ^{1}H NMR spectrum (500 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 3.07-3.08 (1H, t, *J* = 2.4, HC≡C-CH_2-NH-); 3.54-3.55 (2H, t, *J* = 2.4, HC≡C-CH_2-O-); 4.04-4.05 (2H, dd, *J* = 6, *J* = 2.5, CH_2-NH), 4.91-4.92 (2H, d, *J* = 2.4, CH_2-O-), 4.95-4.96 (2H, d, *J* = 2.4, CH_2-O-), 8.43-8.46 (1H, t, *J* = 5.8, NH). ^{13}C NMR spectrum (126 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 30.3 (CH_2-NH); 54.9, 55.1 (CH_2-O); 73.6 (HC≡C-CH_2-NH-); 78.4 (HC≡C-CH_2-O-); 79.0, 79.1 (HC≡C-CH_2-O-); 81.2 (HC≡C-CH_2-NH-); 167.8 (CH_2-NH-C=N- triazine); 171.0, 171.3 (-O-C=N- triazine). Number of signals increased due to hindered rotation around the C–NHR bond. Signals in ^{1}H and ^{13}C NMR spectra were identified analogical to that described in the literature for propargyloxy[S4] and propargylamino[S1] derivates of *s*-triazine. Found (%): C, 59.73; H, 4.16; N, 23.02; Cacl. for $C_{12}H_{10}Cl_4N_2$ (%):C, 59.50; H, 4.16; N, 23.13.

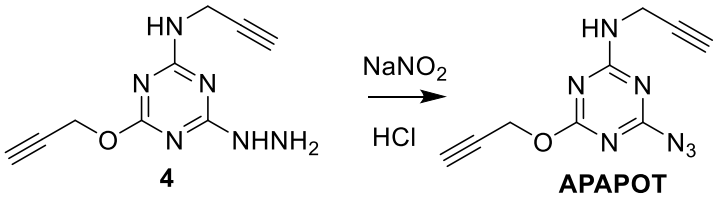
Synthesis of 4-hydrazinyl-*N*-(prop-2-yn-1-yl)-6-(prop-2-yn-1-yloxy)-1,3,5-triazin-2-amine (4).



A solution of compound **3** (2.4 g, 10 mmol) in *i*-PrOH (50 ml) was mixed with hydrazine hydrate (2 ml, 40 mmol). The resulting mixture was refluxed with stirring for 2 h (TLC control). Then it was cooled, the formed precipitate was filtered off and air-dried. The product was purified on a

short chromatography column with silica gel (Silpearl) and EtOAc as an eluent. Yield 1.9 g (88%), mp = 168–170 °C. IR spectrum, ν, cm^{-1}: 3290 (≡CH); 3250 sh (NH); 3326 ($NHNH_2$); 2958, 2853 (CH_2); 2123 (-C≡C-); 1500 ($NHNH_2$); 1448, 1462 (CH_2); 1740, 1620, 1518, 1415, 1341, 1324, 1262, 1243 (C-N of triazine); 1332 (C-O-C). ^{1}H NMR spectrum (500 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 3.07-3.08 (1H, m, HC≡C-CH_2-NH-), 3.46-3.52 (1H, m, HC≡C-CH_2-O-), 3.92-4.02 (2H, m, H_2N-NH-), 4.08-4.35 (2H, m, CH_2-NH), 4.78-5.00 (2H, m, CH_2-O-), 7.43-7.80 (1H, m, NH-NH_2), 8.27-8.54 (1H, m, NH-CH_2-). ^{13}C NMR spectrum (126 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 30.0 (CH_2-NH-); 53.6, 53.8 (CH_2-O-); 72.9, 73.2 (HC≡C-CH_2-NH-); 77.8 (HC≡C-CH_2-O-); 79.7, 79.8 (HC≡C-CH_2-O-); 82.2 (HC≡C-CH_2-NH-); 166.3, 166.4, 166.9, 167.2 (NH_2-NH-C=N- triazine), 168.7, 168,5 (-O-C=N- triazine); 169.1, 169.5, 169.9 (CH_2-NH-C=N- triazine). Number of signals increased due to hindered rotation around the C–NHR bond. Signals in ^{1}H and ^{13}C NMR spectra were identified analogical to that described in the literature for propargyloxy[S4] and propargylamino[S1] derivates of hydrazino-*s*-triazine. Found (%): C, 49.21; H, 5.03; N, 38.77; Cacl. for $C_9H_{10}N_6O$ (%):C, 49.54; H, 4.62; N, 38.51.

Synthesis of 4-azido-*N*-(prop-2-yn-1-yl)-6-(prop-2-yn-1-yloxy)-1,3,5-triazin-2-amine (APAPOT)



Concentrated HCl (1.0 ml, 10 mmol) was added to a suspension of compound **4** (0.94 g, 4 mmol) in water (5 ml), and mixture was stirred until homogenization. Then a solution of $NaNO_2$ (0.30 g, 4 mmol) in water (5 ml) was added with cooling in an ice bath, and the mixture was stirred for 30 min. The formed precipitate was filtered off, air-dried, washed several times with saturated $NaHCO_3$ solution. The residue was dissolved in CH_2Cl_2, the solution was passed through a thin layer of silica gel (Silpearl), and the solvent was evaporated under reduced pressure without heating. Yield 0.75 g (76%), mp = 130–131 °C. IR spectrum, ν, cm^{-1}: 3273 (≡CH); 3239 sh (NH_2); 2156, 1200 (N_3); 2958, 2853 (CH_2); 2129 (-C≡C-); 1452, 1470 (CH_2); 1332 (C-O-C); 1740, 1620, 1518, 1415, 1341, 1324, 1262, 1243 (C-N of triazine). ^{1}H NMR spectrum (500 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 3.12 (1H, m, HC≡C-CH_2-NH-), 3.32-3.58 (1H, m, HC≡C-CH_2-O-), 4.04-4.09 (2H, m, CH_2-NH), 4.94-4.99 (2H, m, CH_2-O-), 8.66-8.70 (1H, m, NH-CH_2-). ^{13}C NMR spectrum (126 MHz, DMSO-d_6), δ, ppm (*J*, Hz): 30.3, 30.4 (CH_2-NH); 55.1, 55.3 (CH_2-O); 73.8 (HC≡C-CH_2-NH-); 78.6 (HC≡C-CH_2-O-), 78.8, 78.9 (HC≡C-CH_2-O-); 80.9 (HC≡C-CH_2-NH-); 167.3 (N_3-C=N- of triazine); 170.3, 170.5 (-O-C=N- of triazine); 170.6,170.8 (-NH-C=N- of triazine). Number of signals increased due to hindered rotation around the C–NHR bond. Signals in ^{1}H and ^{13}C NMR spectra were identified analogical to that described in the literature for propargyloxy[S4] and propargylamino[S1] derivates of azido-*s*-triazine. Found (%): C, 46.27; H, 3.10; N, 42.94; Cacl. for $C_9H_{10}N_6O$ (%):C, 47.16; H, 3.08; N, 42.78.

^{1}H and ^{13}C NMR spectra

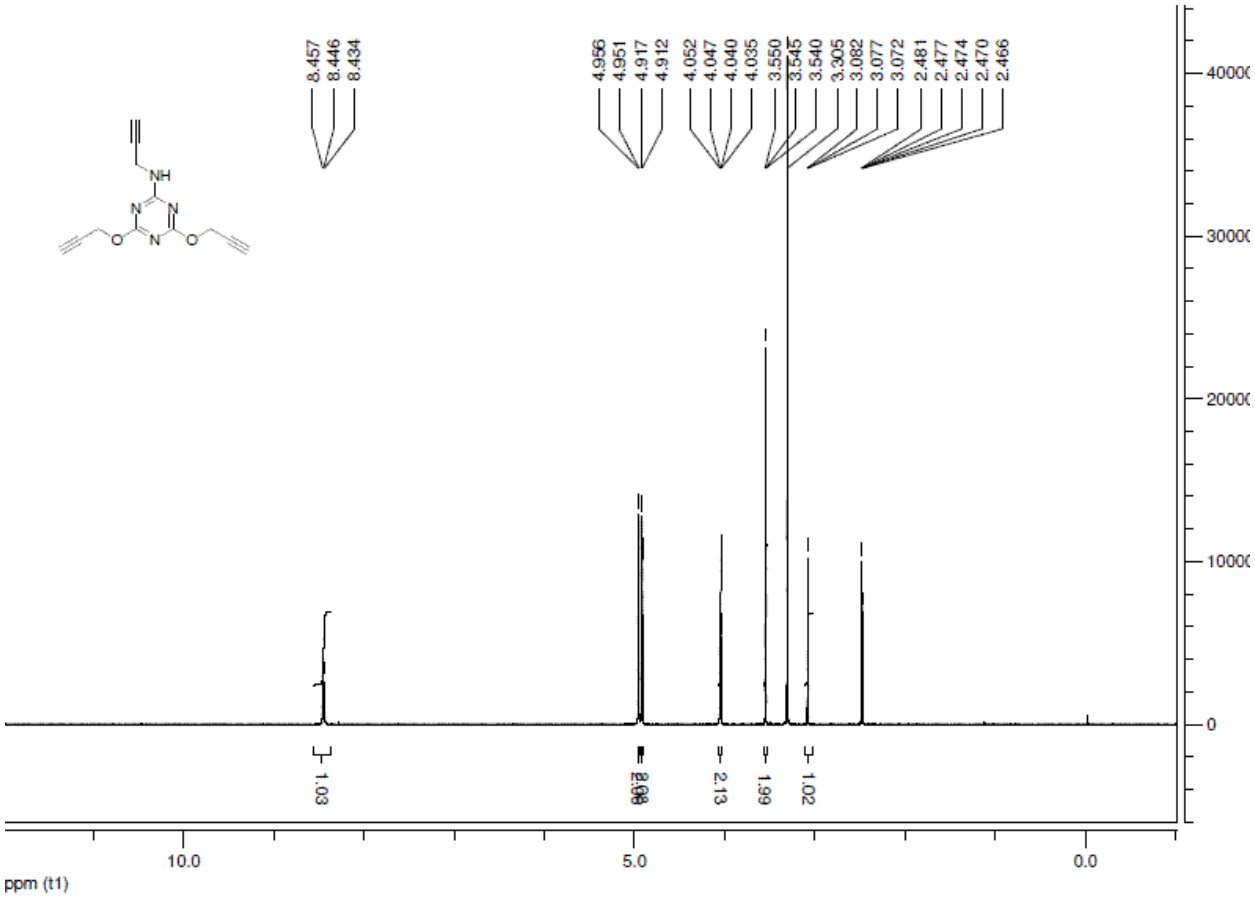


Figure S1. ^{1}H NMR spectrum of **3** in DMSO-d_6

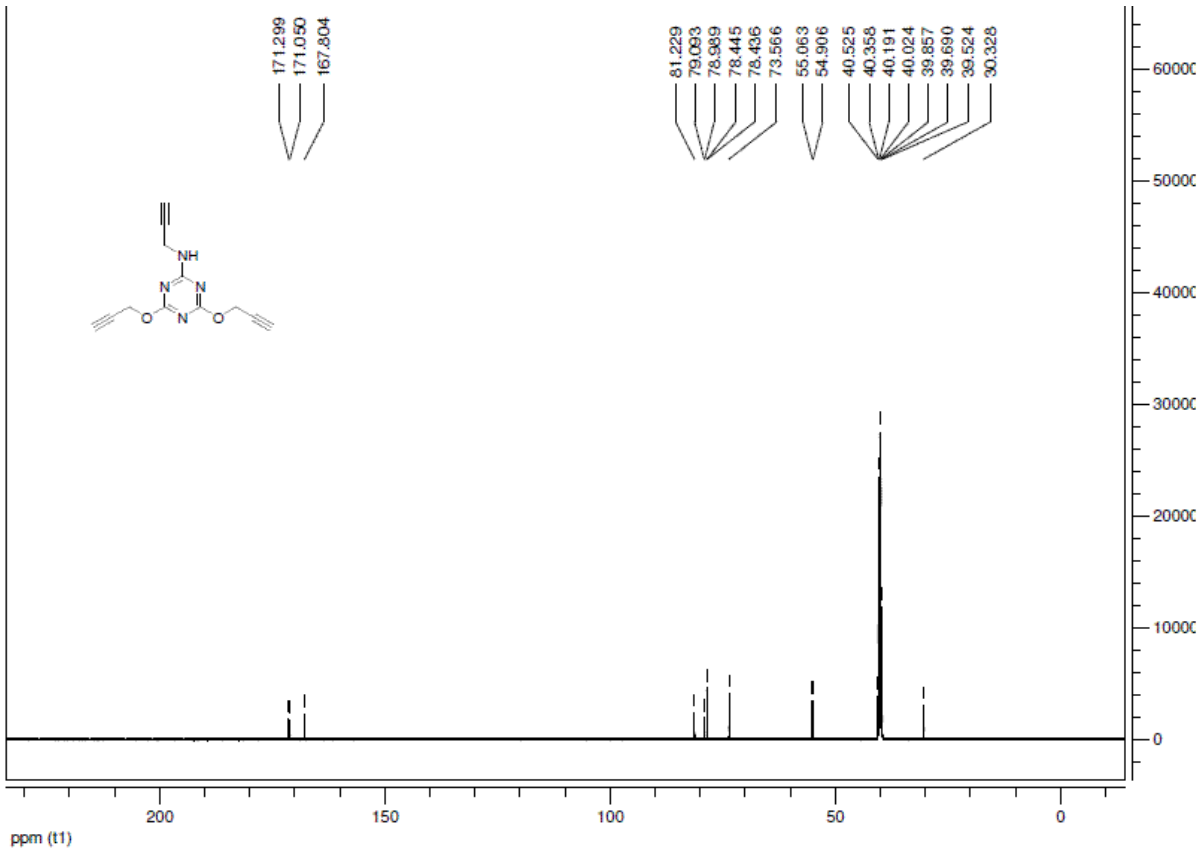


Figure S2. ^{13}C NMR spectrum of **3** in DMSO-d_6

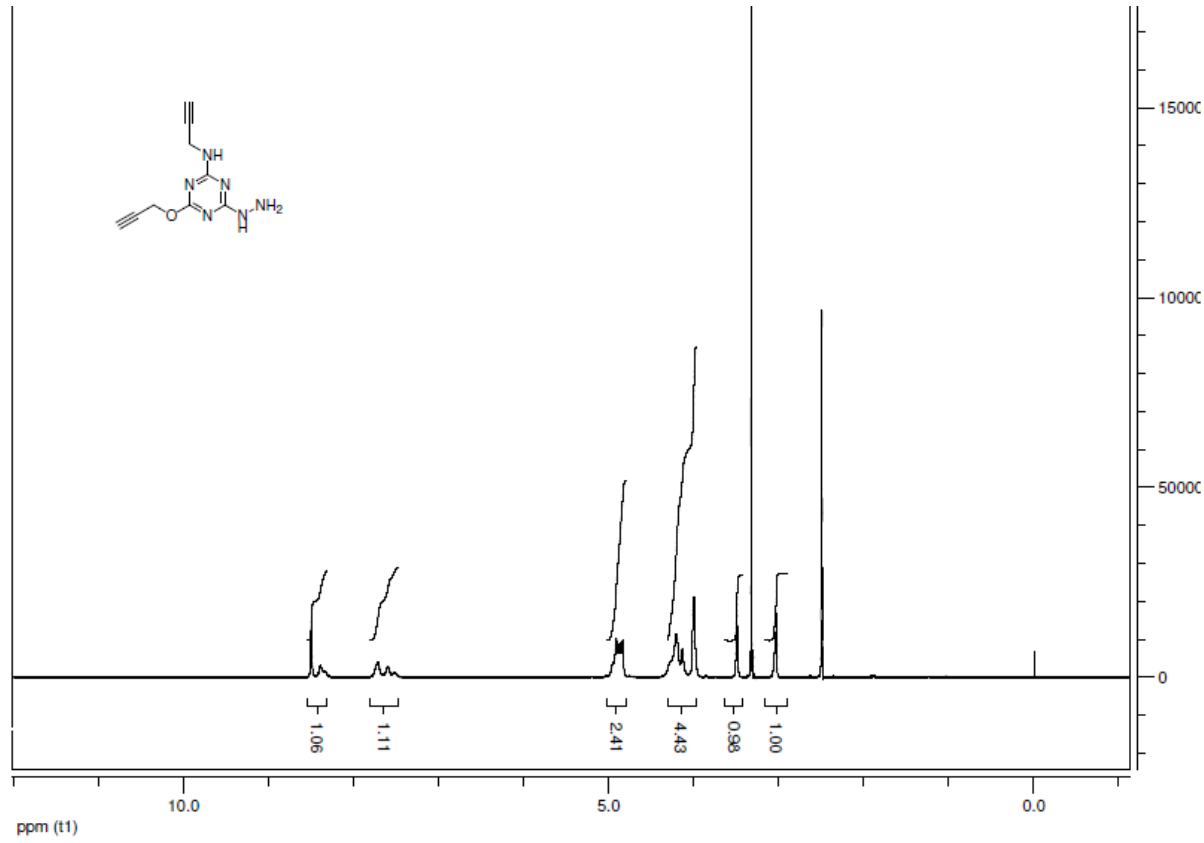


Figure S3. ^{1}H NMR spectrum of **4** in DMSO-d_6

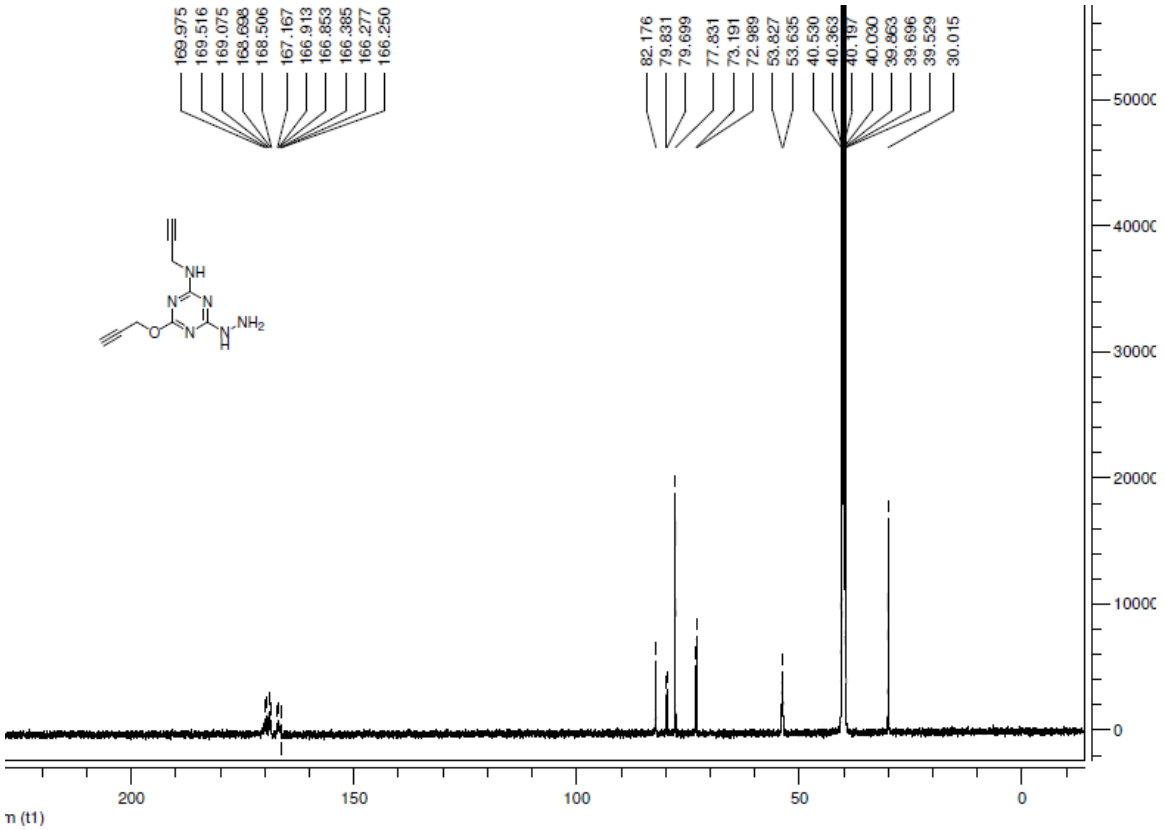


Figure S4. ^{13}C NMR spectrum of **4** in DMSO-d_6

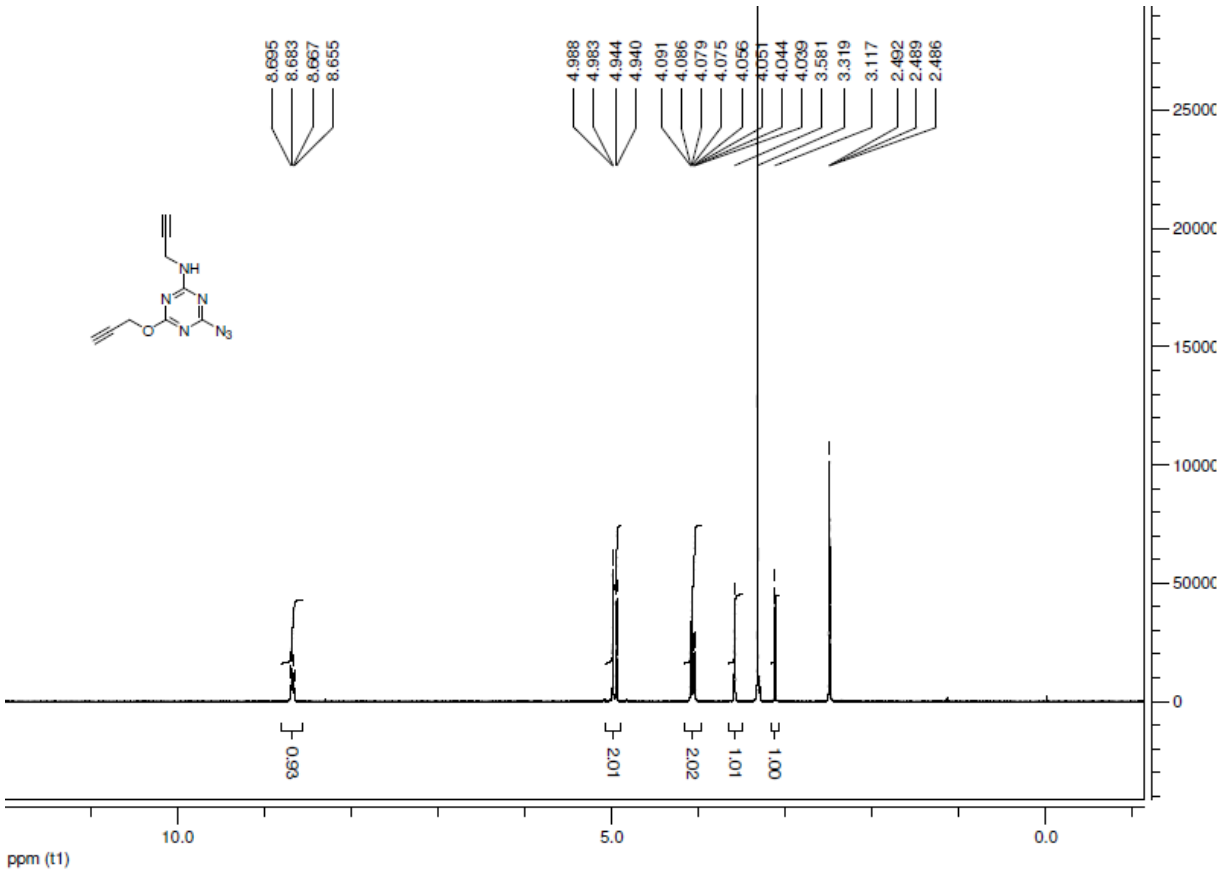


Figure S5. ^{1}H NMR spectrum of **APAPOT** in DMSO-d_6

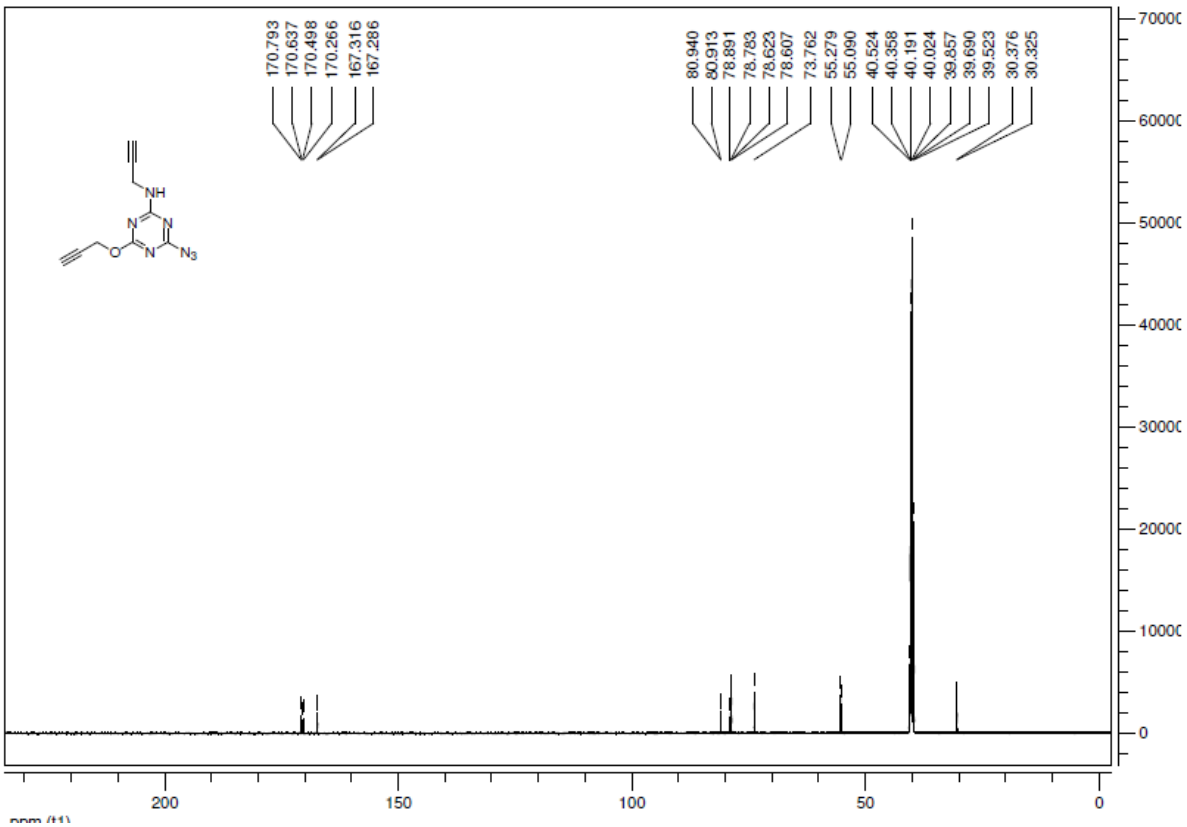


Figure S6. ^{13}C NMR spectrum of **APAPOT** in DMSO-d_6

Calculation of kinetic parameters of azide-alkyne cycloaddition (AAC).

Equation (1) was used to calculate reaction rate constant (**k**).

$$k(T) = \frac{k_B T}{h} \cdot \frac{RT}{P_0} \cdot \exp(-\frac{\Delta G^{\neq}}{RT}) \quad (1),$$

where k_B is Boltzmann constant, T is temperature, h is Planck constant, R is gas constant, P_0 is pressure (1 atm), $\Delta G^{\neq}$ is Gibbs energy of activation.

To determine the content of 1,4- and 1,5-disubstituted 1,2,3-triazoles in ABPOT and APBAT polycycloaddition products, differential equations system (2-8) was solved:

$$\frac{d[B]}{dt} = -k_{1,4} \cdot [B] \cdot [A] - k_{1,5} \cdot [B] \cdot [A] \quad (2)$$

$$\frac{d[A]}{dt} = -k_{1,4} \cdot [B] \cdot [A] - k_{1,5} \cdot [B] \cdot [A] - k_{1,4} \cdot [BT_4] \cdot [A] - k_{1,5} \cdot [BT_4] \cdot [A] - k_{1,4} \cdot [BT_5] \cdot [A] - k_{1,5} \cdot [BT_5] \cdot [A] \quad (3)$$

$$\frac{d[BT_4]}{dt} = k_{1,4} \cdot [B] \cdot [A] - k_{1,4} \cdot [BT_4] \cdot [A] - k_{1,5} \cdot [BT_4] \cdot [A] \quad (4)$$

$$\frac{d[BT_5]}{dt} = k_{1,5} \cdot [B] \cdot [A] - k_{1,4} \cdot [BT_5] \cdot [A] - k_{1,5} \cdot [BT_5] \cdot [A] \quad (5)$$

$$\frac{d[T_4T_4]}{dt} = k_{1,4} \cdot [BT_4] \cdot [A] \quad (6)$$

$$\frac{d[T_4T_5]}{dt} = k_{1,4} \cdot [BT_5] \cdot [A] + k_{1,5} \cdot [BT_4] \cdot [A] \quad (7)$$

$$\frac{d[T_5T_5]}{dt} = k_{1,5} \cdot [BT_5] \cdot [A] \quad (8),$$

where A and B are azido and ethynyl groups of ABPOT/ABPAT,

BT_4 and BT_5 are 1,4- and 1,5-regioisomers formed involving one ethynyl group of ABPOT/ABPAT,

T_4T_5 is 1,4- and 1,5-regioisomers formed involving two ethynyl groups of ABPOT/ABPAT,

$k_{1,4}$ and $k_{1,5}$ are 1,4- and 1,5-regioisomers formation rate constants.

Thus, the part of 1,5-disubstituted 1,2,3,-triazoles ($\omega_{1,5}$) in the mixture can be determined by (9):

$$\omega_{1,5} = \frac{[BT_5] + [T_4T_5] + [T_5T_4] + 2[T_5T_5]}{[BT_4] + [BT_5] + [T_4T_5] + [T_5T_4] + 2[T_4T_4] + 2[T_5T_5]} \quad (9).$$

To determine the content of reacted propargylamino groups and also of 1,4- and 1,5-disubstituted 1,2,3-triazoles in APAPOT polycycloaddition products, differential equations system (10-19) was solved:

$$\frac{d[B]}{dt} = -k_{1,4O} \cdot [B] \cdot [A] - k_{1,5O} \cdot [B] \cdot [A] - k_{1,4N} \cdot [B] \cdot [A] - k_{1,5N} \cdot [B] \cdot [A] \quad (10)$$

$$\frac{d[A]}{dt} = -k_{1,4O} \cdot [B] \cdot [A] - k_{1,5O} \cdot [B] \cdot [A] - k_{1,4N} \cdot [B] \cdot [A] - k_{1,5N} \cdot [B] \cdot [A] - \\ - k_{1,4N} \cdot [B_N T_{4O}] \cdot [A] - k_{1,5N} \cdot [B_N T_{4O}] \cdot [A] - k_{1,4N} \cdot [B_N T_{5O}] \cdot [A] - k_{1,5N} \cdot [B_N T_{5O}] \cdot [A] - \quad (11) \\ - k_{1,4O} \cdot [B_O T_{4N}] \cdot [A] - k_{1,5O} \cdot [B_O T_{4N}] \cdot [A] - k_{1,4O} \cdot [B_O T_{5N}] \cdot [A] - k_{1,5O} \cdot [B_O T_{5N}] \cdot [A]$$

$$\frac{d[B_N T_{4O}]}{dt} = k_{1,4O} \cdot [B] \cdot [A] - k_{1,4N} \cdot [B_N T_{4O}] \cdot [A] - k_{1,5N} \cdot [B_N T_{4O}] \cdot [A] \quad (12)$$

$$\frac{d[B_N T_{5O}]}{dt} = k_{1,5O} \cdot [B] \cdot [A] - k_{1,4N} \cdot [B_N T_{5O}] \cdot [A] - k_{1,5N} \cdot [B_N T_{5O}] \cdot [A] \quad (13)$$

$$\frac{d[B_O T_{4N}]}{dt} = k_{1,4N} \cdot [B] \cdot [A] - k_{1,4O} \cdot [B_O T_{4N}] \cdot [A] - k_{1,5O} \cdot [B_O T_{4N}] \cdot [A] \quad (14)$$

$$\frac{d[B_O T_{5N}]}{dt} = k_{1,5N} \cdot [B] \cdot [A] - k_{1,4O} \cdot [B_O T_{4N}] \cdot [A] - k_{1,5O} \cdot [B_O T_{4N}] \cdot [A] \quad (15)$$

$$\frac{d[T_{4O} T_{4N}]}{dt} = k_{1,4O} \cdot [B_O T_{4N}] \cdot [A] + k_{1,4N} \cdot [B_N T_{4O}] \cdot [A] \quad (16)$$

$$\frac{d[T_{5O} T_{5N}]}{dt} = k_{1,5O} \cdot [B_O T_{5N}] \cdot [A] + k_{1,5N} \cdot [B_N T_{5O}] \cdot [A] \quad (17)$$

$$\frac{d[T_{5O} T_{4N}]}{dt} = k_{1,5O} \cdot [B_O T_{4N}] \cdot [A] + k_{1,4N} \cdot [B_N T_{5O}] \cdot [A] \quad (18)$$

$$\frac{d[T_{4O} T_{5N}]}{dt} = k_{1,4O} \cdot [B_O T_{5N}] \cdot [A] + k_{1,5N} \cdot [B_N T_{4O}] \cdot [A] \quad (19),$$

where O and N indices correspond to propargyloxy and propargylamino groups of APAPOT.

The part of reacted propargylamino groups (ω_N) can be determined by (20):

$$\omega_N = \frac{[B_O T_{5N}] + [B_O T_{4N}] + [T_{4O} T_{5N}] + [T_{5O} T_{4N}] + [T_{4O} T_{4N}] + [T_{5O} T_{5N}]}{2[B]} \quad (20)$$

Degree of branching of HBP that can be obtained from APAPOT was determined by (21):

$$DB = \frac{2D}{2D + L} = \\ = \frac{[T_{4O} T_{5N}] + [T_{5O} T_{4N}] + [T_{4O} T_{4N}] + [T_{5O} T_{5N}]}{2([T_{4O} T_{5N}] + [T_{5O} T_{4N}] + [T_{4O} T_{4N}] + [T_{5O} T_{5N}]) + [B_O T_{5N}] + [B_O T_{4N}] + [B_N T_{5O}] + [B_N T_{4O}]} \quad (21)$$

where DB is the degree of branching,

D is the amount of dendrite units,

L is the amount of linear units.

Table S1. Gibbs energies and Cartesian coordinates of monomer atoms, transition states (TS) and AAC reaction products of ABPOT, ABPAT and APAPOT optimized at M06-2X/6-311++G(d,p) level of theory.

Compound	Gibbs energy, hartree	Atom	x	y	z
ABPOT 2-azido-4,6-bis(prop-2-yn-1-yloxy)-*s*-triazine	-825.126903	O	2.51876500	-1.39603600	-0.61536600
		N	-1.26440500	2.73058500	0.01699300
		N	-0.11430700	2.33377200	-0.26255800
		N	1.24313000	0.49513400	-0.45103700
		N	0.40856500	-1.67098700	0.05873300
		N	-2.24842600	3.20218200	0.23692300
		N	-0.99084300	0.22737400	0.28805000
		C	-0.73843300	-1.07877900	0.34625400
		C	1.35602400	-0.82484000	-0.32306800
		C	0.04246000	0.95292500	-0.13094400
		C	3.61855200	-0.54087500	-0.94427300
		C	4.17608400	0.11446800	0.23896000
		C	4.66194300	0.63799700	1.20111200
		H	5.08324500	1.10804100	2.05760300
		H	3.30865800	0.20536700	-1.67662600
		H	4.35679600	-1.20822700	-1.38630500
		O	-1.70775100	-1.89886600	0.73902500
		C	-2.99412500	-1.33271500	1.00313700
		C	-3.69501500	-0.94609400	-0.22197400
		C	-4.29641300	-0.64764100	-1.21473700
		H	-4.82332500	-0.37978300	-2.09968000
		H	-3.53927400	-2.12639600	1.51162800
		H	-2.89668700	-0.47287200	1.66758700
		O	2.51876500	-1.39603600	-0.61536600
		N	-1.26440500	2.73058500	0.01699300
		N	-0.11430700	2.33377200	-0.26255800
		N	1.24313000	0.49513400	-0.45103700
		N	0.40856500	-1.67098700	0.05873300
		N	-2.24842600	3.20218200	0.23692300
		N	-0.99084300	0.22737400	0.28805000
		C	-0.73843300	-1.07877900	0.34625400
		C	1.35602400	-0.82484000	-0.32306800
		C	0.04246000	0.95292500	-0.13094400
		C	3.61855200	-0.54087500	-0.94427300
ABPOT_TS_14	-1650.20566	O	3.16232700	-1.25289100	-1.95136800
		N	2.56395600	-6.84626000	-1.57211000
		N	2.11550700	-5.70605200	-1.81518200
		N	2.59465600	-3.46778900	-1.90164100
		N	4.76923600	-2.68898900	-1.36234500
		N	2.84301800	-7.90697000	-1.38466900
		N	4.28538800	-5.00708900	-1.26248800
		C	5.09242800	-3.95217600	-1.14813700
		C	3.50008600	-2.51718100	-1.73295700
		C	3.05723200	-4.69052700	-1.64600900

		C	1.79051400	-0.97344500	-2.25234200
		C	0.93195000	-1.04784800	-1.06293700
		C	0.59439200	-1.21779600	0.10631100
		O	-4.73813300	2.15701400	1.57455600
		N	-1.56364300	-0.39172300	-1.10694400
		N	-1.47879800	-0.78649400	0.09395900
		N	-3.16059100	0.72591300	0.74108400
		N	-3.56741600	0.97028500	3.06307600
		N	-0.89034600	-0.36903500	-2.03183900
		N	-1.89110500	-0.53267500	2.30994700
		C	-2.61140000	0.07374300	3.25159100
		C	-3.78584000	1.25429300	1.78244200
		C	-2.22134600	-0.16155300	1.08250300
		C	-4.97016600	2.57738800	0.22608200
		C	-3.91751500	3.46801000	-0.26255200
		C	-3.07823700	4.21963500	-0.67110700
		H	0.58479100	-1.44997200	1.14871100
		H	1.42691800	-1.65728300	-3.01965800
		H	1.79729600	0.04155100	-2.64587300
		H	-2.32596300	4.88020400	-1.03206100
		H	-5.92071500	3.10664100	0.26701500
		H	-5.06051200	1.70851500	-0.42672300
		O	-2.29351000	-0.27959100	4.49235400
		C	-3.08616800	0.25391000	5.55851600
		H	-3.21882100	1.32809500	5.42633100
		H	-2.49941800	0.06159500	6.45525100
		C	-4.38751000	-0.40678100	5.65586600
		C	-5.44701300	-0.95581100	5.76567500
		H	-6.39075900	-1.43969700	5.85255600
		O	6.32904200	-4.25124900	-0.76486600
		C	7.28174900	-3.18406900	-0.71020800
		H	8.11022600	-3.58915500	-0.13144400
		H	6.85343300	-2.32509900	-0.19278900
		C	7.74113300	-2.79226500	-2.04252600
		C	8.14752300	-2.47767400	-3.12509800
		H	8.49607400	-2.19395800	-4.08962600
ABPOT_TS_15	-1650.20714	O	-2.13003100	0.86120300	-1.40567100
		N	-3.88622300	-2.51706100	2.75292600
		N	-2.98351700	-2.02139500	2.04631800
		N	-2.50758400	-0.58620100	0.32514700
		N	-4.25455200	0.58251000	-0.77419700
		N	-4.59518600	-3.02429700	3.44460500
		N	-4.76117600	-0.90326700	1.00159500
		C	-5.08713200	-0.02766500	0.05038800
		C	-2.97606700	0.25482600	-0.58382800
		C	-3.45820200	-1.12946100	1.08298500
		C	-0.74269500	0.52148300	-1.30594900
		C	-0.48601200	-0.78675200	-1.93135800
		C	-0.63951800	-1.85637600	-2.51692100
		O	5.78421400	-0.63716000	0.46809600

		N	1.88947600	-1.89692800	-2.17451500
		N	1.67746700	-0.75059900	-1.67421100
		N	3.79069600	-0.78183900	-0.64210400
		N	4.34137200	1.04251800	0.76837300
		N	1.24618200	-2.69847100	-2.68893800
		N	2.23467700	0.98747600	-0.32344900
		C	3.15037800	1.53707200	0.47162700
		C	4.59343600	-0.12376500	0.17934200
		C	2.61977200	-0.16842300	-0.84618100
		C	6.09253700	-1.93270600	-0.05728400
		C	5.37766700	-2.99715400	0.64666000
		C	4.81831000	-3.88332900	1.22799300
		H	-1.16160100	-2.65239400	-2.99763300
		H	-0.41764600	0.52177400	-0.26694100
		H	-0.21393400	1.30768000	-1.83975100
		H	4.31041500	-4.66519500	1.74108400
		H	7.16576700	-2.03733100	0.09292000
		H	5.86461700	-1.96819400	-1.12315300
		O	2.77852600	2.69462000	1.00922300
		C	3.73975900	3.39588700	1.80529000
		H	4.21602400	2.71140300	2.50786500
		H	3.15429500	4.13529000	2.34934300
		C	4.75128600	4.05935000	0.98290700
		C	5.57223300	4.62996800	0.32218200
		H	6.30551100	5.12651300	-0.26779300
		O	-6.39074000	0.21037200	-0.04739800
		C	-6.81270900	1.21247200	-0.97895400
		H	-7.88381300	1.04935300	-1.08635600
		H	-6.31730300	1.06446000	-1.93898400
		C	-6.55517500	2.56392100	-0.48233300
		C	-6.37439300	3.67772200	-0.07888400
		H	-6.20035900	4.66480100	0.27846900
ABPOT_prod_14	-1650.3364	O	2.65446000	-1.85593900	-1.42951400
		N	3.80119900	0.05776900	3.75010000
		N	3.28198800	-0.77200200	2.97353200
		N	2.94523700	-1.35617200	0.78485700
		N	3.82811800	-0.01402200	-0.96014900
		N	4.21447900	0.72289800	4.54039400
		N	4.18355400	0.60295100	1.30062200
		C	4.31824500	0.76990300	-0.01483900
		C	3.15109300	-1.06068400	-0.48805700
		C	3.49032800	-0.47839000	1.62651300
		C	1.83542500	-2.95208700	-1.01687000
		C	0.45937100	-2.47778000	-0.68425600
		C	-0.12554000	-1.26729400	-0.89803800
		O	-5.65356400	-0.08674700	0.72310100
		N	-1.55042600	-2.67131100	0.10339300
		N	-1.38319500	-1.42532200	-0.38873900
		N	-3.55411700	-0.82238000	0.20169600
		N	-4.28003200	1.39060100	-0.24055400

		N	-0.44939900	-3.30007400	-0.07178800
		N	-2.08618500	0.71930500	-0.83996800
		C	-3.08029700	1.60702900	-0.75016000
		C	-4.45553500	0.15069300	0.21236000
		C	-2.40234700	-0.45785000	-0.33828700
		C	-5.94745000	-1.43300700	1.12679400
		C	-6.20359400	-2.29817400	-0.02316800
		C	-6.43621900	-3.01559400	-0.95417200
		H	0.20356400	-0.34251200	-1.33799700
		H	2.27223900	-3.46287800	-0.15896300
		H	1.81980600	-3.62364700	-1.87445600
		H	-6.62847000	-3.65540400	-1.78249800
		H	-6.84223600	-1.34099100	1.73970800
		H	-5.12646000	-1.83219900	1.72303500
		O	5.00840300	1.85074800	-0.35987200
		C	5.27992200	2.04804800	-1.75201300
		H	5.60348200	3.08532700	-1.82063300
		H	4.36988700	1.90516200	-2.33541000
		C	6.33432700	1.15715100	-2.23541000
		C	7.21510900	0.45289700	-2.64062800
		H	7.98986000	-0.18260200	-2.99880400
		O	-2.78788400	2.80144500	-1.24712200
		C	-3.76875000	3.83721600	-1.10615100
		H	-4.74986400	3.46518500	-1.40271400
		H	-3.44335700	4.61329400	-1.79674800
		C	-3.81643400	4.36026600	0.25840600
		C	-3.85009100	4.81710000	1.36564100
		H	-3.88369900	5.21284700	2.35299000
ABPOT_prod_15	-1650.33485	O	-1.94406800	-1.47009000	0.85908500
		N	-3.52330400	2.80893700	-2.45914600
		N	-2.65117100	2.05753100	-1.97265400
		N	-2.25010500	0.29219800	-0.56996400
		N	-4.04276300	-0.75872200	0.57287700
		N	-4.20148300	3.53735900	-2.95609900
		N	-4.47288000	1.06801300	-0.87519900
		C	-4.84199000	0.10576500	-0.03008700
		C	-2.75748200	-0.60729700	0.25707400
		C	-3.16756700	1.10040600	-1.10008200
		C	-0.53896500	-1.31096000	0.65574300
		C	-0.05203500	-0.21351300	1.55085600
		C	-0.71183900	0.47157400	2.52842800
		O	5.45605200	1.19662200	0.01227700
		N	1.26799100	1.34423100	2.48218600
		N	1.19158400	0.36070300	1.54421600
		N	3.34303200	0.85165200	0.80724300
		N	4.39681400	-0.63382300	-0.71164600
		N	0.13486400	1.40573600	3.06320600
		N	2.19884900	-1.08104500	0.05553200
		C	3.29158600	-1.35351800	-0.66507900
		C	4.35641900	0.46159300	0.04680000

		C	2.30694100	0.02909500	0.75920500
		C	5.43917800	2.44855600	0.71655000
		C	4.67039800	3.46166800	-0.00360700
		C	4.05939700	4.30741600	-0.59259200
		H	-1.72554200	0.35436600	2.87274200
		H	-0.31979900	-1.09924000	-0.38808300
		H	-0.09532100	-2.26727700	0.92446400
		H	3.50390300	5.05334000	-1.10984700
		H	6.48690100	2.73728500	0.77676500
		H	5.03236300	2.30802800	1.71839500
		O	3.19840800	-2.46017000	-1.39016600
		C	5.36587000	-3.47710800	-1.24233100
		C	6.18847300	-3.99372900	-0.54074600
		H	6.92110000	-4.44250900	0.08734700
		C	4.36153800	-2.87614800	-2.11851600
		H	4.78733700	-2.02867700	-2.65643500
		H	3.98759000	-3.61364600	-2.82654900
		O	-6.14688900	0.06031300	0.20909600
		C	-6.63454900	-1.00613200	1.03160000
		H	-7.64324100	-0.69927500	1.30298400
		H	-6.02179700	-1.09763200	1.92884900
		C	-6.66986100	-2.27906400	0.31240800
		C	-6.73039600	-3.32434800	-0.27039700
		H	-6.77220200	-4.25309000	-0.78819600
ABPAT 6-azido-N^2,N^4-di(prop-2-yn-1-yl)-*S*-triazin-2,4-diamine	-785.390744	N	-1.28453600	2.88614500	0.02954800
		N	-0.15419900	2.47822300	-0.29641400
		N	1.19794300	0.64175400	-0.50008900
		N	0.38197800	-1.52255800	0.08206800
		N	-2.25490800	3.36761800	0.29114800
		N	-1.02198600	0.38454100	0.30623400
		C	-0.76766900	-0.92894000	0.40338300
		C	1.32492800	-0.68637800	-0.36313500
		C	0.00529400	1.09211700	-0.15127000
		C	3.69351200	-0.45583900	-0.99048400
		C	4.44951000	-0.13931100	0.22935400
		C	5.06539400	0.10002600	1.23032200
		H	5.60713400	0.32308600	2.11847700
		H	3.38461900	0.46877300	-1.47764200
		H	4.33186000	-1.00737100	-1.68277000
		C	-3.11987300	-1.25951100	1.03209100
		C	-3.85697400	-1.22833000	-0.23930600
		C	-4.45231900	-1.21783800	-1.28040600
		H	-4.97856200	-1.20052500	-2.20505100
		H	-3.63245200	-1.91681100	1.73603400
		H	-3.09930200	-0.25827900	1.46264100
		N	2.50281900	-1.24596800	-0.73390400
		H	2.61458600	-2.21112800	-0.46093700
		N	-1.75158500	-1.72410000	0.89370600
		H	-1.58737100	-2.71330800	0.77987800
ABPAT_TS_14	-1570.73138	N	-4.75383400	-3.05599300	-2.29397700

		N	-4.23517400	-3.00767600	-1.16391000
		N	-3.53720100	-1.64038500	0.53596400
		N	-3.78596800	0.72627900	0.35508200
		N	-5.20599200	-3.22558000	-3.29867100
		N	-4.50778100	-0.69156800	-1.41391600
		C	-4.32127800	0.51268200	-0.84136900
		C	-3.41407800	-0.39031400	0.99918100
		C	-4.09106800	-1.70228500	-0.66559700
		C	-2.20761500	-1.29480600	2.93484000
		C	-0.81225300	-1.49045900	2.46886200
		C	0.16290700	-2.06125400	1.98499700
		N	0.98755300	0.36858400	2.45268200
		N	1.71081300	-0.58533100	2.04496300
		N	2.90541200	0.89902000	0.66573300
		N	4.48974100	-0.04989700	-0.85014300
		N	-0.07858300	0.49847300	2.85477300
		N	3.22408400	-1.45903900	0.59783300
		C	4.13271700	-1.23737900	-0.37086600
		C	3.83915100	0.98133600	-0.29356000
		C	2.66281400	-0.35133200	1.05452100
		C	3.53983100	3.41304500	-0.19194500
		C	4.07049200	4.59725700	-0.86454800
		C	4.51223300	5.56353000	-1.41971400
		H	0.82151200	-2.77856700	1.54806000
		H	-2.77090400	-2.21419300	2.78257700
		H	-2.20570200	-1.05746700	3.99922900
		H	4.90025600	6.42560400	-1.90832900
		H	3.73279300	3.47699800	0.88294800
		H	2.45453800	3.36801100	-0.31714000
		C	-4.80008300	2.91532500	-1.01099600
		H	-4.75255100	3.64166300	-1.82382800
		H	-3.93596900	3.07502700	-0.36609600
		C	-6.03217900	3.12380400	-0.23666400
		C	-7.04792600	3.28713400	0.37982500
		H	-7.94516500	3.42811100	0.93404800
		C	5.87248400	-2.26635000	-1.76601100
		H	5.72169200	-1.44436400	-2.46584100
		H	5.93385400	-3.19128700	-2.34152300
		C	7.12999900	-2.05941600	-1.03315600
		C	8.15203800	-1.90659500	-0.42443400
		H	9.05743800	-1.76422800	0.11602200
		N	-2.89123900	-0.22404100	2.23630700
		H	-2.65290700	0.72791000	2.47315500
		N	4.70885500	-2.34455700	-0.90336700
		H	4.54933300	-3.19348900	-0.38158100
		N	4.15032700	2.21278800	-0.74004500
		H	4.87379600	2.28559700	-1.43796500
		N	-4.69720500	1.58583900	-1.58252000
		H	-5.25777500	1.36271400	-2.39144600
ABPAT_TS_15	-1570.73886	N	-3.95002000	-1.68165800	3.48016700

		N	-3.06661200	-1.33336100	2.67584500
		N	-2.63932300	-0.47009300	0.59812100
		N	-4.44035200	0.11350800	-0.85550300
		N	-4.64702500	-2.02456900	4.27958900
		N	-4.88657700	-0.79002900	1.29985800
		C	-5.26130800	-0.30195900	0.10259800
		C	-3.13824100	0.00686200	-0.54850600
		C	-3.57233400	-0.83990400	1.46249400
		C	-0.83774200	0.19617100	-1.40277300
		C	-0.48636500	-1.15046600	-1.90331100
		C	-0.59377900	-2.28233600	-2.37469000
		N	1.93516700	-2.15369400	-2.09234600
		N	1.67239000	-0.97248200	-1.71853900
		N	3.71528300	-0.88929500	-0.56034400
		N	4.18761500	1.08517400	0.70016000
		N	1.33481200	-3.04149400	-2.50971400
		N	2.14663100	0.89969500	-0.51800600
		C	3.00647000	1.54069100	0.29624800
		C	4.48642900	-0.13740200	0.23728200
		C	2.56744400	-0.29921300	-0.89215800
		C	6.11849900	-1.96559100	0.15846900
		C	7.43764700	-2.26266000	0.71343100
		C	8.51994200	-2.49813200	1.17194200
		H	-1.08448900	-3.14806000	-2.75793000
		H	-0.51637400	0.29811800	-0.36751500
		H	-0.30521500	0.95178900	-1.97936000
		H	9.48048500	-2.71402200	1.57582200
		H	6.15903200	-1.99164000	-0.93428100
		H	5.40254400	-2.73233700	0.46719700
		C	4.37021800	4.41494900	0.51029000
		C	5.06811600	5.03061000	-0.24636500
		H	5.69258800	5.57085600	-0.91736300
		C	3.49626100	3.66720700	1.42611900
		H	4.10787700	3.08912500	2.11886700
		H	2.89641600	4.36688500	2.01026400
		C	-7.16286100	0.45833400	-1.25333400
		H	-8.16010500	0.06126600	-1.44925200
		H	-6.54471200	0.26208300	-2.12940000
		C	-7.24705200	1.90897800	-1.03003100
		C	-7.32605000	3.08913400	-0.83128400
		H	-7.38886400	4.13693900	-0.65738400
		N	-6.59781700	-0.26583900	-0.13060200
		H	-7.17191700	-0.41837600	0.68516600
		N	-2.26378200	0.44554900	-1.48284800
		H	-2.67262700	0.66221700	-2.37947300
		N	2.59766000	2.75361000	0.74741500
		H	1.78812000	3.12908000	0.27683700
		N	5.67045000	-0.65841800	0.61043400
		H	6.26597300	-0.09177800	1.19345900
ABPAT_prod_14	-1570.8666	N	3.12000800	3.57481600	-0.14765500

		N	2.73238600	2.65473200	0.59552400
		N	2.90248300	0.42478000	1.08465600
		N	4.33561900	-0.98652100	-0.20434400
		N	3.39196700	4.47407700	-0.74747900
		N	4.17128800	1.33482900	-0.70605900
		C	4.65134000	0.09144200	-0.91106700
		C	3.45623900	-0.76111500	0.78484600
		C	3.31151900	1.40811400	0.29704600
		C	2.04632100	-1.74514100	2.53862700
		C	0.68177600	-1.68531500	1.92774900
		C	-0.04622500	-0.61707800	1.48918100
		N	-1.15316500	-2.52285600	1.12338100
		N	-1.18449400	-1.17911400	0.99565500
		N	-3.28359900	-1.25364800	-0.00834800
		N	-4.31841000	0.80008100	-0.65953300
		N	-0.03897700	-2.82557700	1.67935400
		N	-2.16949400	0.80642400	0.36885000
		C	-3.23650100	1.41280600	-0.19342300
		C	-4.28553100	-0.53544900	-0.54218100
		C	-2.28419100	-0.50535500	0.41397600
		C	-5.43275500	-2.67208200	-0.88864900
		C	-6.68127600	-3.14236500	-1.48495200
		C	-7.70906900	-3.51911800	-1.97351800
		H	0.13818100	0.44201100	1.47019900
		H	2.21885400	-0.87111200	3.16512700
		H	2.11409800	-2.63904000	3.15798800
		H	-8.61871600	-3.86270300	-2.40587600
		H	-5.37993400	-2.97534500	0.16079700
		H	-4.57812900	-3.13101900	-1.39220000
		C	6.29356400	-1.25033200	-2.14949900
		H	6.60371600	-1.28953900	-3.19483300
		H	5.64999200	-2.10883400	-1.95733200
		C	7.47786500	-1.32320900	-1.28179800
		C	8.44948300	-1.36527300	-0.57994100
		H	9.30694100	-1.40615100	0.04871500
		C	-4.30988900	3.57152500	-0.65594500
		H	-4.83173400	3.07797400	-1.47599000
		H	-3.94775900	4.53463100	-1.01863600
		C	-5.24280300	3.78412400	0.45972400
		C	-5.98998800	3.96379500	1.38038800
		H	-6.65610600	4.11761200	2.19579300
		N	3.11153100	-1.81635500	1.54761200
		H	3.42584300	-2.71628700	1.21830800
		N	-3.16056700	2.76132600	-0.29764000
		H	-2.40919700	3.18612800	0.22526000
		N	-5.34673900	-1.22224200	-0.99649600
		H	-6.12106300	-0.69522600	-1.36913000
		N	5.50942500	-0.04562100	-1.95258700
		H	5.85091100	0.82314000	-2.33581700
ABPAT_prod_15	-1570.861922	N	-6.53535500	-1.29885400	-0.61716500

		N	-5.54492500	-1.88082100	-0.13999400
		N	-3.33342600	-1.68949400	0.42259100
		N	-2.18363100	0.38178500	0.09753400
		N	-7.48624200	-0.88558500	-1.02714000
		N	-4.47561300	0.17334100	-0.51301900
		C	-3.31698500	0.85126100	-0.40471700
		C	-2.24378500	-0.90797600	0.49166100
		C	-4.39318600	-1.07654000	-0.07847600
		C	-0.93033900	-2.77050200	1.42249200
		C	-0.11875200	-3.60283600	0.50831800
		C	0.28449500	-4.60156200	-0.09266700
		N	2.30689800	-3.17365500	-0.53565900
		N	1.67692100	-2.27819000	0.10427600
		N	3.38154400	-0.74680200	-0.44352700
		N	2.99917600	1.55895500	0.05458700
		N	2.08627900	-4.27429200	-0.81714300
		N	1.36092700	-0.07296800	0.59557000
		C	1.81111500	1.19414700	0.52979700
		C	3.73904400	0.54330000	-0.41053400
		C	2.17896500	-0.97806500	0.07541300
		C	5.95390500	-0.12260400	-1.25107800
		C	6.74473500	-0.54846000	-0.08774900
		C	7.39294900	-0.87908500	0.86562100
		H	0.17323500	-5.59681100	-0.46318600
		H	-1.91195300	-3.24002100	1.51154100
		H	-0.45128900	-2.78879600	2.40506200
		H	7.96252100	-1.18057600	1.71225700
		H	6.61690300	0.29541800	-2.01028100
		H	5.44830900	-0.98643400	-1.68243700
		C	1.02323700	4.13190000	-0.42569100
		C	0.79517100	4.60434000	-1.50494500
		H	0.60748800	5.02065300	-2.46613600
		C	1.29855000	3.55955700	0.90062100
		H	2.35615700	3.69122800	1.13117000
		H	0.71112500	4.09383400	1.64726200
		C	-2.21210300	3.02118900	-0.64113700
		H	-2.32767900	3.89685600	-1.28097300
		H	-1.28801700	2.52185900	-0.93812900
		C	-2.10056600	3.45198000	0.76221500
		C	-2.04281300	3.78372800	1.91466200
		H	-2.00436100	4.08044900	2.93626100
		N	-1.11187700	-1.40617500	1.00610600
		H	-0.28290700	-0.80598300	0.94333700
		N	4.94799400	0.87134400	-0.92484800
		H	5.23933400	1.82175900	-0.75162600
		N	0.97978400	2.14857500	1.00449800
		H	0.01836600	1.87216400	1.17296400
		N	-3.32673000	2.12587900	-0.87435300
		H	-4.24112000	2.51047700	-1.05612900
APAPOT	-805.259461	N	1.05863300	2.88025600	0.03637100

4-azido-*N*-(prop-2-yn-1-yl)-6-(prop-2-yn-1-yloxy)-*s*-triazin-2-amine		N	-0.05181800	2.39316600	0.32526100
		N	-1.28802700	0.46854900	0.46058100
		N	-0.33503400	-1.62312100	-0.13625100
		N	2.00119400	3.42846800	-0.19072700
		N	0.95570200	0.37049900	-0.30408800
		C	0.78654000	-0.95536300	-0.42420000
		C	-1.32100200	-0.85073400	0.28850200
		C	-0.11677900	1.00689800	0.14534900
		C	-3.58600600	-0.72411400	0.95485700
		C	-4.21262700	-0.07969700	-0.19970900
		C	-4.75402300	0.43378600	-1.13755200
		H	-5.22318700	0.89800700	-1.97210000
		H	-3.30578500	0.02551200	1.69535300
		H	-4.27209900	-1.44340200	1.39948500
		C	3.16170600	-1.13179300	-1.02674100
		C	3.87512400	-1.02366500	0.25358000
		C	4.45349200	-0.94849200	1.30134900
		H	4.96503100	-0.87563200	2.23157400
		H	3.72525500	-1.77111700	-1.70761600
		H	3.08452900	-0.14416100	-1.48210100
		N	1.82482200	-1.68237800	-0.89579200
		H	1.71141100	-2.68240000	-0.81983700
		O	-2.44525000	-1.50198000	0.58189400
APAPOT_N_TS_14	-1610.47035	N	-4.07316900	-2.25484700	3.17051200
		N	-3.48421400	-2.29954800	2.07180100
		N	-3.41162900	-1.47552000	-0.06290600
		N	-5.01944000	0.13356700	-0.77329900
		N	-4.51144300	-2.30429700	4.19288000
		N	-5.08366200	-0.70480400	1.44147100
		C	-5.51882100	0.06455500	0.44459900
		C	-3.95356100	-0.66500600	-0.97434600
		C	-4.03220600	-1.44513600	1.10847800
		C	-2.12565200	-1.24424800	-2.50407300
		C	-0.98054600	-0.40527800	-2.09222700
		C	-0.37302900	0.55029300	-1.61253000
		N	1.48539600	-1.11472700	-2.36441900
		N	1.66982800	0.05361500	-1.91130800
		N	3.58889600	-0.67097900	-0.76048700
		N	4.57199200	0.86755700	0.77552600
		N	0.59912900	-1.74996400	-2.71402000
		N	2.64165000	1.49362600	-0.45577700
		C	3.61598700	1.70747600	0.42715100
		C	4.51285100	-0.31759800	0.14106300
		C	2.69442600	0.28538600	-1.00169600
		C	5.51295200	-2.53044300	-0.18476800
		C	6.65233900	-3.28735200	0.32923500
		C	7.58938200	-3.90131000	0.75544000
		H	-0.11626700	1.47601500	-1.14554600
		H	-2.07020200	-1.44063900	-3.57559600
		H	-2.06905300	-2.20334800	-1.98964100

		H	8.41883300	-4.45334800	1.12944900
		H	5.59525000	-2.42098100	-1.26988800
		H	4.58419500	-3.07343900	0.01089500
		C	-7.05830900	1.72174300	-0.23247500
		H	-8.03660500	2.03002800	0.13325300
		H	-7.16914300	1.20850300	-1.18849100
		C	-6.19148000	2.89097900	-0.38745900
		C	-5.51092100	3.87027600	-0.50786400
		H	-4.89708700	4.73298000	-0.61437400
		C	4.62046800	3.25058800	1.90679400
		H	4.77642000	2.44097400	2.62078300
		H	4.25474200	4.13350400	2.42889700
		C	5.87392700	3.56119700	1.21762600
		C	6.90114300	3.84905800	0.67121600
		H	7.81169200	4.09604100	0.17913700
		O	3.57168900	2.91109300	0.99899200
		N	5.46098000	-1.21969700	0.44463400
		H	6.17209700	-0.94549900	1.10458200
		O	-6.57467300	0.81484100	0.75928000
		N	-3.41479500	-0.64368400	-2.21351300
		H	-3.74134900	0.10856400	-2.80229500
APAPOT_N_TS_15	-1610.473433	N	-6.24760700	-1.23909600	-1.14207500
		N	-5.35522600	-1.78086000	-0.46136900
		N	-3.28701700	-1.52132500	0.48728100
		N	-2.10837900	0.53369900	0.21780100
		N	-7.11187800	-0.86697800	-1.73828100
		N	-4.25220000	0.26855600	-0.75127600
		C	-3.14048400	0.95382000	-0.47801100
		C	-2.23431000	-0.72092200	0.69679700
		C	-4.24299900	-0.95659500	-0.23640500
		C	-1.07012100	-2.51680100	1.89117400
		C	-0.41719000	-3.43058100	0.92722200
		C	-0.16113800	-4.45229400	0.28654900
		N	1.95647000	-3.21286500	-0.30140200
		N	1.47237600	-2.27740700	0.41269200
		N	3.13144500	-0.84643300	-0.45198700
		N	2.96966700	1.47234500	0.08748400
		N	1.60883600	-4.28029200	-0.57612500
		N	1.39304300	-0.06366100	0.95921700
		C	1.89055300	1.15792100	0.77513200
		C	3.56155800	0.41635600	-0.50318500
		C	2.04059700	-1.01697300	0.29267600
		C	5.53176400	-0.36026000	-1.75163500
		C	6.48810000	-0.86152000	-0.75547200
		C	7.27269100	-1.25541100	0.06132000
		H	-0.39585900	-5.42396800	-0.08897600
		H	-2.05978500	-2.92801400	2.10148700
		H	-0.48959700	-2.52283300	2.81543100
		H	7.96424600	-1.61224500	0.78714300
		H	6.07209400	0.03975800	-2.61085800

		H	4.90411100	-1.18086800	-2.09924500
		O	1.18539800	2.11689700	1.37049600
		C	1.32761900	3.94670700	-0.19171400
		C	1.10998700	4.38101300	-1.28806600
		H	0.92499800	4.75813300	-2.26609500
		C	1.59446900	3.46985000	1.16674500
		H	2.65596300	3.57811400	1.39536700
		H	0.99813300	4.04097000	1.87663900
		O	-3.11040500	2.18462500	-0.99456100
		C	-1.95429300	2.97598600	-0.71004400
		H	-1.99621000	3.79647800	-1.42532000
		H	-1.04598000	2.39528800	-0.87294300
		C	-1.96352200	3.50651300	0.65519100
		C	-1.98609400	3.96814400	1.76171800
		H	-2.01853800	4.36207700	2.74960500
		N	-1.21287500	-1.15503400	1.45142700
		H	-0.37773100	-0.56627500	1.44759200
		N	4.66531900	0.68373100	-1.23325100
		H	5.02726800	1.62083700	-1.13823900
APAPOT_N_prod_14	-1610.60323	N	-2.85115100	3.72010200	0.42567100
		N	-2.53529200	2.84802900	-0.40862200
		N	-2.82129500	0.67696400	-1.06766300
		N	-4.27270900	-0.76360400	0.16022600
		N	-3.05378100	4.57828800	1.10531400
		N	-3.99715700	1.49361500	0.83032500
		C	-4.51804400	0.27033700	0.93856400
		C	-3.41261200	-0.50267500	-0.84431400
		C	-3.16010600	1.61398900	-0.19252100
		C	-2.09525600	-1.40934400	-2.70273700
		C	-0.71728400	-1.45055400	-2.12137100
		C	0.07241900	-0.44790400	-1.63790900
		N	1.08521600	-2.42859400	-1.40650300
		N	1.18889900	-1.09678600	-1.20161000
		N	3.29262200	-1.33827800	-0.23719000
		N	4.43688700	0.61743100	0.49633100
		N	-0.05227800	-2.63950100	-1.95471800
		N	2.29257300	0.79794300	-0.49870300
		C	3.39297000	1.29884800	0.06715500
		C	4.33974400	-0.71192100	0.31205100
		C	2.33117200	-0.51789700	-0.60859700
		C	5.36774400	-2.90552200	0.75789000
		C	4.98350000	-3.40583800	2.08366200
		C	4.68209200	-3.80386300	3.17387000
		H	-0.05262600	0.61744300	-1.55450500
		H	-2.24508700	-0.48421300	-3.25755300
		H	-2.21520300	-2.25100800	-3.38405500
		H	4.40416600	-4.16110200	4.13693000
		H	6.35552700	-3.28670700	0.49317700
		H	4.65573700	-3.25653500	0.01071800
		C	-6.01044000	-1.13179700	2.11431100

		H	-6.42496400	-1.10681400	3.12100700
		H	-5.28528200	-1.94271900	2.03633700
		C	-7.08329400	-1.32097300	1.13681000
		C	-7.98625900	-1.48233800	0.36531900
		H	-8.78020100	-1.62223000	-0.32917700
		C	4.54620000	3.24826300	0.73444300
		H	4.86227100	2.73507000	1.64346400
		H	4.22514400	4.25979500	0.97796600
		C	5.64555600	3.28939300	-0.23033300
		C	6.54824900	3.36025000	-1.01551400
		H	7.34727200	3.41377600	-1.71635000
		O	3.37786600	2.62241200	0.19876100
		N	5.39716200	-1.45323700	0.69631000
		H	6.11135900	-0.95498600	1.20665100
		O	-5.35629500	0.12924800	1.96515200
		N	-3.13839800	-1.51185300	-1.69029800
		H	-3.48786100	-2.41940200	-1.42268700
APAPOT_N_prod_15	-1610.59902	N	-3.97573200	-2.88317800	2.47913700
		N	-3.04548600	-2.18389000	2.02890900
		N	-2.49181900	-0.45067600	0.64068200
		N	-4.19378400	0.68430200	-0.58501700
		N	-4.71328500	-3.57205000	2.94899500
		N	-4.76760700	-1.10385800	0.85978500
		C	-5.05216300	-0.13320600	-0.00695500
		C	-2.91437900	0.48368700	-0.21380500
		C	-3.47046500	-1.19973800	1.13115900
		C	-0.57071100	1.14046900	-0.56237400
		C	-0.03342700	0.07291600	-1.47422100
		C	-0.67654800	-0.66927300	-2.42208300
		N	1.36308400	-1.38574700	-2.45599000
		N	1.25098400	-0.40659400	-1.51829700
		N	3.45568400	-0.75385800	-0.87347700
		N	4.44696400	0.76185100	0.67495300
		N	0.21530600	-1.53716000	-2.99147800
		N	2.20228000	1.06957300	-0.02130200
		C	3.29266600	1.39445300	0.67882500
		C	4.48062300	-0.31328900	-0.13661600
		C	2.37160700	-0.01281000	-0.76225800
		C	5.79622000	-2.25789500	-0.87938100
		C	5.61824300	-3.39069200	0.03707500
		C	5.48255200	-4.30876900	0.79626500
		H	-1.71180300	-0.64297100	-2.71778400
		H	-0.37898100	0.87658100	0.47674000
		H	-0.07303500	2.09101300	-0.74784200
		H	5.35016900	-5.12646000	1.46431800
		H	6.78671100	-2.30439400	-1.33518400
		H	5.05220300	-2.30647600	-1.67478000
		O	3.13656800	2.47070600	1.44648500
		C	5.24803300	3.60893900	1.32075700
		C	6.04309000	4.19215400	0.63947300

		H	6.74865500	4.70266100	0.02780800
		C	4.27521200	2.93181100	2.17862100
		H	4.74781500	2.09802200	2.69901300
		H	3.86613700	3.63199100	2.90525300
		O	-6.34860000	-0.02693200	-0.29627800
		C	-6.74715700	1.03441000	-1.16496000
		H	-7.76717700	0.78340000	-1.45204700
		H	-6.11155400	1.05344800	-2.05110100
		C	-6.72179100	2.33804300	-0.49990700
		C	-6.73879600	3.41077600	0.03445500
		H	-6.74371900	4.36082600	0.51369600
		N	-1.99549200	1.30814900	-0.75734400
		H	-2.34172400	1.96599400	-1.43843800
		N	5.65143800	-0.97347100	-0.21260100
		H	6.35796600	-0.67950800	0.44558300
APAPOT_O_TS_14	-1610.469184	N	3.31228400	2.26597000	2.80897600
		N	2.80196200	1.20410000	2.40437100
		N	2.94666800	-0.50342700	0.88257500
		N	4.70900300	-0.55539000	-0.70905200
		N	3.67513200	3.21942200	3.25674400
		N	4.55994800	1.23619000	0.85129100
		C	5.13791100	0.58870600	-0.17887700
		C	3.61140600	-1.03513000	-0.13698100
		C	3.48385300	0.63079400	1.32305600
		C	1.93208700	-2.69762800	-0.17979500
		C	0.77589400	-1.96070700	-0.70618200
		C	0.12916600	-1.11997500	-1.32683300
		N	-1.66063200	-2.56457100	-0.10591900
		N	-1.88046000	-1.64138000	-0.94415800
		N	-3.79441800	-0.97321400	0.24691000
		N	-4.84440100	1.04942700	-0.44395000
		N	-0.75959900	-3.15168800	0.28487000
		N	-2.89830200	0.28555200	-1.56572800
		C	-3.89024000	1.14620000	-1.35196400
		C	-4.74233300	-0.03682900	0.34095300
		C	-2.91913400	-0.74470600	-0.72869700
		C	-5.82891400	-1.38406500	2.08578900
		C	-6.61187700	-2.41016600	1.38360300
		C	-7.26135600	-3.23640300	0.80611500
		H	-0.15757800	-0.29456300	-1.94128000
		H	1.91525500	-2.68701000	0.91010100
		H	1.91263700	-3.72776900	-0.53202200
		H	-7.82928000	-3.97410300	0.29078300
		H	-6.31560000	-1.13209500	3.02910700
		H	-4.83706400	-1.77536700	2.31229300
		C	7.09072900	0.50108100	-1.66914200
		H	7.57641300	1.25262400	-2.29359100
		H	6.46309500	-0.11847700	-2.30969600
		C	8.10987600	-0.33592000	-1.02153400
		C	8.94641600	-1.00416700	-0.48131000

		H	9.68285200	-1.60582100	-0.00398000
		C	-4.87752800	3.20063900	-1.97236000
		H	-5.86288300	2.74457200	-1.86937900
		H	-4.84645200	3.80294300	-2.87909100
		C	-4.58639800	4.03685600	-0.80675000
		C	-4.34968600	4.75168100	0.12576800
		H	-4.13641700	5.37658400	0.96019100
		O	-3.88759900	2.19239500	-2.17844900
		N	-5.66923400	-0.16292900	1.31649200
		H	-6.43998400	0.48595000	1.26114900
		N	6.22733500	1.18100700	-0.71985500
		H	6.60246300	1.95202400	-0.18764200
		O	3.17463600	-2.17546200	-0.66168400
APAPOT_O_TS_15	-1610.47229	N	-3.67761600	-2.51054600	2.73824800
		N	-2.80104800	-1.98197400	2.02839100
		N	-2.37403200	-0.45255400	0.37562600
		N	-4.13834900	0.81571800	-0.58502000
		N	-4.36837500	-3.05117700	3.42517900
		N	-4.60162800	-0.77848100	1.12813000
		C	-4.96515600	0.16485700	0.23584600
		C	-2.86609300	0.45426000	-0.45996300
		C	-3.30377800	-1.02393600	1.13768500
		C	-0.65129200	0.72885800	-1.24319600
		C	-0.44121200	-0.53360100	-1.97182300
		C	-0.63844400	-1.55452500	-2.62726100
		N	1.89974900	-1.66059500	-2.38970700
		N	1.73087600	-0.55025700	-1.80318500
		N	3.86094800	-0.70917600	-0.82359400
		N	4.48154300	1.00887400	0.70553900
		N	1.22502600	-2.41436500	-2.93577100
		N	2.36049100	1.07917000	-0.35458100
		C	3.30022600	1.54582300	0.46347600
		C	4.71384300	-0.12477200	0.02029100
		C	2.71035300	-0.05182500	-0.95853700
		C	6.23248700	-2.03290300	-0.27704000
		C	5.72978000	-3.09080500	0.61007600
		C	5.32401600	-3.94537300	1.34698700
		H	-1.19448200	-2.30448600	-3.14231400
		H	-0.29086200	0.64563100	-0.21943400
		H	-0.12314100	1.54228700	-1.73513600
		H	4.95503500	-4.70489900	1.99450000
		H	7.31539400	-2.12019300	-0.37655500
		H	5.79197600	-2.14958100	-1.26726600
		C	4.98887400	3.95537400	1.17694300
		C	5.84322200	4.54021400	0.57308500
		H	6.60205000	5.05129500	0.02976600
		C	3.93594000	3.27996500	1.93708600
		H	4.37334000	2.53428500	2.60202200
		H	3.37541100	4.00752400	2.52227900
		C	-6.78712200	1.47093300	-0.74881000

		H	-6.53393600	1.19570400	-1.77642100
		H	-6.31183600	2.43632700	-0.55372000
		C	-8.23656200	1.58717900	-0.60330500
		C	-9.42528500	1.67613200	-0.47721200
		H	-10.48079200	1.76066800	-0.37103400
		O	-2.03323300	1.10002800	-1.26965400
		N	-6.27305200	0.46953000	0.17284600
		H	-6.89978500	-0.01966600	0.79230900
		O	2.95950400	2.67250300	1.09073900
		N	5.92632200	-0.69578900	0.19957400
		H	6.47269600	-0.30892500	0.95461500
APAPOT_O_prod_14	-1610.603243	N	-2.81302700	3.59787400	0.12912000
		N	-2.47054500	2.65221400	-0.60676100
		N	-2.74394700	0.43139600	-1.08445400
		N	-4.27469100	-0.89622500	0.15420100
		N	-3.03868700	4.51318300	0.72220400
		N	-4.01125200	1.41616700	0.66298900
		C	-4.56329000	0.20017600	0.85214500
		C	-3.35582400	-0.71270100	-0.78704600
		C	-3.12229900	1.44723600	-0.31258300
		C	-2.04112700	-1.68753500	-2.49971200
		C	-0.66171200	-1.64007700	-1.93589100
		C	0.08362700	-0.59430600	-1.46997400
		N	1.23026200	-2.50854200	-1.31618700
		N	1.25541700	-1.17386200	-1.09094900
		N	3.41028700	-1.29116000	-0.22304800
		N	4.45403100	0.72200500	0.50466700
		N	0.08879000	-2.78511000	-1.82041400
		N	2.25908100	0.77731800	-0.38980400
		C	3.34853900	1.33959200	0.13780300
		C	4.43678000	-0.60714400	0.29527500
		C	2.38049100	-0.53064400	-0.53294200
		C	5.62023700	-2.73627500	0.65497300
		C	5.30822200	-3.28028300	1.98246300
		C	5.06428800	-3.71344500	3.07361500
		H	-0.10230000	0.46033500	-1.37060800
		H	-2.24807100	-0.81614100	-3.11858200
		H	-2.15092900	-2.60079300	-3.08006900
		H	4.83739700	-4.10355200	4.03729300
		H	6.62176000	-3.04906400	0.35489600
		H	4.90962400	-3.12076900	-0.07688900
		C	-6.30708800	-1.06270700	2.03762900
		H	-6.57905300	-1.13175600	3.09208000
		H	-5.71967700	-1.94393800	1.77992400
		C	-7.52379500	-1.02466500	1.21516800
		C	-8.52027700	-0.97609700	0.54976400
		H	-9.39989500	-0.94037900	-0.04789500
		C	4.40094900	3.34874100	0.79441100
		H	4.79482800	2.83997500	1.67507500
		H	4.02632700	4.33149100	1.07629400

		C	5.44631600	3.48260100	-0.22066900
		C	6.30215400	3.62865000	-1.04684400
		H	7.06020500	3.74818800	-1.78408300
		O	3.25165700	2.65668800	0.30077400
		N	5.55618000	-1.28407200	0.61786800
		H	6.25661300	-0.74989100	1.11065600
		N	-5.46356500	0.10584500	1.85665800
		H	-5.76351700	0.98726500	2.24595800
		O	-3.05025800	-1.79880000	-1.47979600
APAPOT_O_prod_15	-1610.59956	N	-3.44884900	2.87441700	-2.41288400
		N	-2.60210200	2.09374000	-1.93646300
		N	-2.24747000	0.31137800	-0.54161500
		N	-4.06265100	-0.70865400	0.60059100
		N	-4.10943100	3.62695400	-2.90053200
		N	-4.44657400	1.15281900	-0.83354700
		C	-4.85430400	0.19206800	0.01747500
		C	-2.78163500	-0.58423900	0.27938800
		C	-3.14460600	1.14571900	-1.06150000
		C	-0.57546000	-1.33926500	0.66805400
		C	-0.07210900	-0.27049800	1.58876700
		C	-0.72844000	0.40748900	2.57448600
		N	1.26837400	1.24061100	2.56303800
		N	1.18184100	0.27890600	1.60566300
		N	3.34038700	0.74778800	0.88340800
		N	4.36670600	-0.73408400	-0.67508100
		N	0.13042900	1.31325300	3.13596600
		N	2.16783000	-1.15934700	0.09997100
		C	3.25069100	-1.43138500	-0.63340100
		C	4.36486400	0.35333500	0.12010000
		C	2.29894300	-0.05697900	0.81903600
		C	5.58444700	2.38393900	0.78808400
		C	5.26467200	3.48406400	-0.13000500
		C	5.01335600	4.37561100	-0.89134500
		H	-1.74795000	0.30260900	2.90548400
		H	-0.34724100	-1.10879200	-0.36966900
		H	-0.14944700	-2.30861200	0.91762800
		H	4.77905400	5.16914000	-1.56047800
		H	6.59485500	2.51229200	1.17966900
		H	4.88964400	2.39183900	1.62816400
		C	5.30640300	-3.53999300	-1.31579600
		C	6.15489100	-4.06833800	-0.65453400
		H	6.90684900	-4.53046800	-0.05993000
		C	4.26903200	-2.93019800	-2.14810100
		H	4.67624400	-2.07819900	-2.69371100
		H	3.87650500	-3.66206300	-2.85228700
		C	-6.79967000	-0.92900100	1.01882000
		H	-7.68846000	-0.55124600	1.52660800
		H	-6.10052400	-1.28214200	1.77672500
		C	-7.17084100	-2.04256600	0.13544200
		C	-7.48171200	-2.93957600	-0.59718900

		H	-7.74929900	-3.74068300	-1.24439700
		O	-1.98335100	-1.47659100	0.86384300
		N	-6.17383600	0.17361200	0.31007100
		H	-6.74812300	0.76955100	-0.26746200
		O	3.13085400	-2.52412500	-1.38350800
		N	5.49816000	1.08027700	0.14927100
		H	6.19703700	0.81969300	-0.53071600

Table S2. Imaginary frequencies of the transition states AAC reactions ABPOT, ABPAT and APAPOT calculated at M06-2X/6-311++G(d,p) level of theory.

Compound	Imaginary frequencies, cm^{-1}
ABPOT_TS_14	-444.21
ABPOT_TS_15	-439.79
ABPAT_TS_14	-471.46
ABPAT_TS_15	-457.23
APAPOT_N_TS_14	-456.60
APAPOT_N_TS_15	-451.24
APAPOT_O_TS_14	-451.99
APAPOT_O_TS_15	-441.85

References

[S1] A. V. Shastin, A. O. Petrov, G. V. Malkov and T. N. Gavrishova, *Chem. Heterocycl. Compd.*, 2021, **57**, 1.

[S2] M. Chioua, A. González-Camuñas, M. T. Catarozzo, S. Alcaro, F. Ortuso, M. Yáñez and J. Marco-Contelles, *ChemistrySelect*, 2019, **4**, 8334.

[S3] S. N. Danilov, L. N. Yastrebov, A. L. Galka and A. S. Zanina, *Zh. Org. Khim.*, 1979, **15**, 1146.

[S4] G. V. Malkov, A. V. Shastin, Y. I. Estrin, E. R. Badamshina and Y. M. Mikhailov, *Russ. Chem. Bull.*, 2011, **60**, 1940.