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Supporting information

Accelerating the discovery of energetic melt-castable materials by a high-throughput virtual screening and experimental approach

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Methods

1. Machine learning

We gathered more than 1000 data of energetic materials from literatures for training machine learning models covering density, detonation velocity, detonation pressure, melting point and decomposition temperature. To improve the accuracy of T_m models, non-energetic compounds (around 4500 samples) from Molmall database[1] was also involved. Features (molecular descriptors) including custom descriptors and Electrotopological fingerprint were extracted by RDkit library[2]. Machine-learning models were trained by kernel ridge regression (KRR) algorithm implemented in Scikit-learn package[3]. In KRR algorithm, prediction value (y*) can be expressed as the weighted average (α) of inner product between the new sample (x*) and training samples (x) given a kernel function (k) (1). Thus, the learning process is indeed calculating coefficient matrix (α) by equation (2), in which X, Y, λ and I are sample matrix, label matrix, regularization parameter and identity matrix, respectively. Hyper-parameters including kernel function were tuned up by grid-search method and 5-fold cross-validation. Coefficient of determination (R^2) was chosen as refit score (3). Apart from R^2, mean absolute error was also calculated for evaluating the model accuracy (4). Feature importance were acquired after training the T_m model by random forest algorithm in Scikit-learn.

$$y^* = \sum_{i=1}^{N} \alpha_i k(x^*, x_i) \tag{1}$$

$$\alpha \triangleq (k(X, X^T) + \lambda I)^{-1} Y \tag{2}$$

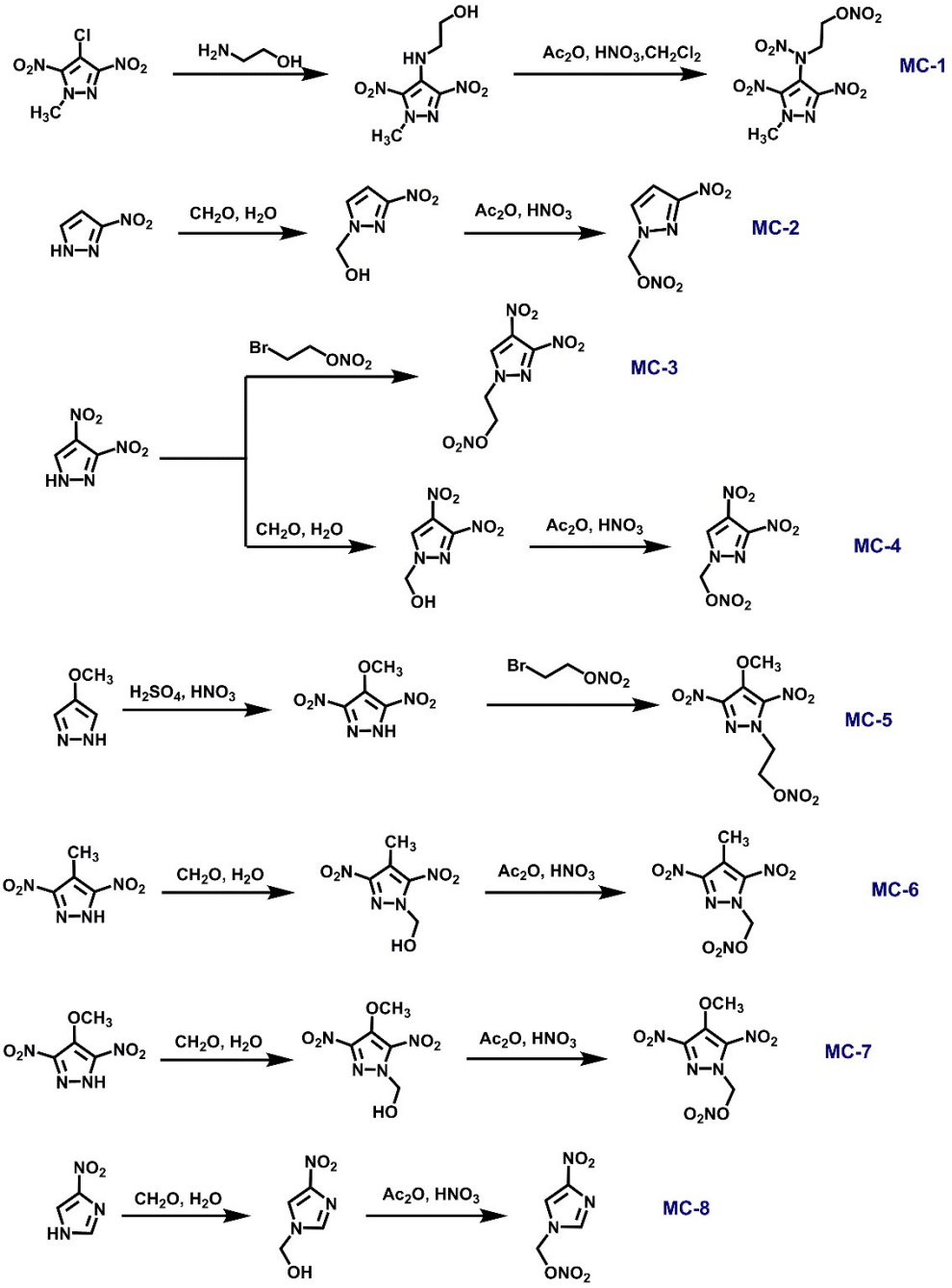
$$R^2 = 1 - \frac{\sum_{i=1}^{N} (y_i - y_i^*)}{\sum_{i=1}^{N} (y_i - \bar{y})} \tag{3}$$

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - y_i^*| \tag{4}$$

2. Experimental

Caution! Though no accidental explosion happened in our preparing process, the compounds reported here are metastable substance that may be triggered by mechanical or chemical stimuli. Safety equipment such as protective gloves and coats, face shield and explosion-proof baffle are recommended.

Synthetic routes of compounds MC-1 to MC-8



Synthesis of 2-((1-methyl-3,5-dinitro-1H-pyrazol-4-yl) (nitro) amino) ethyl nitrate (MC-1):

4-(2'-hydroxyethyl)amino-3,5-dinitro-1-methylpyrazole: 1.0 g (4.9 mmol) 4-chloro-

1-methyl-3,5-dinitro-1H-pyrazole[4] and 0.7g (11.5 mmol) ethanolamine were dissolved into 20 mL DMF, then the solution was stirred at 100 °C for 2 hours. Subsequently the reaction product was poured into ice, the precipitate filtered and recrystallized from ethanol to form yellow crystals, yield: 0.62 g (54.9 %).

2-((1-methyl-3,5-dinitro-1H-pyrazol-4-yl)(nitro)amino)ethyl nitrate: 0.5 g (2.2 mmol) 4-(2'-hydroxyethyl)amino-3,5-dinitro-1-methylpyrazole was added in portions into a mixture of 2 mL anhydrous dichloromethane, 1.5 mL fuming nitric acid and 1.3 mL acetic anhydride at 0 °C. After stirring for 3 hours, the reaction was quenched by 60 mL crashed ice and the milky solid is filtered out. The product was washed with water and dried at room temperature with a yield of 0.42 g (60.4%).^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 4.41 (br. s, 3H), 4.59 (br. s, 1H), 4.66 (br. s, 1H),4.87 (br. s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 43.80, 50.78, 70.51, 111.81,141.26,146.04. IR (KBr, cm^{-1}):2908.80, 1650.58, 1603.12, 1530.69, 1443.79, 1417.24, 1338.43, 1270.74, 1146.08, 1123.49, 1020.92, 967.12, 888.12, 842.95, 784.82, 666.01, 491.64. Elemental analysis (%) calcd for MC-1: C 22.44, H 2.20, N 30.53; found: C 22.32, H 2.43, N 30.12.

Synthesis of (3-nitro-1H-pyrazol-1-yl) methyl nitrate (MC-2):

(3-nitro-1H-pyrazol-1-yl) methanol: 1.0 g (8.8 mmol) 3-nitro-1H-pyrazole was added to 30 mL water. Afterwards, 1.5 mL formaldehyde solution and three drops of concentrated hydrochloric acid were added to the reaction mixture. The solution gradually turned into clear and the reaction was stirred for another 48 h at room temperature. After extracted with ethyl acetate, vacuum distillation and dried in air to give (3-nitro-1H-pyrazol-1-yl) methanol as white solid, yield: 1.1 g (87.0%).

(3-nitro-1H-pyrazol-1-yl) methyl nitrate: 1.0g (7.0 mmol) (3-nitro-1H-pyrazol-1-yl) methanol was partially added into the stirred mixture of acetic anhydride (2.0 mL) and fuming nitric acid (1.0 mL) at 0 °C. After several hours, the reaction was quenched with ice water and the precipitate was filtered as white solid product, yield: 0.65g (49.4%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 6.68 (br. s, 2H), 7.16 (br. s, 1H), 8.32 (br. s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 79.52, 103.99, 137.08, 157.26. IR (KBr, cm^{-1}):3156.53, 3135.78, 3058.16, 2937.50, 1666.44, 1556.89, 1512.59, 1383.56, 1306.21, 1288.73, 1235.66, 1181.74, 1047.87, 992.31, 956.1, 822.99, 792.63, 757.07, 656.40, 636.28, 446.06, 414.85. Elemental analysis (%) calcd for MC-2: C 25.54, H

2.14, N 29.79; found: C 25.78, H 1.92, N 29.43.

Synthesis of (3-nitro-1H-pyrazol-1-yl) methyl nitrate (MC-3): 1.6 g (10.0 mmol) 3,4-dinitro-1H-pyrazole[5] was added into 20 mL of methanol. Afterwards, the equimolar amount of KOH and 18-Crown-6 were added to the reaction mixture and then 2.0g of 2-bromoethyl nitrate[5] was added, the reaction was stirred for another 48 h at 80 °C. Then the product was extracted with ethyl acetate (3×40 mL) and purified by column chromatography (petroleum ether: ethyl acetate = 10:1) as slight yellow crystals, yield: 1.0 g (40.5%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 4.71 (br. s, 2H), 4.98 (br. s, 2H) , 9.25 (br. s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 51.51, 70.88, 126.73, 135.16, 147.65. IR (KBr, cm^{-1}):3158.12, 2981.57, 2911.92, 2665.76, 2563.01, 1642.94, 1549.48, 1519.64, 1461.50, 1359.91, 1338.14, 1284.27, 1150.06, 1121.82, 1031.45, 904.86, 863.66, 809.81, 750.37, 715.03, 596.53, 574.10, 503.42, 455.13. Elemental analysis (%) calcd for MC-3: C 24.30, H 2.04, N 28.34; found: C 24.15, H 2.02, N 28.53.

Synthesis of (3,4-dinitro-1H-pyrazol-1-yl) methyl nitrate (MC-4):

(3,4-dinitro-1H-pyrazol-1-yl)methanol: 1.6 g (10.0 mmol) 3,4-dinitro-1H-pyrazole was added to 30 mL water. Afterwards, 1.4 ml formaldehyde solution and three drops of concentrated hydrochloric acid were added to the reaction mixture. The solution gradually turned into clear and the reaction was stirred for another 48 h at room temperature. After extracted with ethyl acetate, vacuum distillation and dried in air to give (3,4-dinitro-1H-pyrazol-1-yl)methanol as pale yellow liquid, yield: 1.49 g (79.0%).

(3,4-dinitro-1H-pyrazol-1-yl) methyl nitrate: 1.4 g (7.5 mmol) (3,4-dinitro-1H-pyrazol-1-yl)methanol was partially added into the stirred mixture of acetic anhydride (2 mL) and fuming nitric acid (1.0 mL) at 0 °C. After 5 hours, the reaction was quenched with ice water and the precipitate was filtered as white solid product, yield: 1.2 g (68.7%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 6.65 (br. s, 2H), 9.40 (br. s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm:79.30, 127.48, 136.73, 148.52. IR (KBr, cm^{-1}):3168.09, 3156.11, 3064.82, 3006.94, 2934.07, 1663.21, 1649.55, 1560.86, 1525.86, 1462.55, 1365.90, 1312.85, 1285.78, 1236.99, 1148.24, 1121.16, 971.17, 864.45,

837.53, 809.80, 768.07, 662.61, 624.08, 584.54, 496.97. Elemental analysis (%) calcd for MC-4: C 20.61, H 1.30, N 30.05; found: C 20.41, H 1.46, N 29.95.

Synthesis of 2-(4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) ethyl nitrate (MC-5)

4-methoxy-3,5-dinitro-1H-pyrazole: 1.0 g (10.2 mmol) 4-methoxy-1H-pyrazole was dissolved into 2mL 98% concentrated sulfuric acid at 0 ^{o}C, then 1 mL 68% concentrated nitric acid were slowly added into above solution. After 5 hours, the reaction was quenched with ice water and the precipitate was filtered as white solid product, yield: 1.8 g (96.0%).

2-(4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) ethyl nitrate: 0.5 g (2.7 mmol) 4-methoxy-3,5-dinitro-1H-pyrazole was added into 20 mL of methanol. Afterwards, the equimolar amount of KOH and 18-Crown-6 were added to the reaction mixture and then 0.6 g of 2-bromoethyl nitrate[6] was added, the reaction was stirred for another 48 h at 80 °C. Then the product was extracted with ethyl acetate (3×40 mL) and purified by column chromatography (petroleum ether: ethyl acetate = 12:1) as white crystals, yield: 0.22 g (30.3%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 4.01(br. s, 3H), 4.99 (br. s, 2H) , 5.01 (br. s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 52.64, 63.72, 70.69, 135.96, 138.56, 144.80. IR (KBr, cm^{-1}):3052.54, 3003.29, 2949.44, 1647.63, 1610.54, 1533.41, 1451.09, 1334.12, 1284.12, 1233.20, 1115.43, 1073.24, 1003.68, 981.16, 959.01, 888.76, 850.65, 766.59, 683.39, 594.00, 525.79, 451.88. Elemental analysis (%) calcd for MC-5: C 26.00, H 2.55, N 25.27; found: C 26.17, H 2.68, N 25.04.

Synthesis of (4-methyl-3,5-dinitro-1H-pyrazol-1-yl) methyl nitrate (MC-6):

(4-methyl-3,5-dinitro-1H-pyrazol-1-yl)methanol: 1.0 g (5.8 mmol) 4-methyl-3,5-dinitro-1H-pyrazole[7] was as added to 30 mL water. Afterwards, 1.4 ml formaldehyde solution and three drops of concentrated hydrochloric acid were added to the reaction mixture. The reaction was stirred for another 48 h at room temperature. After extracted with ethyl acetate, vacuum distillation and dried in air to (4-methyl-3,5-dinitro-1H-pyrazol-1-yl)methanol as white solid, yield: 0.88 g (75.2%).

(4-methyl-3,5-dinitro-1H-pyrazol-1-yl) methyl nitrate: 1.0 g (4.9 mmol) (4-methyl-3,5-dinitro-1H-pyrazol-1-yl)methanol was partially added into the stirred mixture of acetic anhydride (2.5 mL) and fuming nitric acid (1.0 mL) at 0 °C. After 3 hours, the

reaction was quenched with ice water and the product was separated by column chromatography (petroleum ether: ethyl acetate =10:1) as white solid, yield: 0.75 g (61.5%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 2.56 (br. s, 3H), 6.90 (br. s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 10.10, 79.17, 115.96, 144.64, 152.71. IR (KBr, cm^{-1}):3059.36, 2940.07, 1698.87, 1671.33, 1596.81, 1540.15, 1435.60, 1415.17, 1358.62, 1333.30, 1279.56, 1109.01, 1029.79, 971.84, 879.96, 818.93, 790.46, 637.19. Elemental analysis (%) calcd for MC-6: C 24.30, H 2.04, N 28.34; found: C 24.46, H 2.23, N 28.02.

Synthesis of (4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) methyl nitrate (MC-7):

(4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) methanol: 1.0 g (5.3 mmol) 4-methoxy-3,5-dinitro-1H-pyrazole was added to 20 mL water. Afterwards, 1 mL formaldehyde solution and three drops of concentrated hydrochloric acid were added to the reaction mixture. The reaction was stirred for 48 h at 80 ^{o}C. After extracted with ethyl acetate, vacuum distillation and dried in air to give (4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) methanol as pale yellow solid, yield: 0.5 g (43.1%).

(4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) methyl nitrate: 1.0 g (4.6 mmol) (4-methoxy-3,5-dinitro-1H-pyrazol-1-yl) methanol was partially added into the stirred mixture of acetic anhydride (2.5 mL) and fuming nitric acid (1.0 mL) at 0 °C. After 3 hours, the reaction was quenched with ice water and the product was separated by column chromatography (petroleum ether: ethyl acetate = 6:1) as white solid, yield: 1.1 g (91%). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 4.03 (br. s, 3H), 6.86 (br. s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 63.84, 79.62, 136.24, 138.42, 146.13. IR (KBr, cm^{-1}):3073.25, 3009.63, 2943.11, 1669.05, 1609.15, 1529.19, 1459.34, 1336.41, 1284.12, 1255.04, 1054.60, 980.20, 899.35, 837.33, 791.82, 748.23, 683.56, 634.03, 526.17. Elemental analysis (%) calcd for MC-7: C 22.82, H 1.92, N 26.62; found: C 22.51, H 2.03, N 26.33.

Synthesis of (4-nitro-1H -imidazol-1-yl) methyl nitrate (MC-8):

(4-nitro-1H-imidazol-1-yl) methanol: 1.5 g (13.3 mmol) 4-nitro-1H-imidazole was added to 45 mL water. Afterwards, 2 mLformaldehyde solution and three drops of concentrated hydrochloric acid were added to the reaction mixture. The reaction was

stirred for 48 h at 80°C. After extracted with ethyl acetate, vacuum distillation and dried in air to give (4-nitro-1H-imidazol-1-yl) methanol as white solid, yield: 0.8 g (42.1%). **(4-nitro-1H-imidazol-1-yl) methyl nitrate**: 1.0 g (7.0 mmol) (4-nitro-1H-imidazol-1-yl) methanol was partially added into the stirred mixture of acetic anhydride (2.0 mL) and fuming nitric acid (1.0 mL) at 0 °C. After 4 hours, the reaction was quenched with ice water and the product was separated by column chromatography (petroleum ether: ethyl acetate = 4:1) as white solid, yield: 0.71 g (54.0 %). ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm: 6.55 (br. s, 2H), 8.14 (br. s, 1H), 8.59 (br. s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 75.34, 122.30, 138.95, 147.89. IR (KBr, cm^{-1}):3148.88, 3081.38, 3052.08, 2932.60, 2767.18, 1663.41, 1546.33, 1493.96, 1432.49, 1379.15, 1358.29, 1289.46, 1228.69, 1146.16, 1042.31, 985.64, 964.25, 880.39, 822.03, 755.00, 655.67, 616.89, 587.28, 454.11, 411.02. Elemental analysis (%) calcd for MC-8: C 25.54, H 2.14, N 29.79; found: C 25.75, H 2.31, N 29.43.

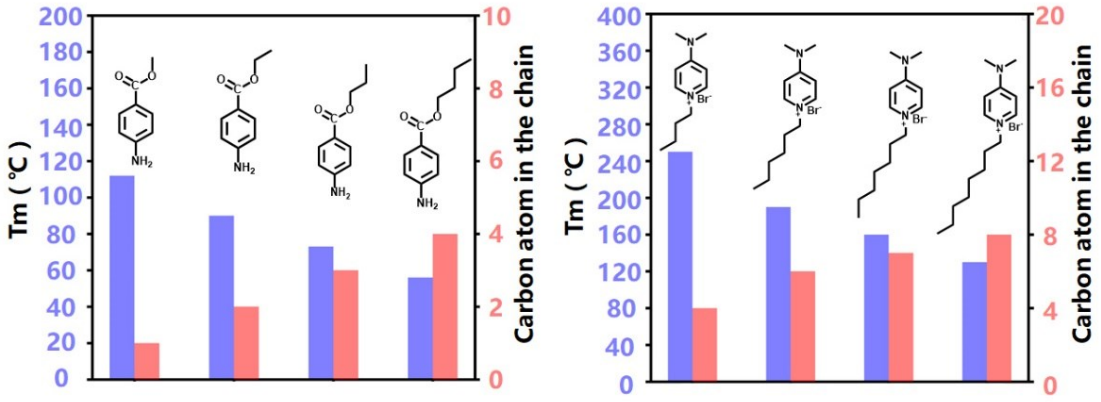
Characterization

^{1}H and ^{13}C spectra were collected on a Bruker Avance Neo 400 NMR spectrometer operating at 400 and 100 MHz, respectively. Infrared (IR) spectra were recorded using a Bruker FTIR instrument with KBr pellets (4000-500 cm^{-1}). Elemental analysis was performed on a varioMICRO cube elemental analyzer. Impact and friction sensitivity measurements were launched using a standard BAM Fall hammer and a BAM friction tester. Single crystal X-ray diffraction data was collected on a XtaLAB diffractometer with Cu-Kα monochromated radiation (λ=1.54178 Å). The crystal structures were solved by direct methods. The structures were refined on F2 by full-matrix least-squares methods using the SHELXTL script package[8]. All non-hydrogen atoms were refined anisotropically. The thermal properties of compounds were measured by METLLER TOLEDO 2 TGA/DSC synchronous thermal analyzer at a heating rate of 10 °C min^{-1}.

The heat of formation of compound was calculated by Gaussian09 (RevD.01) program[9].

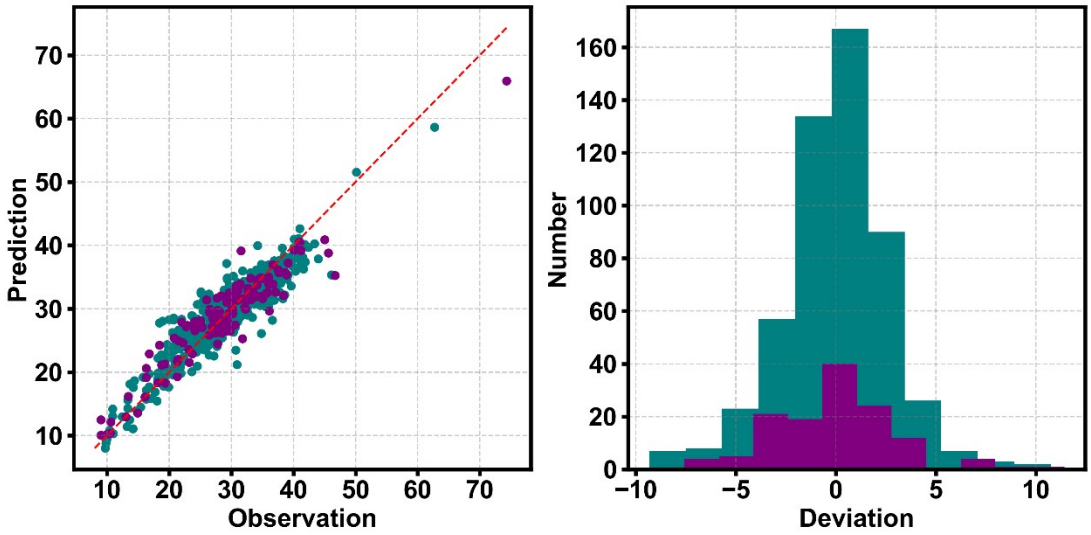
The standard detonation properties were calculated by Explo5 (version 6.02) software.

Figure S1. Effect of side-chain length (carbon atom numbers) on the melting point of neutral and ionic compounds.



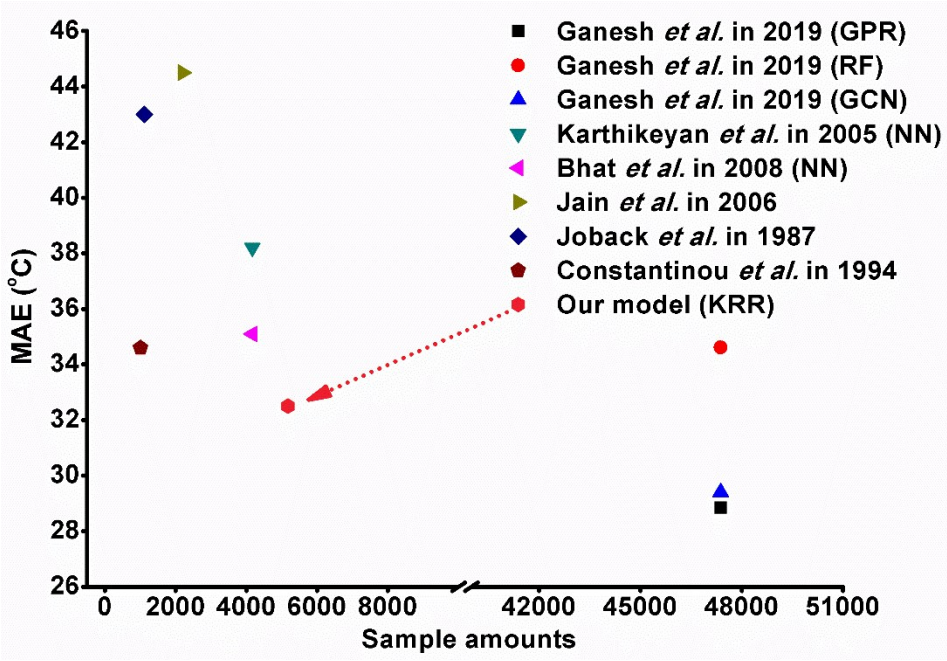
As shown in Figure S1, no matter the compounds are neutral and ionic, there is a general rule that the melt points decrease with increasing side-chain length. Therefore, we think it will be an effective way to introduce some reasonable flexible alkyl chains for developing new energetic melt-castable materials.

Figure S2. Scatter plot of prediction value versus observation value and error distribution for detonation pressure (P) model.



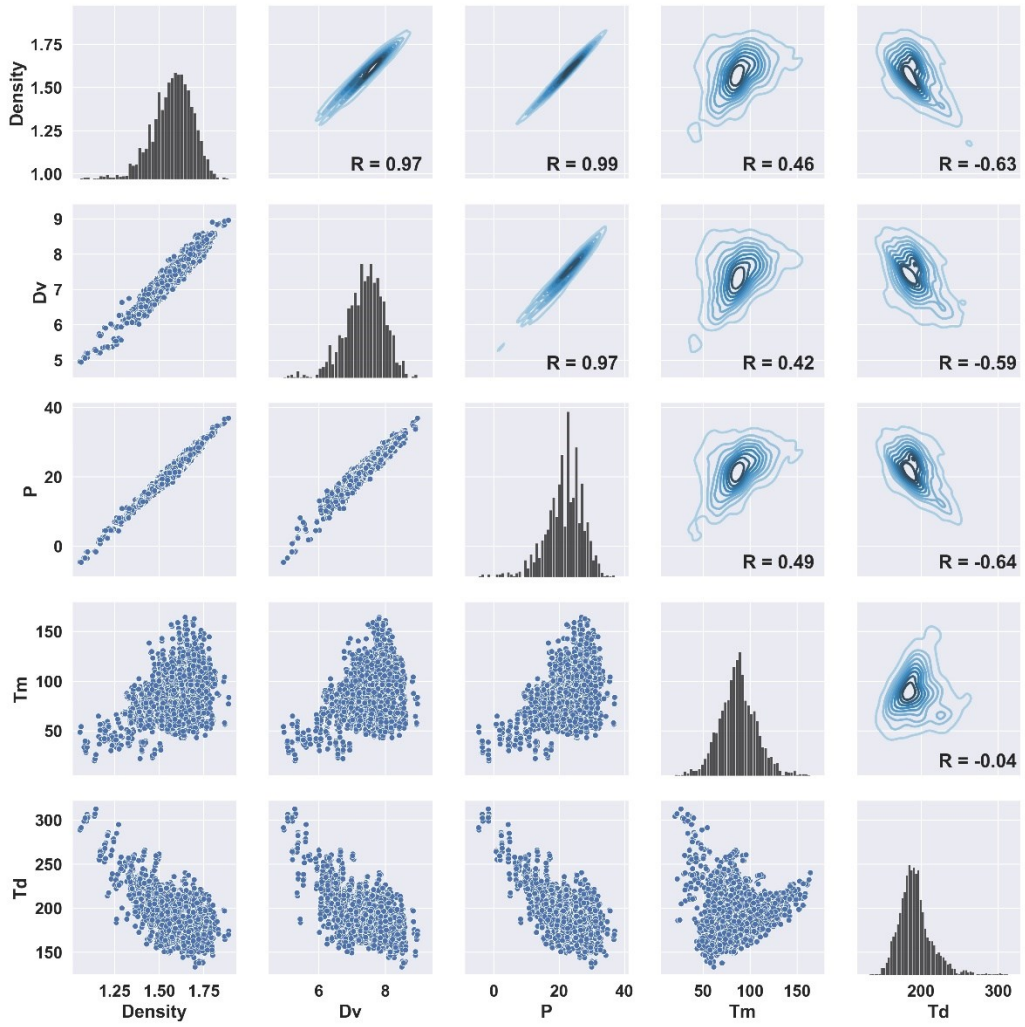
The R2 and MAE of P model on test set are 0.82, 2.379 GPa, respectively. Considering the strong correlation between Dv and P (0.97, Figure S4) and convenient layout, this figure was showed separately in supporting information.

Figure S3. Comparison of prediction accuracy for T_m models.



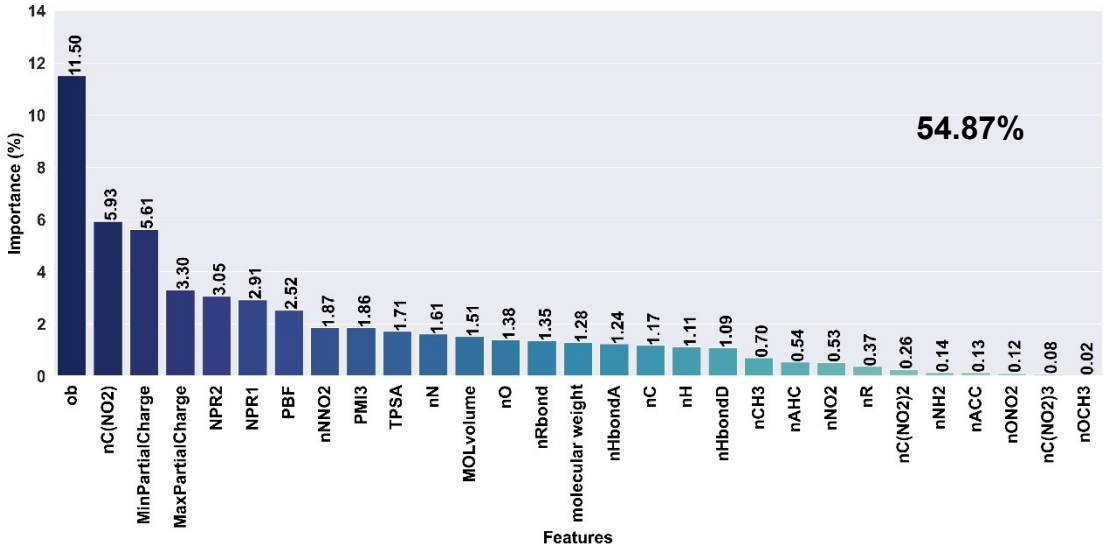
In Figure S3, we compared our T_m model with some reported results[10-15]. Our model has reached to a desirable accuracy.

Figure S4. Property space represented by pair-grid plot.



The diagonal is the sample distribution histogram, the upper and lower off-diagonal are kernel density estimation (KDE) plot (R is the correlation coefficient) and scatter plot that reveal the correlations between different properties. From the diagonal, we can see that the property space is complete and reasonable, since it covers large property range that could provide enough potential molecule for screening. In KDE and scatter plot we can see strong positive correlation between Density and D_v (or P) because R is larger than 0.97. Meanwhile, T_d shows a negative correlation with Density (R = -0.63), D_v (R = -0.59) and P (R = -0.64). The phenomenon is accordance with our common sense that density can evidently impact the energy of energetic material and the thermal stability usually decreases as the energy increases. It must be noted that the property models are mutually independently trained. These results prove that the trained property models are convinced since the knowledge revealed in the models obeys our chemical intuition.

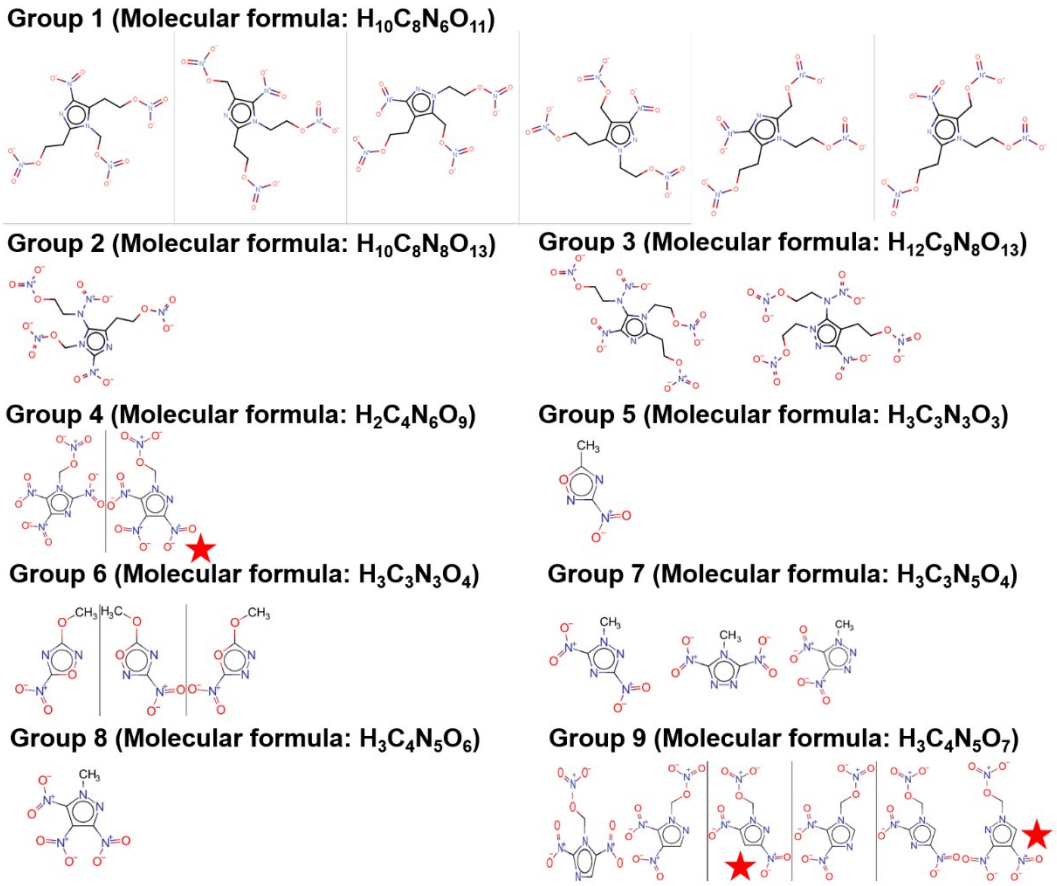
Figure S5. Evaluation on feature importance for T_d models from random forest (RF) algorithm.



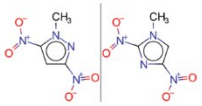
For T_d model, features correlated with molecular stability such as ob (oxygen balance) and nC(NO2) (number of C(NO2) groups) are more weighted with the values of 11.50% and 5.93%, respectively. Since high ob and more nC(NO2) usually indicates the poor thermal stability of compound, thus we think their high importance in features are reasonable. Detailed comparative analysis on the feature importance of T_m (Figure 3B) and T_d models (Figure S5), we can find that the feature importance for T_d and T_m models are quietly different. In addition, this variance also demonstrates the necessity and reliability of custom descriptor set in unrevealing the pattern in different property data.

Figure S6. Searching the most potential molecules for synthetic endeavor from screened 136 candidates

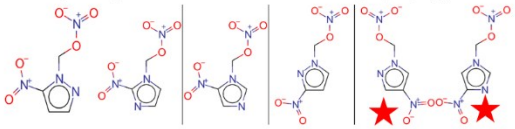
As shown in Figure S6, the screened 136 molecules can be classified into 24 groups from the view of structural isomer. Based on the predicted results of ML models, we can find that the main properties of (including density, Dv, P, Tm and Td) different structural isomers are very close (Table S2). We think that it would be reasonable to select one or two molecules in every structural isomer group for experimental verifications. Thus, the molecules valuable for synthetic endeavor can be narrowed to around 40 from original 136. Considering the reported molecules (such as Group 7 and Group 8) and difficulty of introducing multiple alkyl nitric esters in a molecular skeleton (such as Group 1, 2 and 3, *etc.*), we think that the red star-marked twelve molecules are the most valuable to experimentally synthesize and verify.



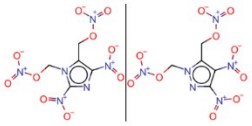
Group 10 (Molecular formula: $H_4C_4N_4O_4$)



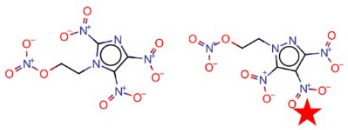
Group 11 (Molecular formula: $H_4C_4N_4O_5$)



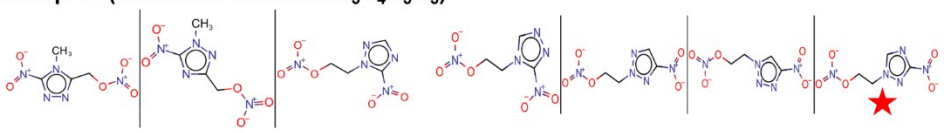
Group 12 (Molecular formula: $H_4C_5N_6O_{10}$)



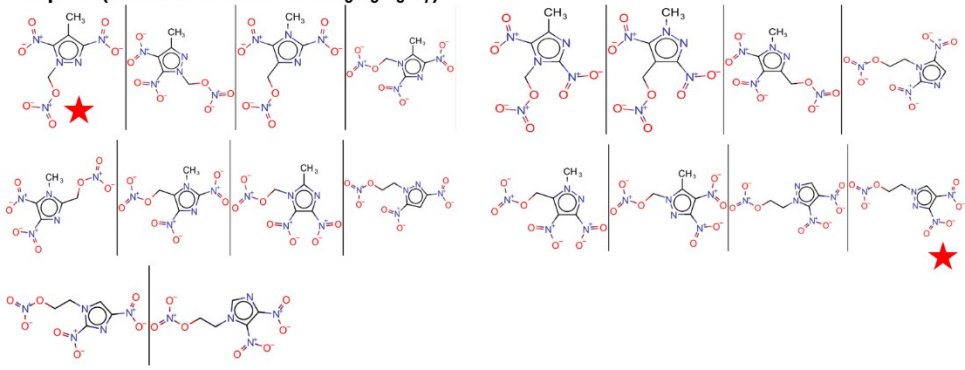
Group 13 (Molecular formula: $H_4C_5N_6O_9$)



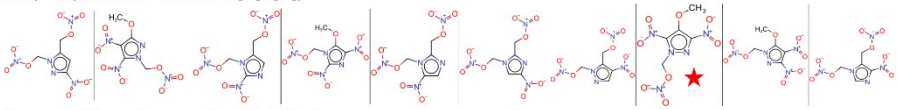
Group 14 (Molecular formula: $H_5C_4N_5O_5$)



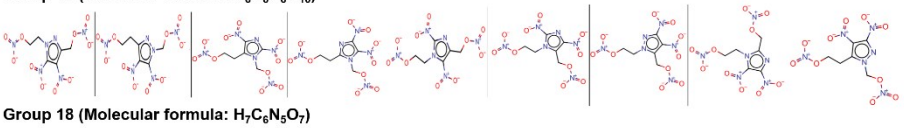
Group 15 (Molecular formula: $H_5C_5N_5O_7$)



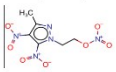
Group 16 (Molecular formula: $H_5C_5N_5O_8$)



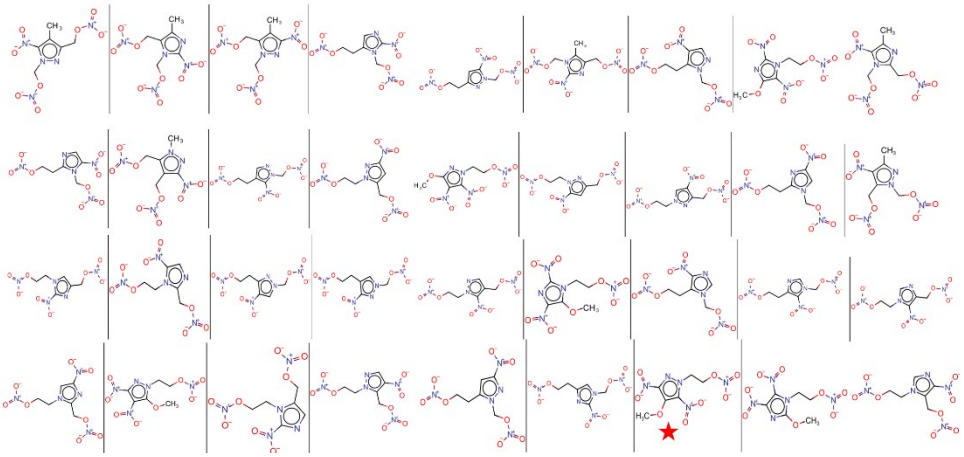
Group 17 (Molecular formula: $H_6C_6N_6O_{10}$)



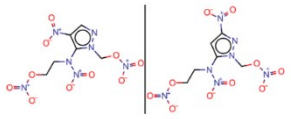
Group 18 (Molecular formula: $H_7C_6N_5O_7$)



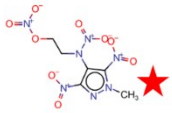
Group 19 (Molecular formula: $H_7C_6N_5O_8$)



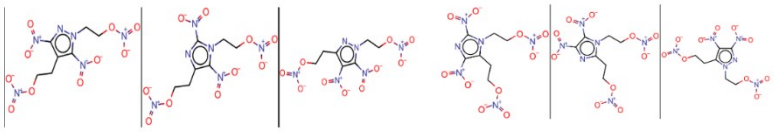
Group 20 (Molecular formula: $H_7C_6N_7O_{10}$)



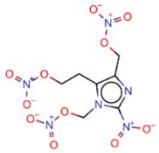
Group 21 (Molecular formula: $H_7C_6N_7O_9$)



Group 22 (Molecular formula: $H_8C_7N_6O_{10}$)



Group 23 (Molecular formula: $H_8C_7N_6O_{11}$)



Group 24 (Molecular formula: $H_9C_7N_7O_{10}$)

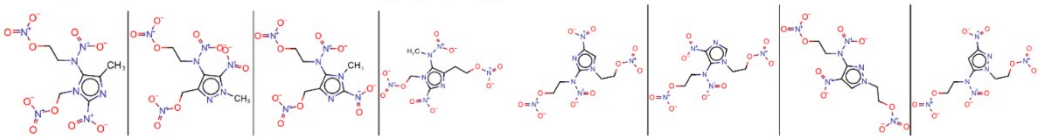
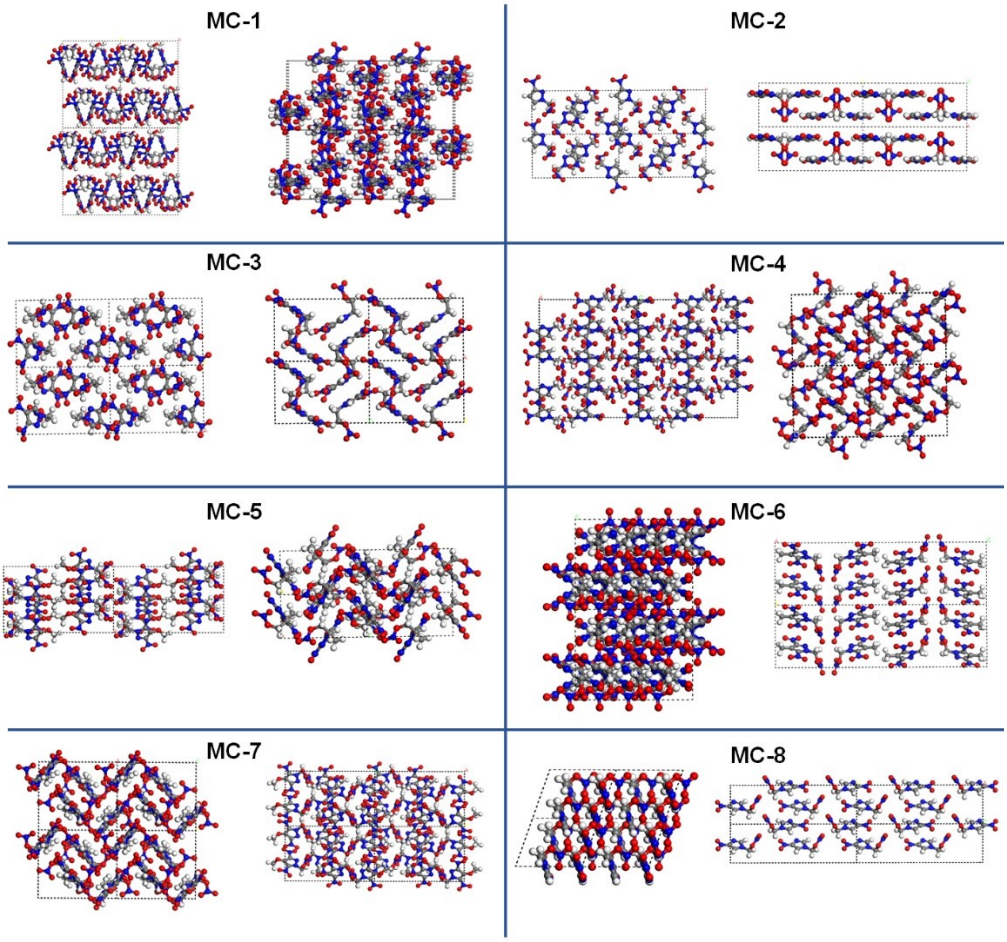


Figure S7. Crystal packing structures of compounds MC-1 to MC-8.



Slow solvent evaporation of dichloromethane solution (MC-3 and MC-8) or ethyl acetate solutions (MC-1, MC-2, MC-4, MC-5, MC-6 and MC-7) at room temperature, we obtained the single crystals of MC-1 to MC-8 and their crystal packing structures are shown in Figure S7. Through analyzing their crystal structures, we find that they usually take mix-crossed crystal packing modes and lack strong hydrogen-bond interactions.

Table S1. Abbreviation and description for custom descriptors

Abbreviation	Description	Abbreviation	Description
nHbondA	Number of hydrogen bond acceptor	nH	Number of hydrogen atom
nHbondD	Number of hydrogen bond donor	nC	Number of carbon atom
nNH2	Number of amino group	nN	Number of nitrogen atom
nAHC	Number of aromatic heterocycle	nO	Number of oxygen atom
nACC	Number of aromatic carbocycle	PBF	Plane of best fit
nRbond	Number of rotatable bond	TPSA	Topological polar surface area
nR	Number of ring	ob	Oxygen balance
nNNO2	Number of nitramine group	Molecular weight	Molecular weight
nC(NO2)3	Number of nitroform group	PMI3	Principal moments of inertia 3
nC(NO2)2	Number of dinitro group	nCH3	Number of methyl group
nC(NO2)	Number of nitro group	nOCH3	Number of methoxy group
MinPartialCharge	Minimum value of partial charge	NPR1	Normalized principal moments ratios 1
MaxPartialCharge	Maximum value of partial charge	NPR2	Normalized principal moments ratios 2
MOLvolume	Molecular volume		

Table S2. Predicted properties for screened 136 molecules

SMILES	Formula	Density	Dv	P	Tm	Td
O=[N+]([O-])OCn1c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	H2C4N6O9	1.866	8.830	35.634	104.105	196.881
O=[N+]([O-])OCn1nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H2C4N6O9	1.860	8.811	35.376	99.729	197.668
O=[N+]([O-])OCc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H4C5N6O10	1.803	8.478	32.570	102.992	195.339
O=[N+]([O-])OCc1c([N+](=O)[O-])c([N+](=O)[O-])nn1CO[N+](=O)[O-]	H4C5N6O10	1.801	8.475	32.386	97.074	190.008
O=[N+]([O-])OCCn1c([N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	H4C5N6O9	1.800	8.483	32.123	102.242	203.337
O=[N+]([O-])OCn1c([N+](=O)[O-])cnc1[N+](=O)[O-]	H3C4N5O7	1.778	8.440	31.892	102.847	213.572
O=[N+]([O-])OCCn1nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H4C5N6O9	1.791	8.478	31.746	100.810	202.646
O=[N+]([O-])OCn1ncc([N+](=O)[O-])c1[N+](=O)[O-]	H3C4N5O7	1.781	8.484	31.595	100.351	202.168
O=[N+]([O-])OCn1nc([N+](=O)[O-])cc1[N+](=O)[O-]	H3C4N5O7	1.779	8.472	31.538	98.789	209.626
O=[N+]([O-])OCn1cnc([N+](=O)[O-])c1[N+](=O)[O-]	H3C4N5O7	1.784	8.475	31.497	103.558	198.187
O=[N+]([O-])OCn1cc([N+](=O)[O-])nc1[N+](=O)[O-]	H3C4N5O7	1.778	8.457	31.420	101.952	209.308
O=[N+]([O-])OCn1cc([N+](=O)[O-])c([N+](=O)[O-])n1	H3C4N5O7	1.783	8.515	31.339	98.713	199.223

Cn1nc([N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H3C4N5O6	1.760	8.330	30.597	109.334	212.287
O=[N+]([O-])OCCN(c1c([N+](=O)[O-])cnn1CO[N+](=O)[O-])[N+](=O)[O-]	H7C6N7O10	1.744	8.211	30.000	99.639	193.533
O=[N+]([O-])OCCN(c1cc([N+](=O)[O-])nn1CO[N+](=O)[O-])[N+](=O)[O-]	H7C6N7O10	1.736	8.186	29.779	108.655	203.215
Cn1nc([N+](=O)[O-])nc1[N+](=O)[O-]	H3C3N5O4	1.731	8.329	29.667	100.758	195.780
O=[N+]([O-])OCCn1nc(CO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H6C6N6O10	1.752	8.184	29.597	91.577	191.370
O=[N+]([O-])OCCc1nn(CO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H6C6N6O10	1.751	8.240	29.557	92.384	191.807
O=[N+]([O-])OCCc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H6C6N6O10	1.748	8.173	29.539	100.161	199.591
O=[N+]([O-])OCCc1nc([N+](=O)[O-])c([N+](=O)[O-])n1CO[N+](=O)[O-]	H6C6N6O10	1.749	8.188	29.467	91.362	191.684
O=[N+]([O-])OCCn1c([N+](=O)[O-])nc(CO[N+](=O)[O-])c1[N+](=O)[O-]	H6C6N6O10	1.745	8.220	29.465	92.916	194.196
O=[N+]([O-])OCCn1c([N+](=O)[O-])nc([N+](=O)[O-])c1CO[N+](=O)[O-]	H6C6N6O10	1.745	8.158	29.430	98.631	197.038
Cn1c([N+](=O)[O-])nnc1[N+](=O)[O-]	H3C3N5O4	1.727	8.346	29.377	104.266	198.593
Cn1nnc([N+](=O)[O-])c1[N+](=O)[O-]	H3C3N5O4	1.708	8.299	29.374	88.674	190.227
O=[N+]([O-])OCCn1nc([N+](=O)[O-])c([N+](=O)[O-	H6C6N6O10	1.747	8.175	29.327	90.695	190.909

])c1CO[N+](=O)[O-]						
Cn1nc([N+](=O)[O-])c(N(CCO[N+](=O)[O-])[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N7O9	1.715	8.211	29.233	105.555	197.348
O=[N+]([O-])OCCn1c(CO[N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	H6C6N6O10	1.744	8.177	29.176	93.577	195.804
O=[N+]([O-])OCCc1c([N+](=O)[O-])c([N+](=O)[O-])nn1CO[N+](=O)[O-]	H6C6N6O10	1.742	8.165	29.115	97.683	201.388
O=[N+]([O-])OCc1cc([N+](=O)[O-])nn1CO[N+](=O)[O-]	H5C5N5O8	1.721	8.122	28.763	91.061	194.796
COc1nn(CO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O8	1.728	7.932	28.722	97.608	191.842
O=[N+]([O-])OCc1cnc([N+](=O)[O-])n1CO[N+](=O)[O-]	H5C5N5O8	1.718	8.137	28.720	91.283	195.671
O=[N+]([O-])OCCc1nc([N+](=O)[O-])n(CO[N+](=O)[O-])c1N(CCO[N+](=O)[O-])[N+](=O)[O-]	H10C8N8O13	1.720	8.017	28.696	99.772	193.115
COc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H5C5N5O8	1.727	7.919	28.624	98.029	191.998
O=[N+]([O-])OCc1ncc([N+](=O)[O-])n1CO[N+](=O)[O-]	H5C5N5O8	1.722	8.156	28.610	89.568	195.407
O=[N+]([O-])OCc1nc([N+](=O)[O-])cn1CO[N+](=O)[O-]	H5C5N5O8	1.724	8.138	28.545	87.497	190.220
O=[N+]([O-])OCc1c([N+](=O)[O-])cnn1CO[N+](=O)[O-]	H5C5N5O8	1.720	8.124	28.514	91.190	199.945
COc1c([N+](=O)[O-])nn(CO[N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O8	1.721	7.957	28.415	97.658	195.295
COc1c([N+](=O)[O-])c([N+](=O)[O-	H5C5N5O8	1.721	7.906	28.395	97.212	191.918

])nn1CO[N+](=O)[O-]						
Cc1c([N+](=O)[O-])nn(CO[N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.711	8.149	28.285	100.273	204.154
O=[N+]([O-])OCc1c([N+](=O)[O-])ncn1CO[N+](=O)[O-]	H5C5N5O8	1.716	8.138	28.267	89.497	194.505
Cc1nn(CO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.710	8.118	28.254	104.451	203.091
Cn1c([N+](=O)[O-])nc(CO[N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.710	8.066	28.217	104.712	202.848
Cc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H5C5N5O7	1.710	8.084	28.184	106.861	205.651
Cc1nc([N+](=O)[O-])n(CO[N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.694	8.047	28.124	104.996	215.099
Cn1nc([N+](=O)[O-])c(CO[N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.700	8.036	28.061	102.881	204.506
Cn1nc(CO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.707	8.074	28.048	101.412	202.259
O=[N+]([O-])OCCn1c([N+](=O)[O-])cnc1[N+](=O)[O-]	H5C5N5O7	1.714	8.085	28.010	95.362	216.219
Cn1c(CO[N+](=O)[O-])nc([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.711	8.073	27.981	105.202	200.984
Cn1c([N+](=O)[O-])nc([N+](=O)[O-])c1CO[N+](=O)[O-]	H5C5N5O7	1.707	8.061	27.966	105.074	204.169
Cc1nc([N+](=O)[O-])c([N+](=O)[O-])n1CO[N+](=O)[O-]	H5C5N5O7	1.700	8.084	27.929	101.687	203.571
O=[N+]([O-])OCCn1nc([N+](=O)[O-])cc1[N+](=O)[O-]	H5C5N5O7	1.718	8.106	27.860	96.815	212.151
Cn1nc([N+](=O)[O-])c([N+](=O)[O-])c1CO[N+](=O)[O-]	H5C5N5O7	1.704	8.071	27.819	103.782	201.281
Cc1c([N+](=O)[O-	H5C5N5O7	1.700	8.076	27.814	102.011	204.387

])c([N+](=O)[O-])nn1CO[N+](=O)[O-]						
O=[N+]([O-])OCCn1ncc([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.715	8.123	27.692	104.783	208.299
O=[N+]([O-])OCCn1cc([N+](=O)[O-])c([N+](=O)[O-])n1	H5C5N5O7	1.716	8.098	27.516	95.159	206.668
O=[N+]([O-])OCCn1cc([N+](=O)[O-])nc1[N+](=O)[O-]	H5C5N5O7	1.708	8.077	27.502	99.154	215.930
O=[N+]([O-])OCCn1cnc([N+](=O)[O-])c1[N+](=O)[O-]	H5C5N5O7	1.711	8.101	27.492	103.421	205.910
Cc1nc([N+](=O)[O-])n(CO[N+](=O)[O-])c1N(CCO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.673	7.924	27.421	101.513	194.376
Cn1nc(CO[N+](=O)[O-])c(N(CCO[N+](=O)[O-])[N+](=O)[O-])c1[N+](=O)[O-]	H9C7N7O10	1.675	7.921	27.124	101.984	192.273
O=[N+]([O-])OCCc1c(CO[N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H8C7N6O11	1.703	7.931	27.047	89.291	190.545
Cn1c([N+](=O)[O-])nc(CO[N+](=O)[O-])c1N(CCO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.671	7.901	26.983	103.741	194.211
CN(c1c(CCO[N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.674	7.941	26.958	101.358	191.823
O=[N+]([O-])OCCN(c1nc([N+](=O)[O-])cn1CCO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.685	7.913	26.914	100.063	197.495
O=[N+]([O-])OCn1nccc1[N+](=O)[O-]	H4C4N4O5	1.679	7.990	26.902	79.611	209.231
O=[N+]([O-])OCCN(c1c([N+](=O)[O-])ncn1CCO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.686	7.887	26.882	98.377	194.674

O=[N+]([O-])OCCN(c1nn(CCO[N+](=O)[O-])cc1[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.694	7.888	26.834	100.045	192.068
O=[N+]([O-])OCCN(c1cc([N+](=O)[O-])nn1CCO[N+](=O)[O-])[N+](=O)[O-]	H9C7N7O10	1.685	7.877	26.794	108.303	206.845
O=[N+]([O-])OCn1ccnc1[N+](=O)[O-]	H4C4N4O5	1.678	7.970	26.775	79.835	208.334
O=[N+]([O-])OCCc1c([N+](=O)[O-])nn(CCO[N+](=O)[O-])c1[N+](=O)[O-]	H8C7N6O10	1.700	7.956	26.708	91.380	196.640
O=[N+]([O-])OCn1cncc1[N+](=O)[O-]	H4C4N4O5	1.679	7.978	26.704	81.298	210.710
O=[N+]([O-])OCCc1nc([N+](=O)[O-])n(CCO[N+](=O)[O-])c1[N+](=O)[O-]	H8C7N6O10	1.698	7.960	26.699	90.687	196.590
COc1noc([N+](=O)[O-])n1	H3C3N3O4	1.690	7.779	26.674	62.822	195.691
COc1nc([N+](=O)[O-])no1	H3C3N3O4	1.690	7.778	26.665	63.047	195.930
COc1nnc([N+](=O)[O-])o1	H3C3N3O4	1.691	7.776	26.658	61.105	195.125
O=[N+]([O-])OCCc1nn(CCO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H8C7N6O10	1.698	7.930	26.577	89.798	198.182
O=[N+]([O-])OCCc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CCO[N+](=O)[O-]	H8C7N6O10	1.693	7.860	26.507	100.021	208.984
O=[N+]([O-])OCn1ccc([N+](=O)[O-])n1	H4C4N4O5	1.683	7.996	26.422	89.714	205.057
O=[N+]([O-])OCn1cc([N+](=O)[O-])cn1	H4C4N4O5	1.678	8.007	26.404	88.575	203.188
O=[N+]([O-])OCCc1c([N+](=O)[O-])nn(CCO[N+](=O)[O-])c1N(CCO[N+](=O)[O-])[N+](=O)[O-]	H12C9N8O13	1.684	7.784	26.398	97.663	194.305
Cn1c(CO[N+](=O)[O-])nnc1[N+](=O)[O-]	H5C4N5O5	1.670	8.011	26.383	92.358	191.837

O=[N+]([O-])OCCc1nc([N+](=O)[O-])c([N+](=O)[O-])n1CCO[N+](=O)[O-]	H8C7N6O10	1.691	7.835	26.376	95.968	203.234
O=[N+]([O-])OCCc1c([N+](=O)[O-])c([N+](=O)[O-])nn1CCO[N+](=O)[O-]	H8C7N6O10	1.690	7.828	26.355	95.445	203.173
O=[N+]([O-])OCCc1nc([N+](=O)[O-])c(N(CCO[N+](=O)[O-])[N+](=O)[O-])n1CCO[N+](=O)[O-]	H12C9N8O13	1.681	7.787	26.053	95.768	190.293
Cn1nc(CO[N+](=O)[O-])nc1[N+](=O)[O-]	H5C4N5O5	1.658	8.030	26.048	91.916	190.090
O=[N+]([O-])OCn1cnc([N+](=O)[O-])c1	H4C4N4O5	1.673	7.988	26.034	92.825	205.005
Cc1nc(CO[N+](=O)[O-])n(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.657	7.811	26.023	94.629	190.261
Cc1nn(CO[N+](=O)[O-])c(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.655	7.813	25.851	92.305	190.073
O=[N+]([O-])OCCn1ncnc1[N+](=O)[O-]	H5C4N5O5	1.662	8.026	25.801	76.154	190.085
Cc1c(CO[N+](=O)[O-])nn(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.657	7.875	25.778	93.768	193.143
Cc1nc([N+](=O)[O-])n(CO[N+](=O)[O-])c1CO[N+](=O)[O-]	H7C6N5O8	1.653	7.852	25.771	91.628	192.248
Cc1c([N+](=O)[O-])nn(CO[N+](=O)[O-])c1CO[N+](=O)[O-]	H7C6N5O8	1.653	7.817	25.749	96.078	192.642
O=[N+]([O-])OCCn1cnnc1[N+](=O)[O-]	H5C4N5O5	1.662	8.005	25.705	76.320	190.189
O=[N+]([O-])OCCc1cnc([N+](=O)[O-])n1CO[N+](=O)[O-]	H7C6N5O8	1.671	7.825	25.591	80.123	192.996
Cn1nc([N+](=O)[O-])cc1[N+](=O)[O-]	H4C4N4O4	1.666	7.849	25.503	107.723	236.562

O=[N+]([O-])OCCc1cc([N+](=O)[O-])n(CO[N+](=O)[O-])n1	H7C6N5O8	1.669	7.873	25.485	85.275	193.512
Cc1c(CO[N+](=O)[O-])nc([N+](=O)[O-])n1CO[N+](=O)[O-]	H7C6N5O8	1.652	7.861	25.478	93.683	192.288
Cn1cc([N+](=O)[O-])nc1[N+](=O)[O-]	H4C4N4O4	1.664	7.825	25.466	109.456	237.285
O=[N+]([O-])OCCc1c([N+](=O)[O-])cnn1CO[N+](=O)[O-]	H7C6N5O8	1.662	7.768	25.462	90.787	204.326
COc1nc([N+](=O)[O-])n(CCO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.666	7.612	25.450	92.129	197.484
O=[N+]([O-])OCCn1ncc([N+](=O)[O-])n1	H5C4N5O5	1.660	8.036	25.440	90.030	190.466
O=[N+]([O-])OCCc1ncc([N+](=O)[O-])n1CO[N+](=O)[O-]	H7C6N5O8	1.669	7.842	25.419	83.942	195.726
O=[N+]([O-])OCCn1cc([N+](=O)[O-])nn1	H5C4N5O5	1.658	8.011	25.401	88.191	190.166
Cn1nc([N+](=O)[O-])c(CO[N+](=O)[O-])c1CO[N+](=O)[O-]	H7C6N5O8	1.651	7.814	25.400	92.358	191.954
O=[N+]([O-])OCCn1cnc([N+](=O)[O-])n1	H5C4N5O5	1.663	8.004	25.395	84.645	191.310
O=[N+]([O-])OCCc1cnn(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.668	7.897	25.381	92.065	190.236
O=[N+]([O-])OCCn1nc([N+](=O)[O-])cc1CO[N+](=O)[O-]	H7C6N5O8	1.668	7.821	25.357	82.480	193.850
COc1nn(CCO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.668	7.609	25.325	96.001	200.365
O=[N+]([O-])OCCn1nc(CO[N+](=O)[O-])cc1[N+](=O)[O-]	H7C6N5O8	1.670	7.865	25.304	88.624	192.408
O=[N+]([O-])OCCn1cc([N+](=O)[O-])c(CO[N+](=O)[O-])n1	H7C6N5O8	1.671	7.809	25.286	82.341	192.415

O=[N+]([O-])OCCc1nc([N+](=O)[O-])cn1CO[N+](=O)[O-]	H7C6N5O8	1.666	7.804	25.286	84.373	196.382
O=[N+]([O-])OCCn1cc(CO[N+](=O)[O-])nc1[N+](=O)[O-]	H7C6N5O8	1.657	7.777	25.276	91.242	201.640
O=[N+]([O-])OCCn1c([N+](=O)[O-])cnc1CO[N+](=O)[O-]	H7C6N5O8	1.664	7.815	25.243	86.817	200.621
O=[N+]([O-])OCCc1nn(CO[N+](=O)[O-])cc1[N+](=O)[O-]	H7C6N5O8	1.669	7.873	25.229	87.400	191.415
O=[N+]([O-])OCCc1cn(CO[N+](=O)[O-])nc1[N+](=O)[O-]	H7C6N5O8	1.669	7.855	25.222	86.164	190.873
O=[N+]([O-])OCCn1ncc(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.668	7.872	25.205	92.188	190.864
COc1c([N+](=O)[O-])nc([N+](=O)[O-])n1CCO[N+](=O)[O-]	H7C6N5O8	1.659	7.580	25.200	97.316	199.099
O=[N+]([O-])OCCc1c([N+](=O)[O-])ncn1CO[N+](=O)[O-]	H7C6N5O8	1.658	7.771	25.181	90.722	203.076
Cc1nc([N+](=O)[O-])no1	H3C3N3O3	1.651	7.871	25.179	68.223	205.714
O=[N+]([O-])OCCc1ncn(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.664	7.884	25.164	90.234	191.092
O=[N+]([O-])OCCn1cc([N+](=O)[O-])nc1CO[N+](=O)[O-]	H7C6N5O8	1.663	7.785	25.150	84.785	196.692
COc1c([N+](=O)[O-])c([N+](=O)[O-])nn1CCO[N+](=O)[O-]	H7C6N5O8	1.667	7.594	25.147	96.184	198.435
O=[N+]([O-])OCCn1c(CO[N+](=O)[O-])cnc1[N+](=O)[O-]	H7C6N5O8	1.661	7.836	25.116	83.735	195.558
O=[N+]([O-])OCCn1ncc([N+](=O)[O-])c1CO[N+](=O)[O-]	H7C6N5O8	1.662	7.816	25.088	86.164	199.948
O=[N+]([O-])OCCc1cc([N+](=O)[O-])nn1CO[N+](=O)[O-]	H7C6N5O8	1.659	7.824	25.074	89.746	202.177
O=[N+]([O-	H7C6N5O8	1.659	7.858	25.030	85.393	193.480

])OCCc1cn(CO[N+](=O)[O-])c([N+](=O)[O-])n1						
COc1c([N+](=O)[O-])nn(CCO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.663	7.620	24.990	95.981	201.035
COc1nc([N+](=O)[O-])c([N+](=O)[O-])n1CCO[N+](=O)[O-]	H7C6N5O8	1.656	7.583	24.987	88.502	196.733
O=[N+]([O-])OCCn1cnc([N+](=O)[O-])c1CO[N+](=O)[O-]	H7C6N5O8	1.658	7.792	24.970	85.875	198.462
O=[N+]([O-])OCCn1cnc(CO[N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O8	1.657	7.850	24.969	94.504	190.922
Cc1nn(CCO[N+](=O)[O-])c([N+](=O)[O-])c1[N+](=O)[O-]	H7C6N5O7	1.651	7.775	24.902	101.815	211.477
O=[N+]([O-])OCCc1nc([N+](=O)[O-])c(CCO[N+](=O)[O-])n1CO[N+](=O)[O-]	H10C8N6O11	1.662	7.645	24.468	90.551	193.437
O=[N+]([O-])OCCc1nc(CO[N+](=O)[O-])c([N+](=O)[O-])n1CCO[N+](=O)[O-]	H10C8N6O11	1.663	7.621	24.440	97.614	197.297
O=[N+]([O-])OCCc1c([N+](=O)[O-])nn(CCO[N+](=O)[O-])c1CO[N+](=O)[O-]	H10C8N6O11	1.653	7.686	24.436	94.283	195.999
O=[N+]([O-])OCCc1c(CO[N+](=O)[O-])c([N+](=O)[O-])nn1CCO[N+](=O)[O-]	H10C8N6O11	1.661	7.648	24.325	90.059	191.712
O=[N+]([O-])OCCc1c([N+](=O)[O-])nc(CO[N+](=O)[O-])n1CCO[N+](=O)[O-]	H10C8N6O11	1.660	7.629	24.277	92.611	196.876
O=[N+]([O-])OCCc1nc([N+](=O)[O-])c(CO[N+](=O)[O-])n1CCO[N+](=O)[O-]	H10C8N6O11	1.660	7.637	24.256	90.815	193.641

Table S3. Single crystal X-ray diffraction data of MC-1

CCDC	2047538
Formula	$C_6H_7N_7O_9$
Mr	321.19
Crystal system	monoclinic
Space group	P 2_1/c
a [Å]	13.4091(4)
b [Å]	11.1765(3)
c [Å]	16.6893(5)
α [°]	90
β [°]	90.5270(10)
γ [°]	90
V [Å^3]	2526.78(13)
Z	8
T(K)	298
ρ[g cm^{-3}]	1.689
Mu [mm^{-1}]	0.159
F(000)	1312.0
θ [°]	2.656 to 26.735
h, k, lmax	16, 14, 21
reflections collected	57641
independent reflections	4133 [R_{int} = 0.0363, R_{sigma} = 0.0231]
data/restraints/parameters	5355/0/399
GOF on F2	1.057
*R*1 [I>2σ(I)]	0.0448
*wR*2 [I>2σ(I)]	0.1102
*R*1(all data)	0.0618
*wR*2(all data)	0.1245

Table S4. Single crystal X-ray diffraction data of MC-2

CCDC	2047548
Formula	$C_4H_4N_4O_5$
Mr	188.11
Crystal system	monoclinic
Space group	P 2_1/c
a [Å]	6.5012(5)
b [Å]	14.8421(11)
c [Å]	7.7354(5)
α [°]	90
β [°]	105.631(2)
γ [°]	90
V [Å^3]	718.80(9)
Z	4
T(K)	170
ρ[g cm^{-3}]	1.738
Mu [mm^{-1}]	0.161
F(000)	384.0
θ [°]	2.745 to 27.047
h, k, lmax	8, 18, 8
reflections collected	7519
independent reflections	1036 [R_{int} = 0.0604, R_{sigma} = 0.0586]
data/restraints/parameters	1551/0/134
GOF on F2	1.177
*R*1 [I>2σ(I)]	0.0703
*wR*2 [I>2σ(I)]	0.1062
*R*1(all data)	0.1168
*wR*2(all data)	0.1230

Table S5. Single crystal X-ray diffraction data of MC-3

CCDC	2047557
Formula	$C_5H_5N_5O_7$
Mr	247.14
Crystal system	orthorhombic
Space group	P 21 21 21
a [Å]	8.32070(10)
b [Å]	9.07030(10)
c [Å]	12.6090(2)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	951.62(2)
Z	4
T(K)	294.64
ρ[g cm^{-3}]	1.725
Mu [mm^{-1}]	1.448
F(000)	504
θ [°]	6.0010 to 77.4910
h, k, lmax	10, 10, 15
reflections collected	9947
independent reflections	1885 [R_{int} = 0.0205, R_{sigma} = 0.0370]
data/restraints/parameters	1989/0/174
GOF on F2	1.121
*R*1 [I>2σ(I)]	0.0330
*wR*2 [I>2σ(I)]	0.0777
*R*1(all data)	0.0361
*wR*2(all data)	0.0869

Table S6. Single crystal X-ray diffraction data of MC-4

CCDC	2047549
Formula	$C_8H_6N_{10}O_{14}$
Mr	466.23
Crystal system	orthorhombic
Space group	Pna21
a [Å]	9.5410(3)
b [Å]	10.2625(3)
c [Å]	17.2833(5)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	1692.29(9)
Z	4
T(K)	295
ρ[g cm^{-3}]	1.830
Mu [mm^{-1}]	1.586
F(000)	944.0
θ [°]	5.01 to 77.79
h, k, lmax	11, 12, 21
reflections collected	15165
independent reflections	2691 [R_{int} = 0.0635, R_{sigma} = 0.0368]
data/restraints/parameters	2882/1/313
GOF on F2	1.113
*R*1 [I>2σ(I)]	0.0645
*wR*2 [I>2σ(I)]	0.1738
*R*1(all data)	0.0678
*wR*2(all data)	0.1860

Table S7. Single crystal X-ray diffraction data of MC-5

CCDC	2047558
Formula	$C_6H_7N_5O_8$
Mr	188.11
Crystal system	monoclinic
Space group	P 2_1/c
a [Å]	18.4801(8)
b [Å]	5.4258(2)
c [Å]	10.9951(4)
α [°]	90
β [°]	103.3230(10)
γ [°]	90
V [Å^3]	1073.33(7)
Z	4
T(K)	176.0
ρ[g cm^{-3}]	1.715
Mu [mm^{-1}]	0.161
F(000)	568.0
θ [°]	3.71 to 27.48
h, k, lmax	23, 6, 14
reflections collected	11585
independent reflections	1908 [R_{int} = 0.0564, R_{sigma} = 0.0463]
data/restraints/parameters	2434/0/173
GOF on F2	0.602
*R*1 [I>2σ(I)]	0.0521
*wR*2 [I>2σ(I)]	0.1447
*R*1(all data)	0.0696
*wR*2(all data)	0.1839

Table S8. Single crystal X-ray diffraction data of MC-6

CCDC	2047559
Formula	$C_5H_5N_5O_7$
Mr	247.14
Crystal system	orthorhombic
Space group	P b c a
a [Å]	6.1341(5)
b [Å]	9.4426(8)
c [Å]	31.793(3)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	1841.5(3)
Z	8
T(K)	170
ρ[g cm^{-3}]	1.783
Mu [mm^{-1}]	0.168
F(000)	1008.0
θ [°]	3.560 to 26.444
h, k, lmax	6, 11, 39
reflections collected	8540
independent reflections	1176 [R_{int} = 0.0724, R_{sigma} = 0.0605]
data/restraints/parameters	1889/0/155
GOF on F2	1.064
*R*1 [I>2σ(I)]	0.0529
*wR*2 [I>2σ(I)]	0.0966
*R*1(all data)	0.1053
*wR*2(all data)	0.1281

Table S9. Single crystal X-ray diffraction data of MC-7

CCDC	2056920
Formula	$C_5H_5N_5O_8$
Mr	263.14
Crystal system	monoclinic
Space group	P 2_1/n
a [Å]	11.7818(14)
b [Å]	10.1692(12)
c [Å]	16.570(2)
α [°]	90
β [°]	93.178(4)
γ [°]	90
V [Å^3]	1982.3(4)
Z	4
T(K)	170
ρ[g cm^{-3}]	1.763
Mu [mm^{-1}]	0.169
F(000)	1072.0
θ [°]	2.068 to 26.418
h, k, lmax	12, 12, 20
reflections collected	13525
independent reflections	2325 [R_{int} = 0.0821, R_{sigma} = 0.0955]
data/restraints/parameters	4032/0/327
GOF on F2	1.096
*R*1 [I>2σ(I)]	0.0974
*wR*2 [I>2σ(I)]	0.2349
*R*1(all data)	0.1660
*wR*2(all data)	0.2673

Table S10. Single crystal X-ray diffraction data of MC-8

CCDC	2047550
Formula	$C_4H_4N_4O_5$
Mr	188.11
Crystal system	monoclinic
Space group	Cc
a [Å]	5.321(2)
b [Å]	21.200(8)
c [Å]	6.910(3)
α [°]	90
β [°]	109.241(11)
γ [°]	90
V [Å^3]	736.0(5)
Z	4
T(K)	180
ρ[g cm^{-3}]	1.698
Mu [mm^{-1}]	0.157
F(000)	384.0
θ [°]	3.667 to 26.428
h, k, lmax	6, 23, 6
reflections collected	2697
independent reflections	763 [R_{int} = 0.0656, R_{sigma} = 0.0901]
data/restraints/parameters	1231/2/118
GOF on F2	1.060
*R*1 [I>2σ(I)]	0.0732
*wR*2 [I>2σ(I)]	0.1604
*R*1(all data)	0.1291
*wR*2(all data)	0.1972

Table S11. Physicochemical properties of synthesized compounds.

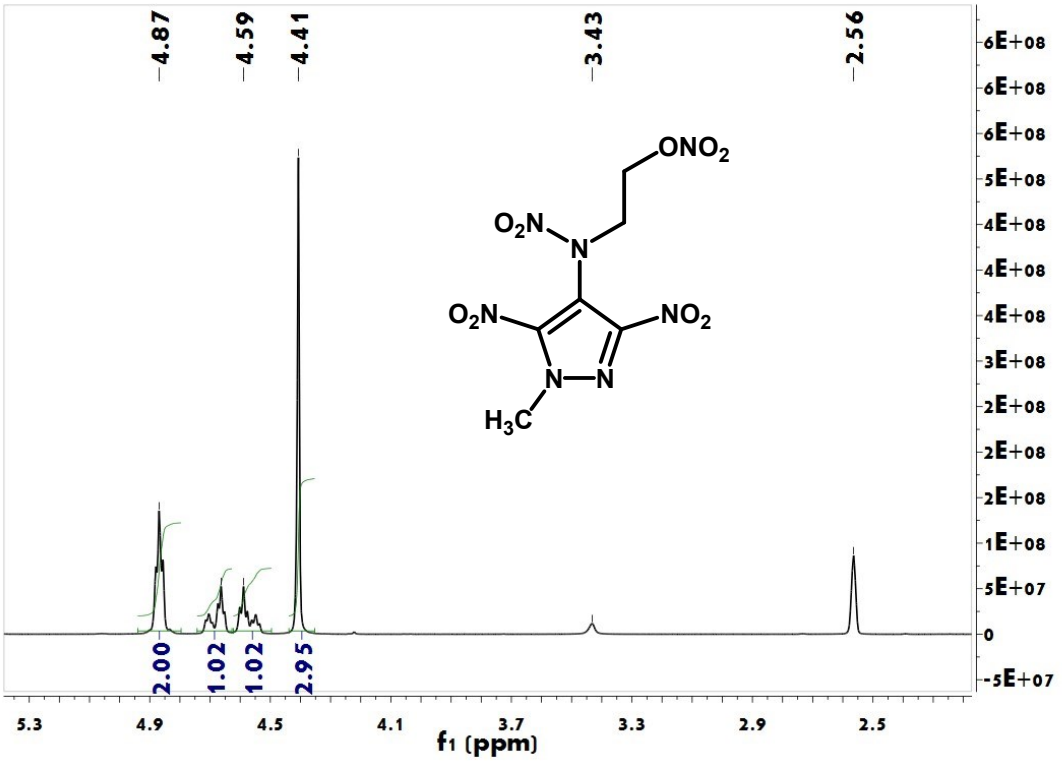
	MC-1	MC-2	MC-3	MC-4	MC-5	MC-6	MC-7	MC-8	TNT
Density [a] ($g\ cm^{-3}$)	1.689	1.714	1.725	1.830	1.692	1.759	1.738	1.675	1.65
$\Delta_f H$ ($kJ\ mol^{-1}$)	97.0	38.3	46.0	71.7	-88.3	16.2	-71.0	-7.7	-67.0
T_m (^oC)	75.9	68.4	65.2	97.1	88.2	90.2	106.9	76.2	80.4
T_d [b] (^oC)	208.7	191.1	221.0	188.0	219.8	180.5	183.2	183.9	295
D_v ($km\ s^{-1}$)	8.139	8.020	8.165	8.705	7.912	8.238	8.175	7.843	6.881
P (GPa)	28.1	26.9	28.8	33.8	26.3	29.4	29.0	25.2	19.5
IS (J)	8	>20	>20	>20	>20	>20	>20	>20	15
FS (N)	96	144	96	160	96	96	96	96	353

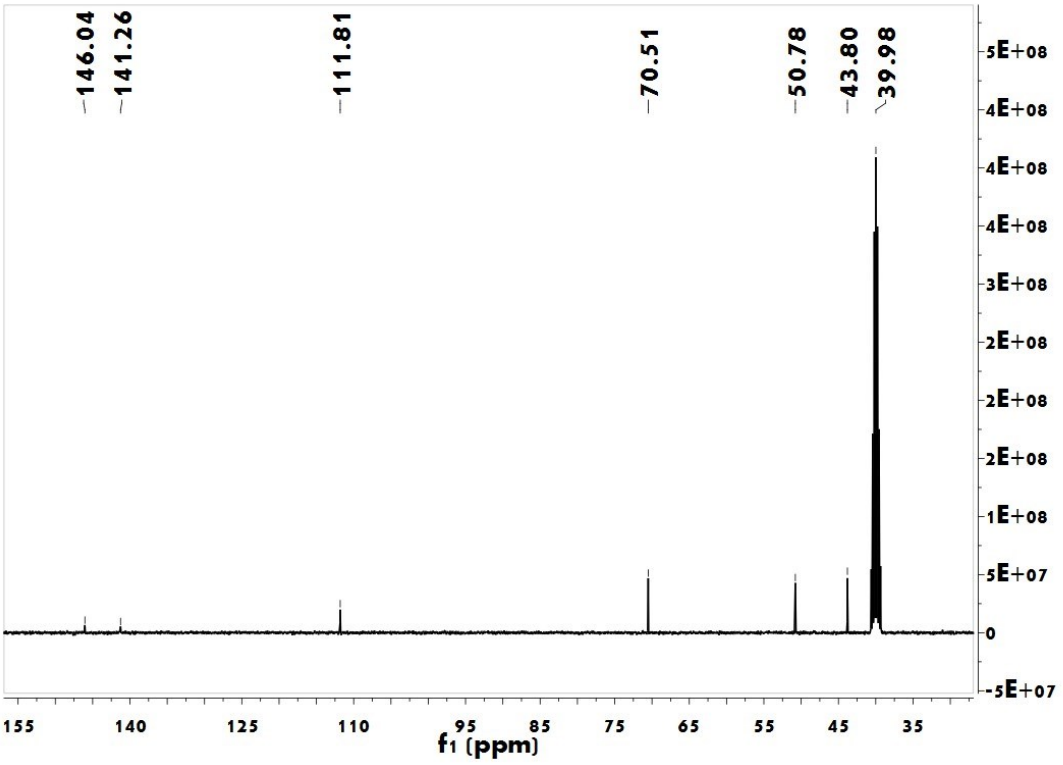
[a] Crystal density at room temperature. For data collected at low temperature, the density was revised by the following equation: $\rho_{rt} = \rho - 0.188*(298.15-T)/1000$.

[b] Peak temperature of decomposition.

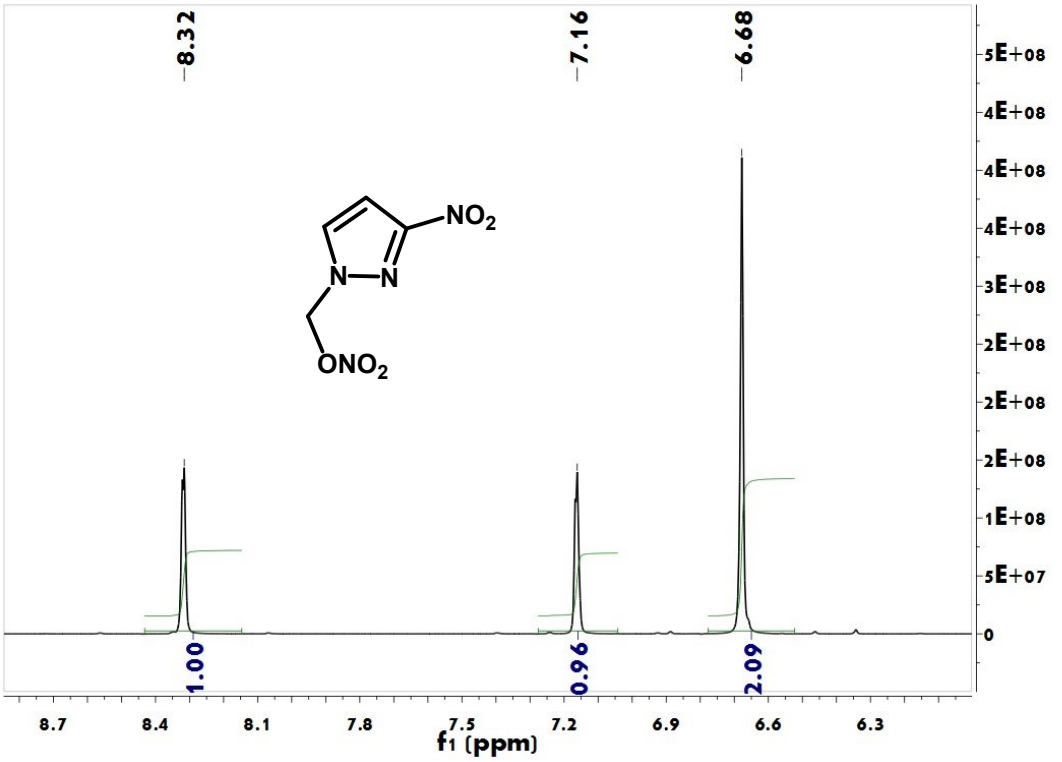
Figure S8. ^{1}H and ^{13}C NMR spectra for synthesized compounds.

MC-1





MC-2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ONO2
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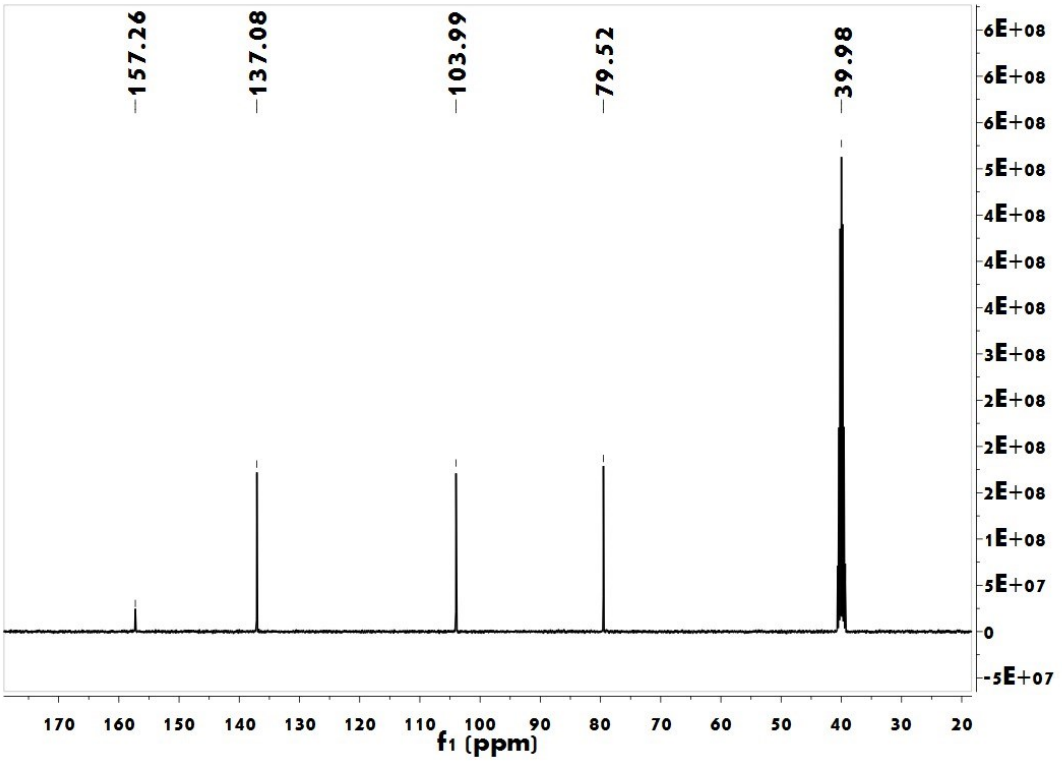
2.09
f1 (ppm)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39.98
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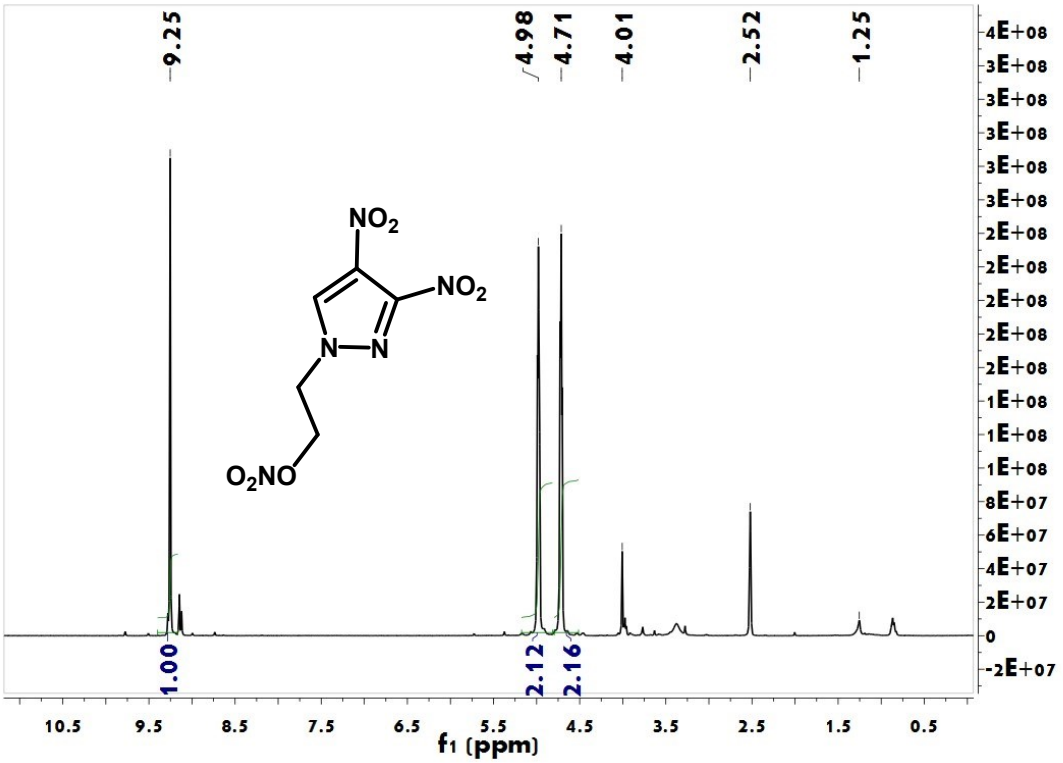
MC-3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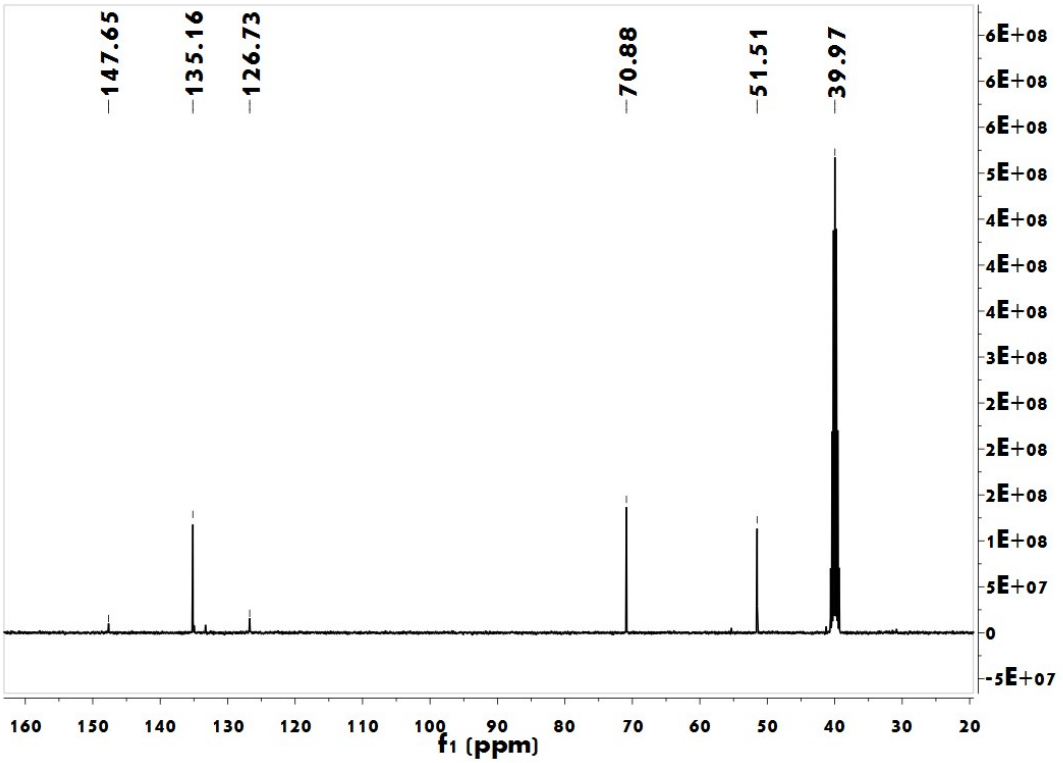
2.16
f1 (ppm)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51.51
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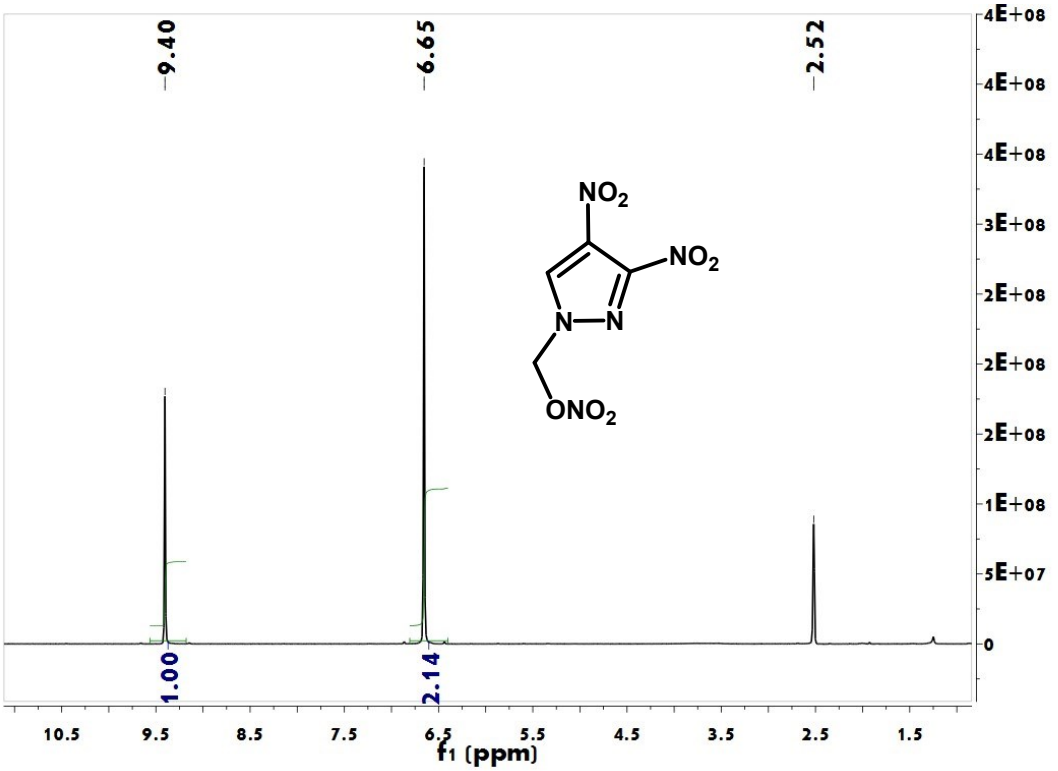
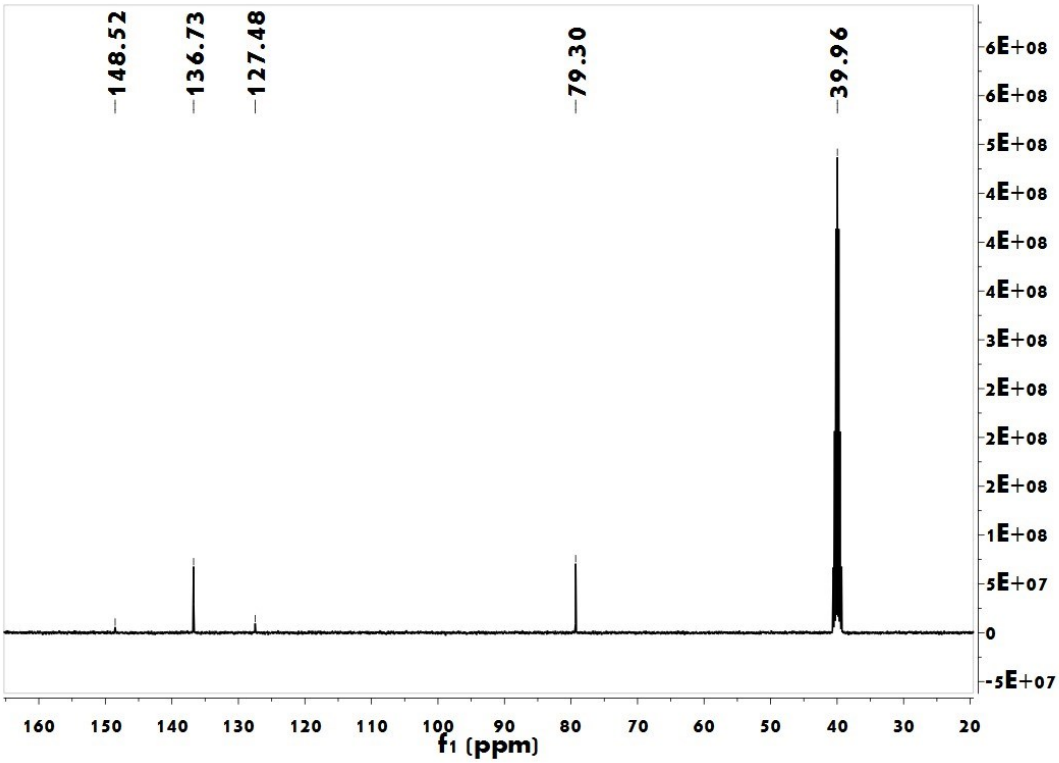
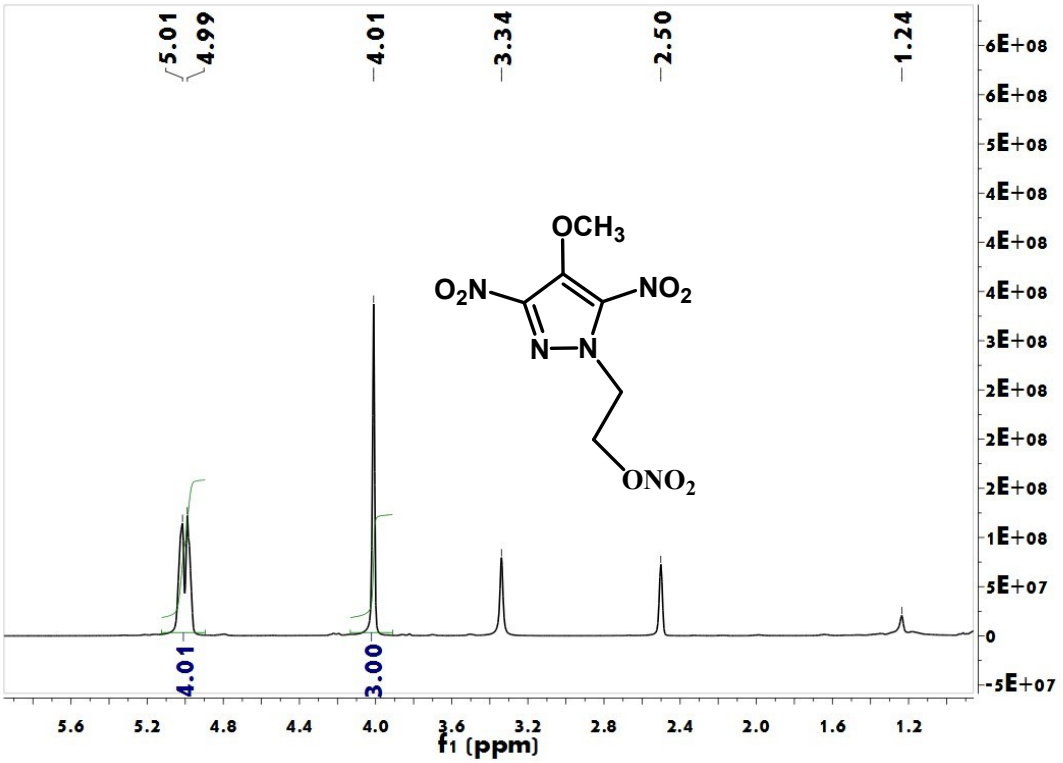
f1 (ppm)

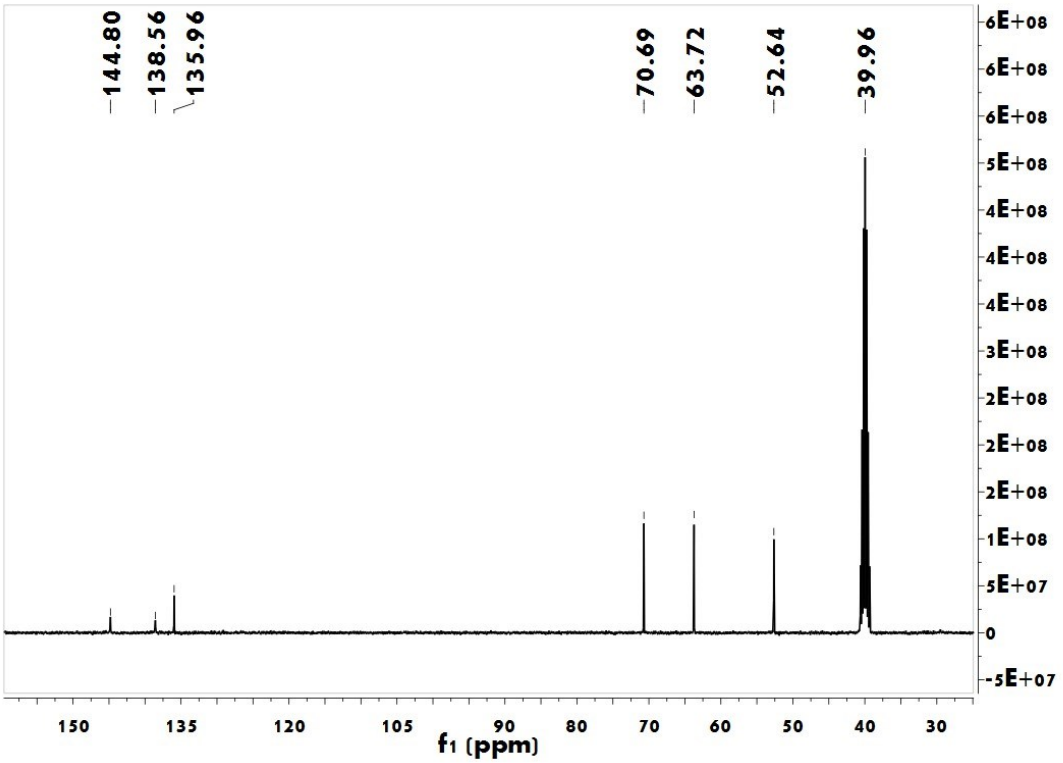
MC-4


9.40
6.65
2.52
NO2
NO2
N
N
ONO2
1.00
2.14
4E+08
3E+08
2E+08
1E+08
5E+07
0
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
f1 (ppm)

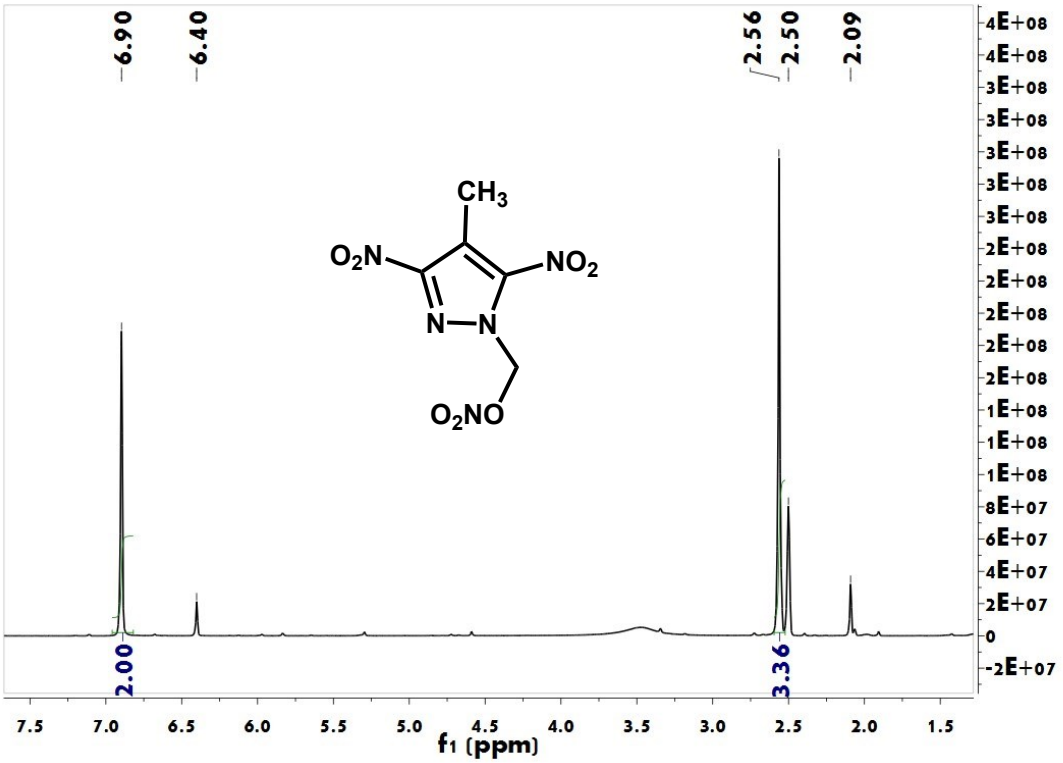

148.52
136.73
127.48
79.30
39.96
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
5E+07
0
-5E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

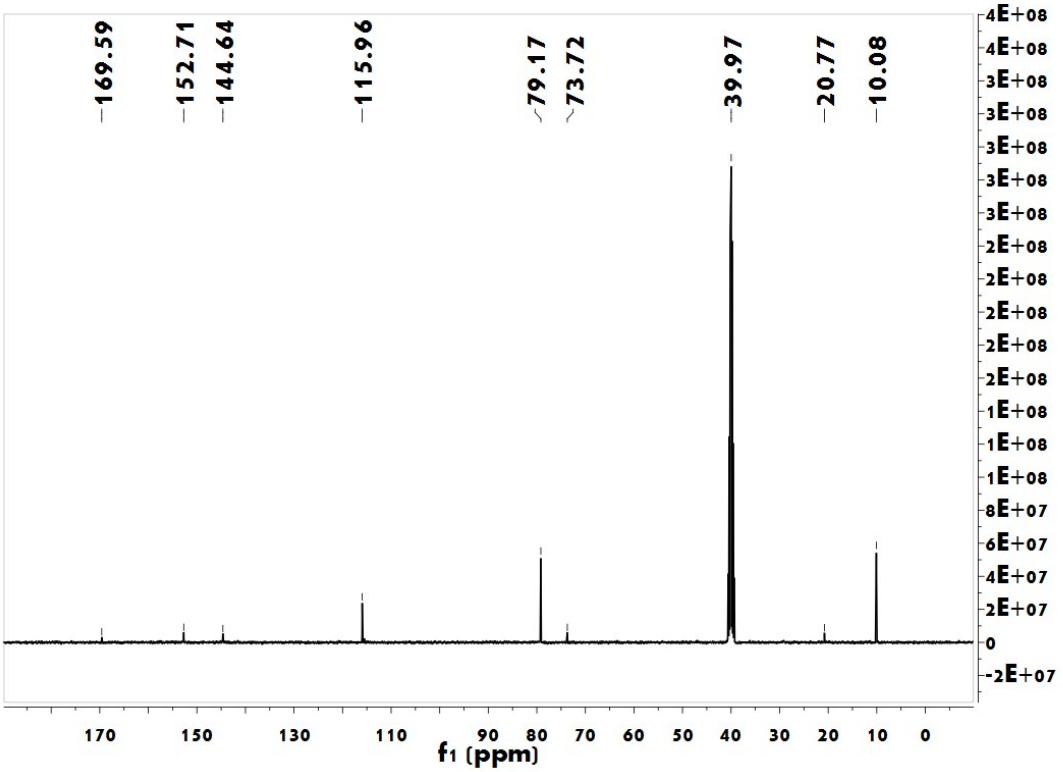
MC-5


5.01
4.99
4.01
3.34
2.50
1.24
OCH3
O2N
NO2
N–N
ONO2
4.01
3.00
f1 (ppm)

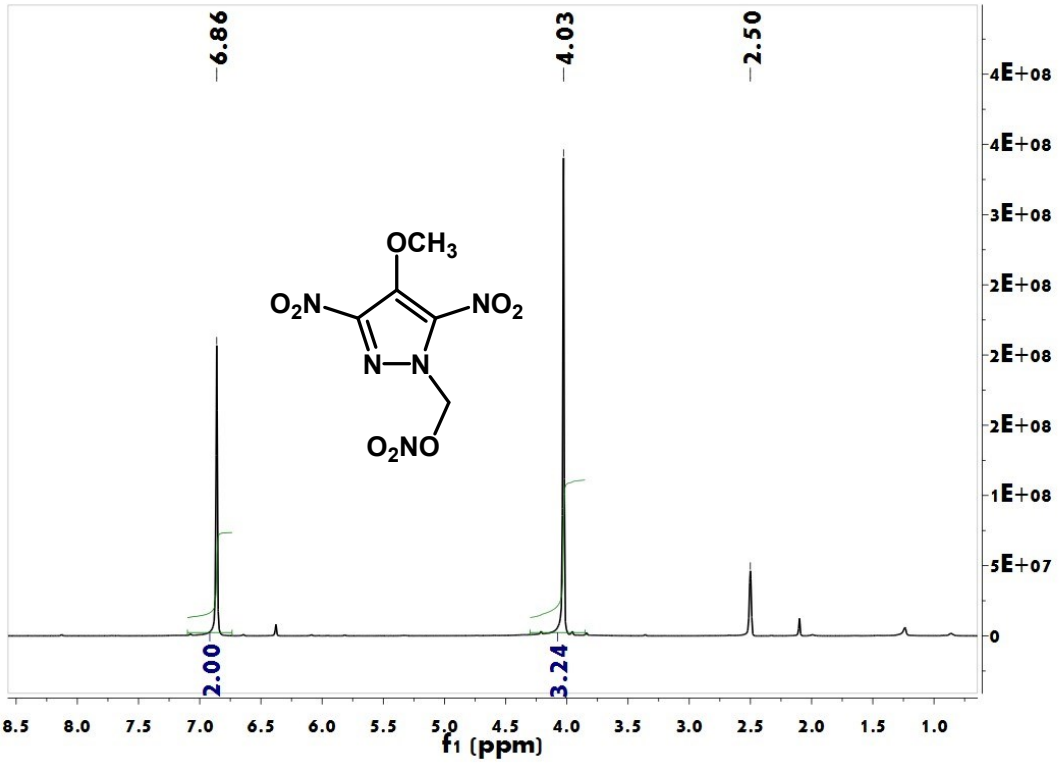

144.80
138.56
135.96
70.69
63.72
52.64
39.96
f1 (ppm)

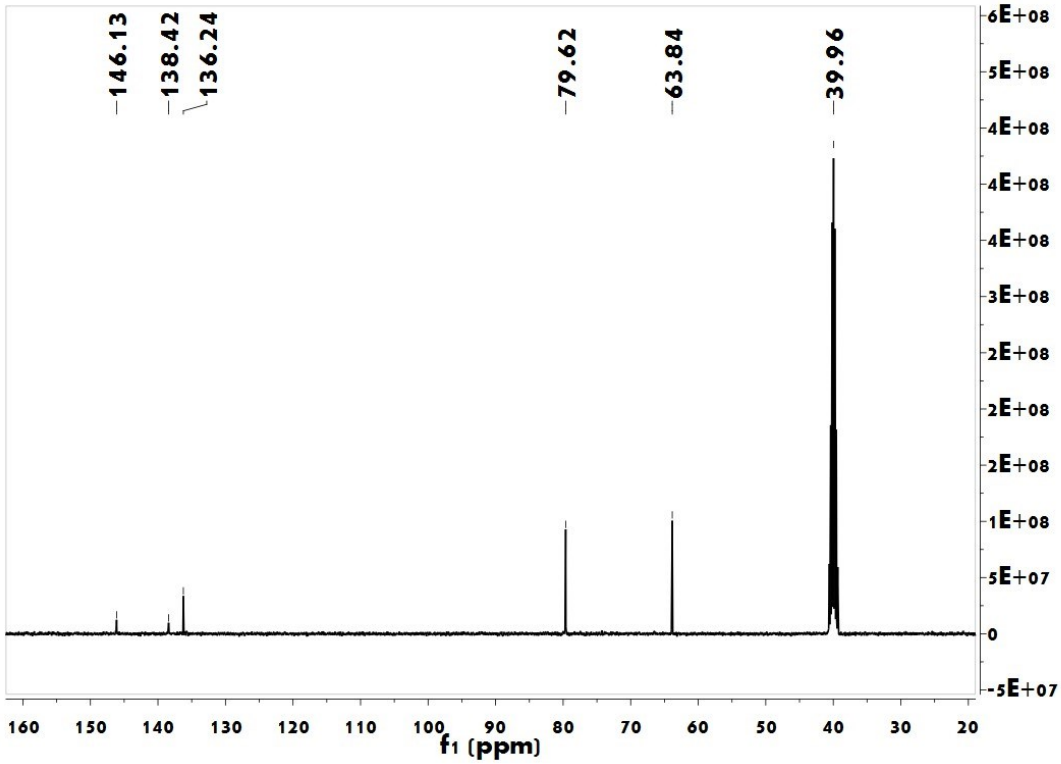
MC-6


6.90
6.40
2.56
2.50
2.09
CH3
O2N
NO2
N–N
O2NO
2.00
3.36
f1 (ppm)

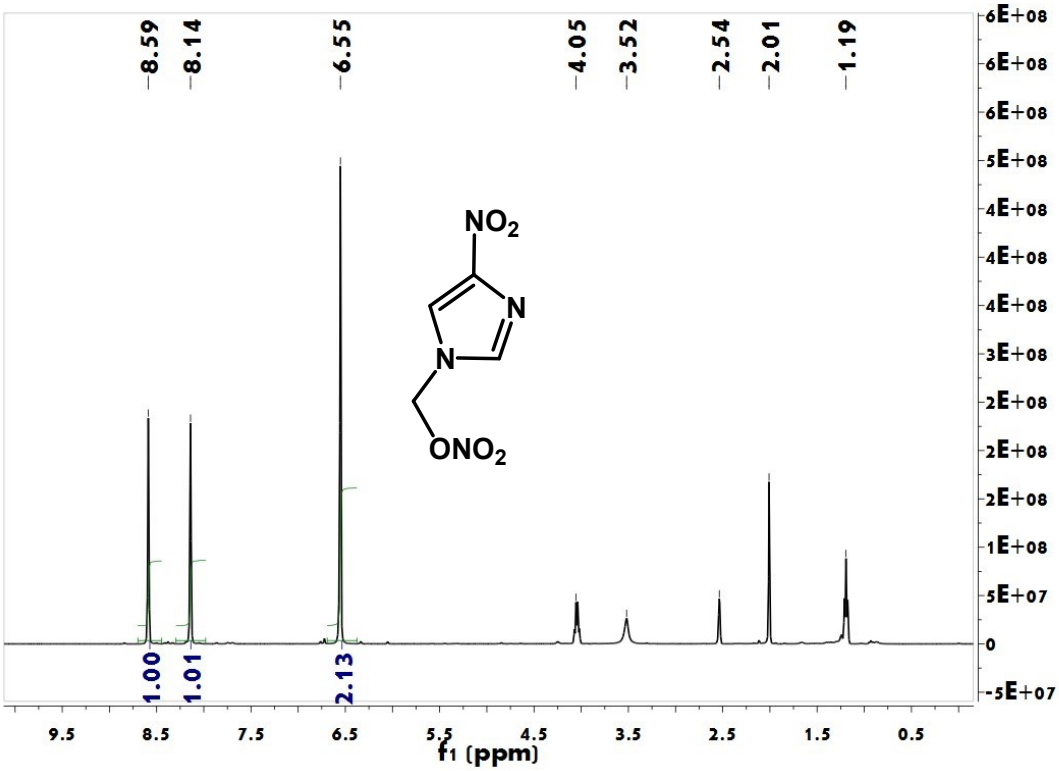

169.59
152.71
144.64
115.96
79.17
73.72
39.97
20.77
10.08
f1 (ppm)

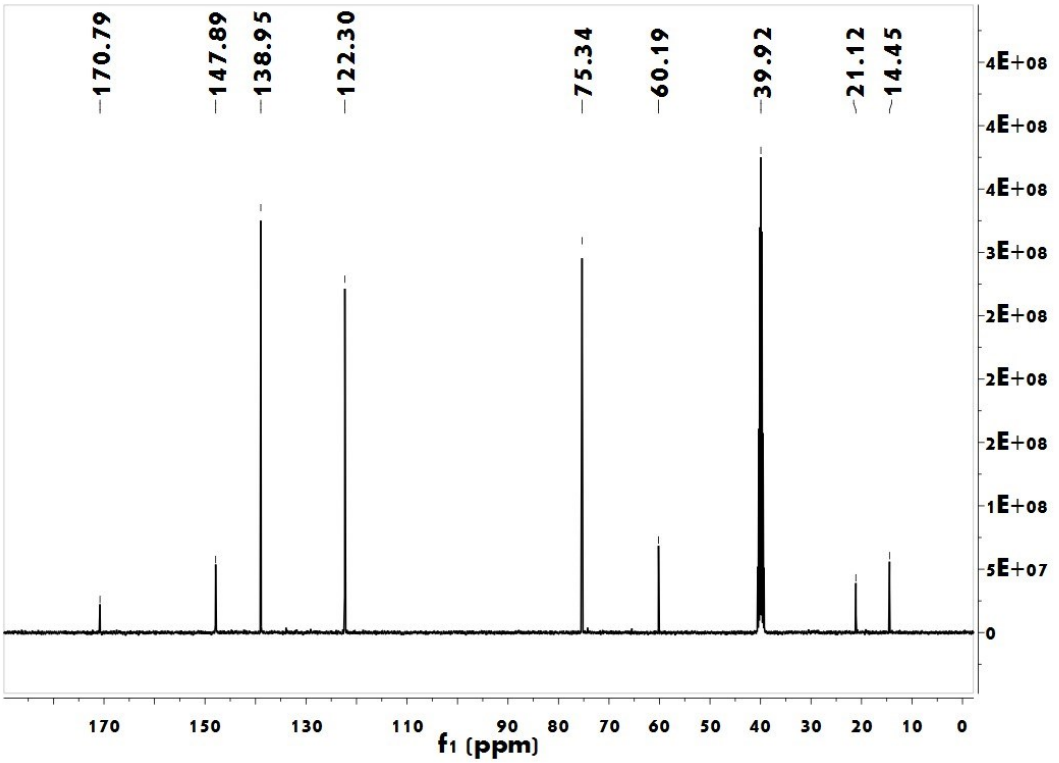
MC-7


6.86
4.03
2.50
OCH3
O2N
NO2
N
N
O2NO
2.00
3.24
f1 (ppm)


146.13
138.42
136.24
79.62
63.84
39.96
f1 (ppm)

MC-8


8.59
8.14
6.55
4.05
3.52
2.54
2.01
1.19
NO2
N
N
ONO2
1.00
1.01
2.13
f1 (ppm)


170.79
147.89
138.95
122.30
75.34
60.19
39.92
21.12
14.45
f1 (ppm)

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