Supporting Information:

Aryl urea substituted fatty acids: a new class of protonophoric mitochondrial uncoupler that utilises a synthetic anion transporter

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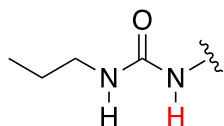[4]School of Chemistry, University of Sydney, Sydney, NSW, 2006, Australia;

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1. Supporting Tables

Compound	R	pKa (TCC)	pKa (DPU)	ΔG_{bind}prop (kJ/mol)	ΔG_{bind}prop (kJ/mol)	ΔG_{bind}prop (kJ/mol)
	N/A	water	water	gas phase	water	n-pentadecane
1		14.00	13.47	-148.55	5.04	-97.35
2		13.88	13.34	-151.88	4.52	-99.30
3		14.08	13.54	-148.25	4.77	-97.14
4		13.37	12.84	-148.75	4.82	-96.21
5		12.81	12.28	-151.88	6.78	-99.45
6		13.55	13.01	-146.84	6.32	-95.02
7		11.60	11.06	-108.21	6.67	-89.07
8		12.76	12.22	-152.47	3.47	-100.66
9		12.14	11.61	-163.69	3.63	-106.40
10		13.33	12.79	-157.78	4.515	-103.19
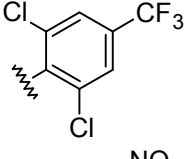
11		13.47	12.93	-158.67	5.74	-101.38
12		10.24	9.7	-121.15	0.92	-78.77
13		11.83	11.3	-176.07	-1.073	-116.88

Table S1: pKa values and propanoate binding free energies of model aryl urea compounds shown to two decimal places. pK_a values are for the urea proton highlighted in red above the main table and were calculated using the G3(MP2)CC(+) composite procedure (see Computational Methodology for details). pKa values calculated using triclocarban and diphenylurea as references are denoted pKa (TCC) and pKa (DPU) respectively. Propanoate binding free energies (ΔG_{bind}prop) were computed at the M06-2X/6-31+G(d) level of theory (see Computational Methodology for details).
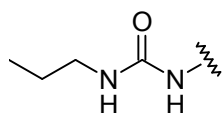
Compound	R	$\Delta G_{Solv}Monomer_{(W-P)}$ (kJ/mol)	$\Delta G_{Solv}Complex_{(W-P)}$ (kJ/mol)
1		9.39	81.47
2		10.37	81.02
3		14.13	73.45
4		45.03	118.48
5		14.22	82.45
6		7.34	80.47
7		21.80	100.53
8		8.53	78.88
9		25.73	90.18
10		11.07	77.84
11		7.51	74.86
12		4.58	99.37
13		16.31	74.98

Table S2: Lipophilicity measures for isolated and complex aryl urea model compounds. The quantities $\Delta G_{Solv}Monomer_{(W-P)}$ and $\Delta G_{Solv}Complex_{(W-P)}$ are described in detail Computational Methodology and are shown to two decimal places.

6-TBAOH	D(ArH1) / (10^{-9} m²/s)	D(ArH2) / (10^{-9} m²/s)	Average ± SD / (10^{-9} m²/s)
50 μM	1.02	0.988	1.01 ± 0.04
5.0 mM	1.12	1.05	1.09 ± 0.05

Table S3 Diffusion coefficients of **6**-TBAOH at two concentrations in CDCl$_3$ at 298 K, determined by diffusion NMR based on two aromatic CH peaks of NM3 from 7.5 to 7.9 ppm.
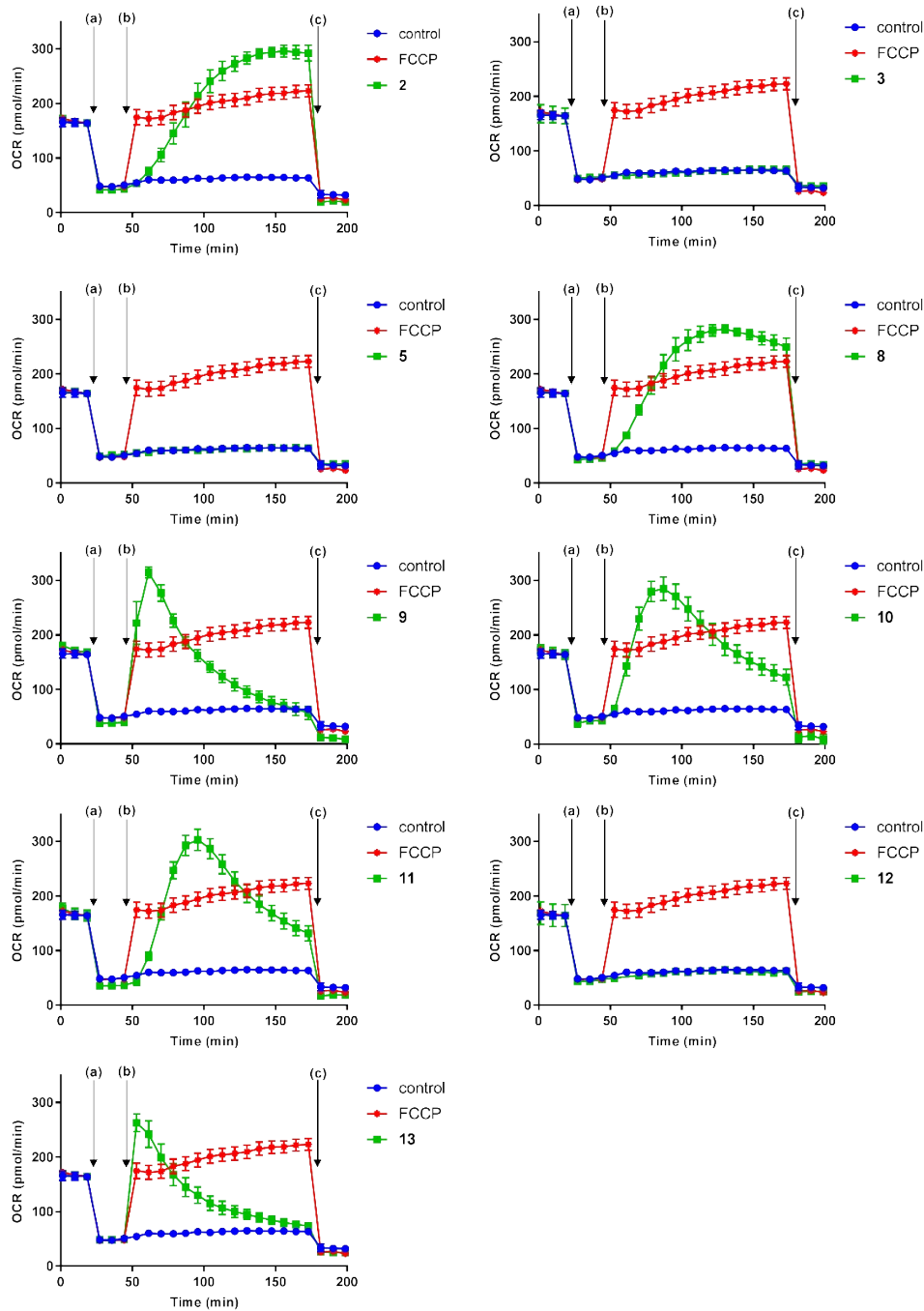
2. Supporting Figures

Figure S1. Uncoupling activity of aryl-urea fatty acids. Oxygen consumption rates (OCR) in MDA-MB-231 cells after sequential addition of the ATP-synthase inhibitor oligomycin (1 µM; arrow a), protonophore FCCP (1 µM) or aryl-ureas (20 µM; arrow b), and then the ETC complex inhibitors rotenone/antimycin A (1 µM). Data represents the mean ± SEM of 3 independent experiments.
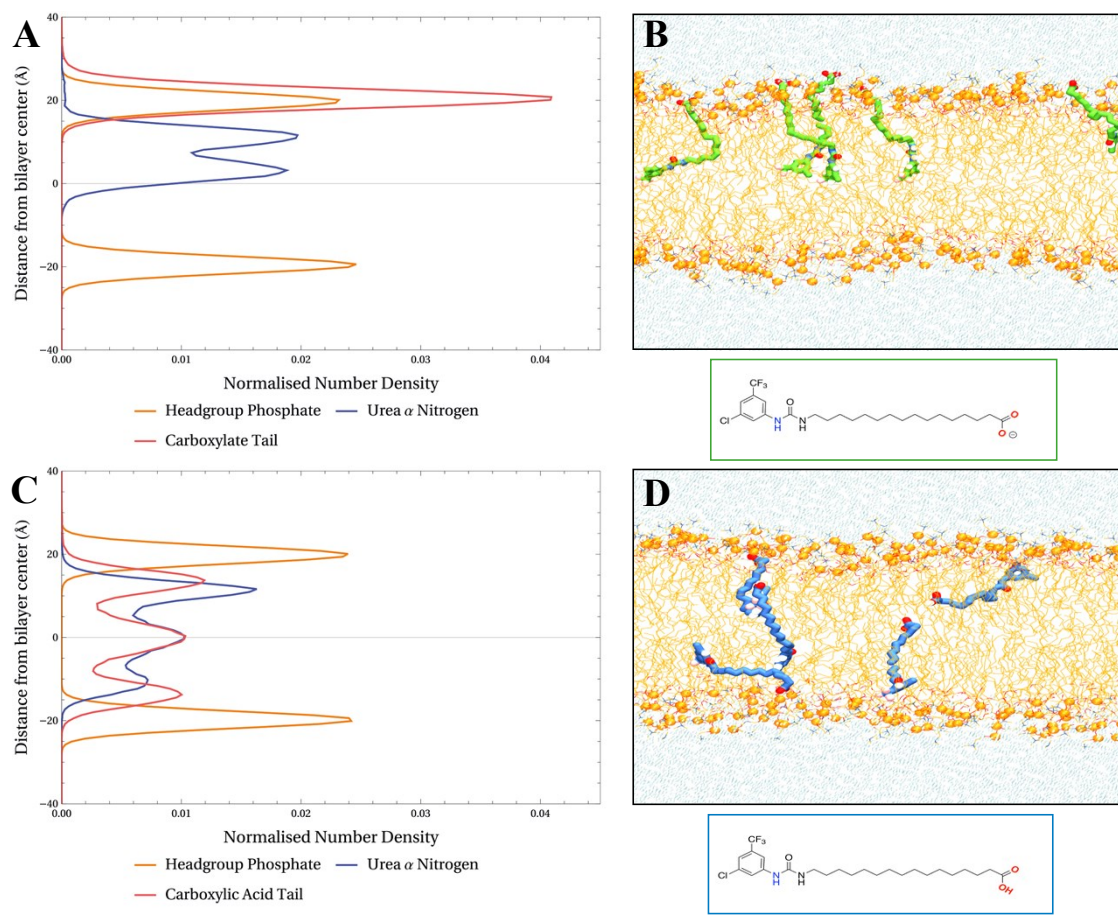
Figure S2: Normalised Z axis number densities and representative simulation snapshots for various species in a DOPC bilayer over the simulation timeframe (4 microseconds per system). Normalized Z axis number densities are shown for the **6-D** and **6** containing systems in a) and c) while the corresponding simulation snapshots are shown in b) and d).
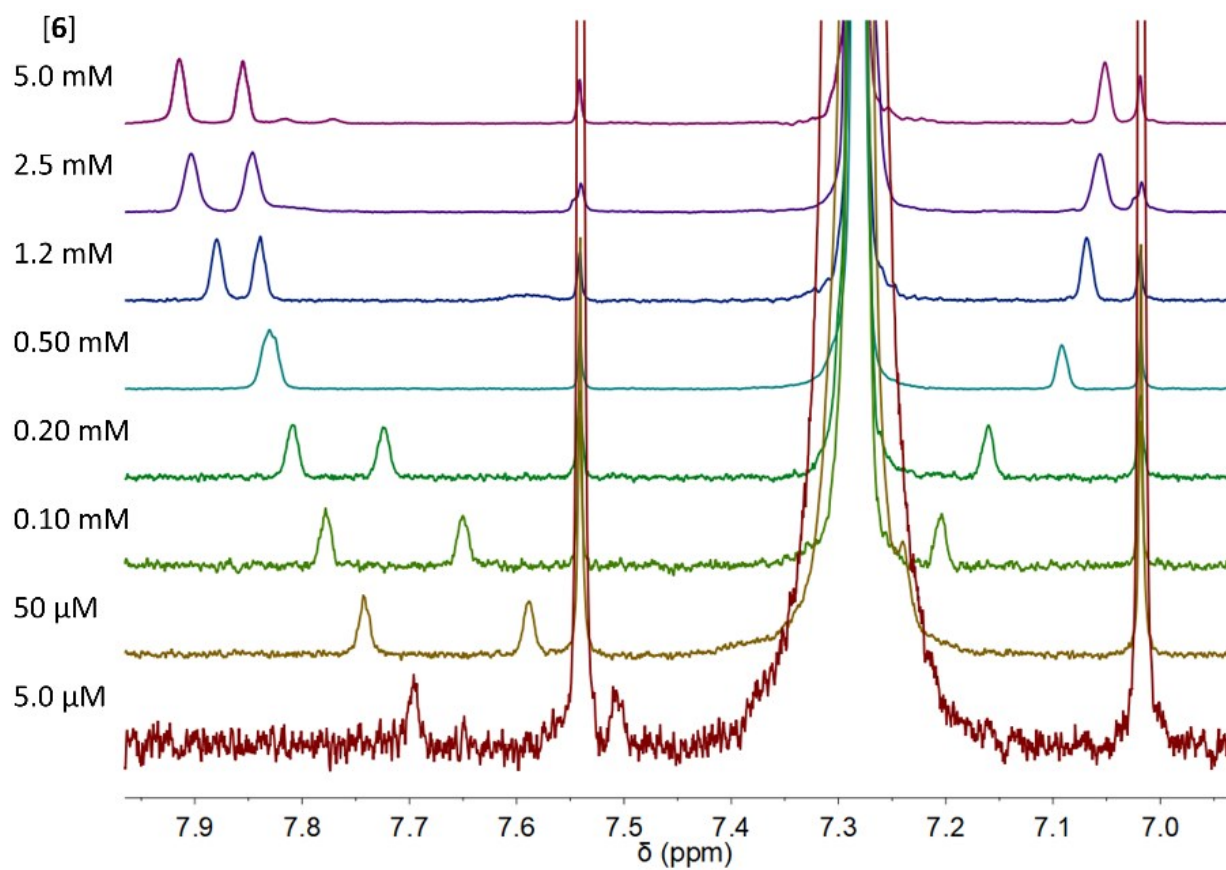
Figure. S3: Concentration-dependent ^{1}H NMR (400 MHz) spectra of **6**-TBAOH in CDCl$_3$ at 298 K.

The plot contains an inset fit results table:

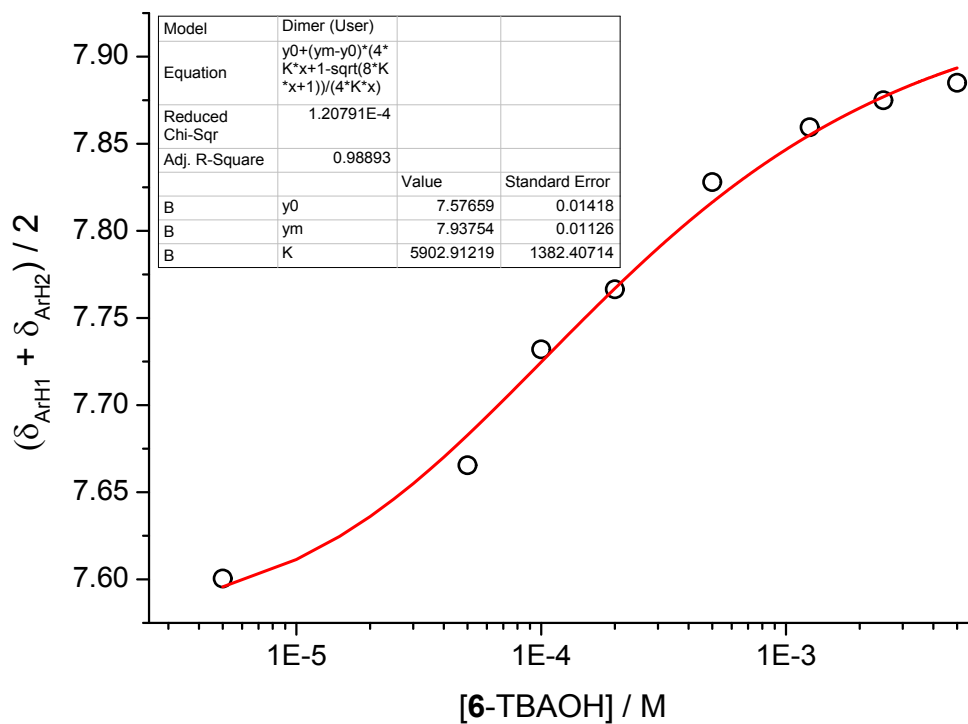| Model	Dimer (User)		
Equation	y0+(ym-y0)*(4*K*x+1-sqrt(8*K*x+1))/(4*K*x)		
Reduced Chi-Sqr	1.20791E-4		
Adj. R-Square	0.98893		
		Value	Standard Error
B	y0	7.57659	0.01418
B	ym	7.93754	0.01126
B	K	5902.91219	1382.40714

Figure S4: Averaged chemical shifts of two aromatic CH peaks from 7.5 to 7.9 ppm at different concentrations of **6**-TBAOH in $CDCl_3$ at 298 K. The data was fitted to a monomer-dimer equilibrium model, giving a dimerisation constant (K_2) of 5.9×10^3 M^{-1}.
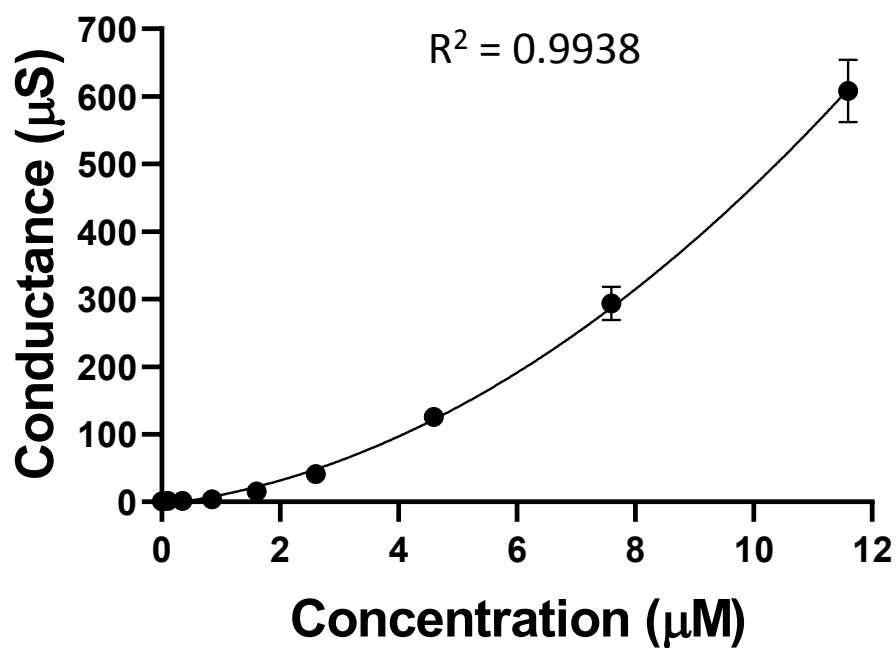
Figure S5. Conductance measures of DOPC tethered bilayer lipid membranes in response to increasing concentrations of **6**. The quadratic regression was made with GraphPad Prism 8.2.1. Data represents the mean ± SEM of 3 independent experiments.

3. Experimental procedures – Biology

Cell culture and cell-based assays.

Human tumour cell lines were obtained from ATCC (Manassas, VA) and were grown at 37°C in a humidified atmosphere of 5% CO2 in air in DMEM supplemented with 10% fetal bovine serum (Thermo Fisher Scientific) and 1% penicillin/streptomycin (Invitrogen). Confluent cells (80-90%) were harvested using Trypsin/EDTA after washing in PBS. Cells were treated with various concentrations of the test compounds in DMSO (final concentration 0.1%); control cells were treated with DMSO alone.

ATP assay: MDA-MB-231 cells were seeded in triplicate in 96-well plates (7.5×10^4 cells/well) and allowed to adhere overnight. After serum starvation for 24 h cells were treated with various concentrations of the test compounds for 24 h; control cells received serum-free DMEM. Cells were incubated with CellTiter-Glo in serum-free medium (RT, 10 min) and luminescence was determined (CellTiter-Glo® luminescent cell viability assay, Promega; Annandale, NSW, Australia).

JC-1 assay: MDA-MB-231 cells were seeded in triplicate in 96-well plates (1×10^4 cells/well) and allowed to adhere overnight. After serum starvation for 24 h cells were treated with various concentrations of the test compounds for 1 h; control cells received serum-free DMEM. Cells were incubated with JC-1 in serum-free medium (37°C, 20 min) and the JC-1 red:green ratio was estimated (JC-1 Mitochondrial Membrane Potential Assay Kit; Cayman Chemical, Ann Arbor, MI).

Mitochondrial function: Mitochondrial function was measured by determining the oxygen consumption rate (OCR) of cells with a Seahorse XF24 extracellular flux analyser (Seahorse Bioscience, MA, USA) according to the manufacturer's protocol. MDA-MB-231 cells were seeded in 24-well XF cell culture microplates (2.5×10^4 cells per well) and allowed to adhere

overnight (37 °C, 5% CO_2). After serum starvation for 24 h, culture media was replaced with buffered XF Base Medium supplemented with 2 mM L-glutamine, 10 mM glucose and 2 mM sodium pyruvate at pH=7.4. The cells were incubated at 37 °C without CO_2 for an hour, and then, the OCR was measured utilizing an XF Cell Mito Stress Test Kit (Seahorse Bioscience, MA, USA). Oligomycin (final concentration 1 µM), carbonylcyanide m-chlorophenylhydrazone (FCCP-final concentration 0.5 µM, or test compounds - final concentrations 20 µM), and rotenone/antimycin A (final concentration 0.5 µM) were added to the sensor cartridge, and the OCR was measured using a modified cycling program.

4. Experimental procedures – Tethered bilayer lipid membranes

Tethered bilayer lipid membranes

Lipid bilayers were anchored to across a gold electrode according to "T10" architecture.[1-2] This consists of 10% benzyl-disulfide (tetra-ethyleneglycol) n=2 C20-phytanyl "tethering" molecules interspersed with 90% benzyl-disulfide-tetra-ethyleneglycol-OH "spacer" molecules. Spacer and tether molcules are all coordinated onto a 2.1 mm2 gold tethering electrode. To these first layer chemistries were added a second layer of mobile phase lipid molecules of 3 mM 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) (Avanti Polar Lipids Inc., Alabaster, USA) which was left to incubate with the tethering molecules for exactly 2 min before a rapid exchange of 3 x 400 µL 100 mM NaCl tris buffer induced the formation of a completed tBLM.

Electrical impedance spectroscopy

Swept frequency electrical impedance spectroscopy ranging from 0.1 Hz to 2000 Hz was applied at 25 mV peak-to-peak, using a Tethapod™ electrical impedance spectrometer (SDx Tethered Membranes Pty Ltd). Impedance and phase profiles were fitted to an equivalent circuit consisting of a constant phase element, representing the tethering gold electrode and reservoir region, in series with a resistor, to represent the impedance of the surrounding electrolyte solution, and a resistor/capacitor representing the lipid bilayer (as described previously[3]). Data fitting utilized a proprietary adaptation of a Levenberg–Marquardt fitting routine incorporated into the TethaQuick™ software (SDx Tethered Membranes Pty Ltd).

5. Experimental procedures – Chemistry

General Chemistry

Compounds **1**, **8**, **11**, **12** and **14** were prepared by previously reported procedures.[4-5] Reagents and anhydrous solvents were purchased from Sigma Aldrich (Castle Hill, NSW, Australia), Fluorochem (Derbyshire, United Kingdom) and Astatech (Bristol, USA), and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) using silica gel 60 F_{254} plates. TLC plates were visualised with UV light and potassium permanganate TLC stain. Reaction products were purified by dry column vacuum chromatography on silica gel using gradient elutions. ^1H and ^{13}C NMR spectra were recorded on an Agilent 500 MHz NMR. Spectra were referenced internally to residual solvent (CDCl$_3$; ^1H δ 7.26, ^{13}C δ 77.10. DMSO-d_6; ^1H δ 2.49, ^{13}C δ 39.52). High resolution mass spectra (HRMS) were recorded on an Agilent Technologies 6510 Q-TOF LCMS. The purity of all test compounds was confirmed to be >95% by absolute quantitative NMR.

Synthesis of aryl ureas 2- 13
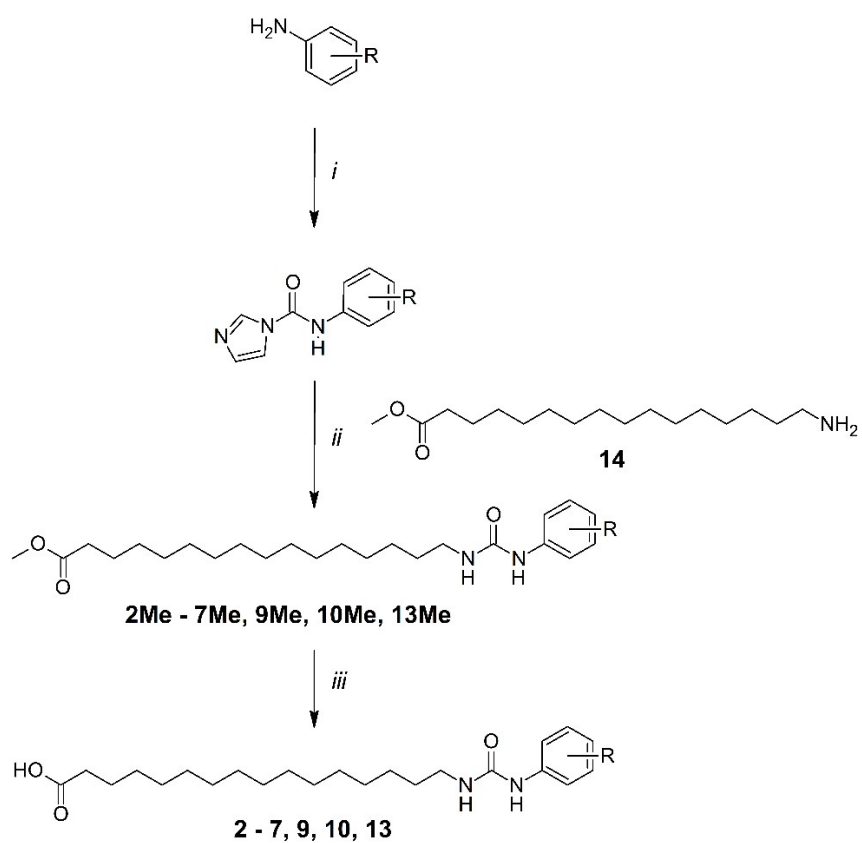
Scheme S1. Synthesis of aryl-urea substituted fatty acids **2-13**. Reagents and conditions (*i*)

dichloromethane, rt, 2 h; (*ii*) dichloromethane, rt, 1 h; (*iii*) 1.5M NaOH, ethanol, rt, 3 h.

General Procedure A: Urea formation

N,N-carbonyldiimidazole (1.0 mmol) was added to a solution of an appropriately substituted aniline (1.0 mmol) in anhydrous dichloromethane (20 mL) under N_2. The solution was stirred at room temperature for 2 hours and the solvent was removed *in vacuo* to provide a crude N-carbamoyl imidazole as a solid. The crude N-carbamoyl imidazole was then added to a solution of amine **14** (0.150g, 0.53 mmol) in dichloromethane (15 mL) and the reaction was stirred at room temperature for 1 hour. Ethyl acetate (50mL) was added and the solution washed with water (3 x 50 mL). The organic layer was dried over sodium sulphate and evaporated *in vacuo*. The crude product was purified by DCVC using gradient elutions of dichloromethane/ethyl acetate (100:0 to 85:15) or dichloromethane/methanol (100:0 to 85:10).
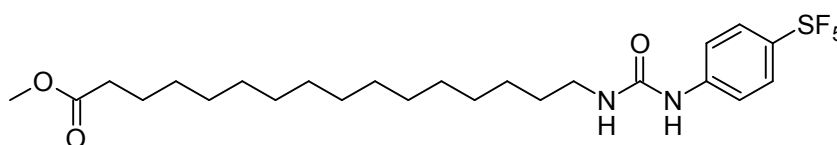
Methyl 16-({[4-(pentafluoro-λ⁶-sulfanyl)phenyl]carbamoyl}amino)hexadecanoate (2-Me).

Product isolated as an impure solid that was used directly in General Procedure B. ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.68 (AA'BB', 2H), 7.46 (AA'BB', 2H), 6.25 (s, 1H), 4.72 (br, 1H), 3.70 (s, 3H), 3.30 (q, J = 6.5 Hz, 2H), 2.34 (t, J = 7.5 Hz, 2H), 1.6 (p, J = 7.0 Hz, 2H), 1.54 (p, J = 7.0 Hz, 2H), 1.33-1.20 (m, 22H). HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{24}$H$_{40}$O$_3$N$_2$F$_5$S 531.2674; found 531.2682.
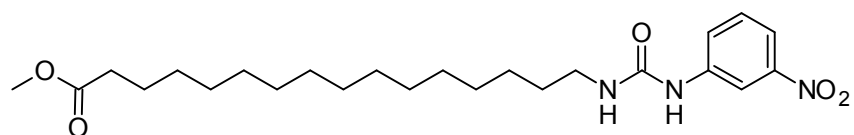
Methyl 16-[(3-nitrophenyl)carbamoylamino]hexadecanoate (3-Me).

White solid, yield = 45 %. Mp = 110-112 °C. ^{1}H NMR (500 MHz, DMSO-d$_6$) δ 8.92 (s, 1H), 8.50 (dd, J = 2.0 Hz, 1H), 7.73 (dd, J = 8.0, 1.5 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 6.31 (t, J = 6.0 Hz, 1H), 3.54 (s, 3H), 3.09 (q, J = 6.5 Hz, 2H), 2.26 (t, J = 7.0 Hz, 2H), 1.48 (p, J = 7.0 Hz, 2H), 1.42 (p, J = 7.0 Hz, 2H), 1.30 − 1.18 (m, 22H). ^{13}C NMR (125MHz, DMSO-d$_6$) δ 176.47, 158.00, 151.22, 145.06, 132.97, 126.69, 118.44, 114.54, 54.29, 36.37, 32.71, 32.13 (4C), 32.10, 32.08, 31.97, 31.85, 31.77, 31.55, 29.44, 27.54. HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{24}$H$_{40}$O$_5$N$_3$ 450.2962; found 450.2985.
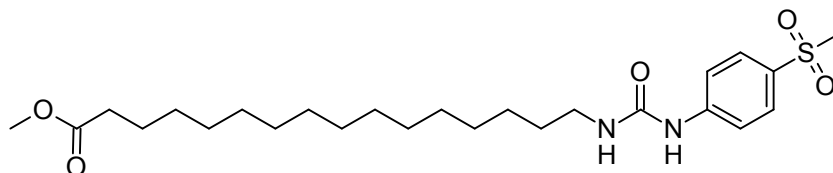
Methyl 16-({[4-(methanesulfonyl)phenyl]carbamoyl}amino)hexadecanoate (4-Me).

White solid, yield = 86%. Mp = 124-125 °C. ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.80 (AA'BB', 2H), 7.54 (AA'BB', 2H), 7.07 (br s, 1H), 5.06 (br s, 1H), 3.68 (s, 3H), 3.27 (q, J = 6.5 Hz, 2H), 3.03 (s, 3H), 2.32 (t, J = 7.5 Hz, 2H), 1.70-1.60 (m, 2H), 1.54 (p, J = 7.0 Hz, 2H), 1.40-1.20 (m, 22H). ^{13}C NMR (125 MHz, CDCl$_3$) δ 174.84, 154.66, 144.89, 133.20, 128.85 (2C), 118.49 (2C), 51.70, 44.94, 40.61, 34.33, 30.14, 29.63, 29.60 (2C), 29.48 (3C), 29.42, 29.34 (2C), 29.28, 27.02, 25.22. HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{25}$H$_{42}$N$_2$O$_5$S 483.2887; found 483.2899.
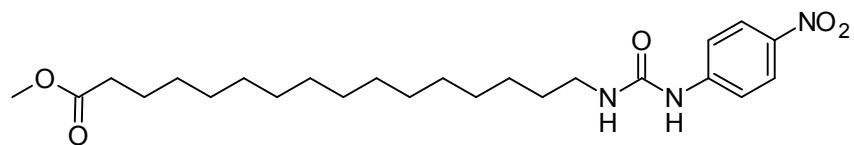
Methyl 16-[(4-nitrophenyl)carbamoylamino]hexadecanoate (5-Me).

White solid, yield = 45%. Mp = 128-130 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.38 (br, 1H), 8.10 (AA'BB', 2H), 7.62 (AA'BB', 2H), 7.11 (br, 1H), 3.60 (s, 3H), 3.08 (q, J = 6.5 Hz, 2H), 2.26 (t, J = 7.0 Hz, 2H), 1.55 − 1.40 (m, 4H), 1.30 − 1.20 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 175.59, 154.90, 147.79, 139.62, 125.29 (2C), 116.44 (2C), 51.59, 33.38, 29.67, 29.16, 29.11 (2C), 29.08 (2C), 28.85, 28.77, 28.66, 28.55, 26.44, 24.54. HRMS (ESI) *m/z* [M+H]$^+$ calcd for $C_{24}H_{40}O_5N_3$ 450.2962; found 450.2970.
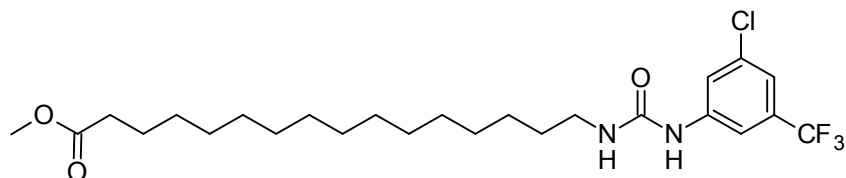
Methyl 16-[[3-chloro-5-(trifluoromethyl)phenyl]carbamoylamino]hexadecanoate (6-Me).

White solid, yield = 54%. Mp = 87-85°C. ^{1}H NMR (500 MHz, CDCl$_3$): δ 7.65 (s, 1H), 7.47 (s, 1H), 7.23 (s, 1H), 6.84 (s, 1H), 4.96 (s, 1H), 3.69 (s, 3H), 3.23 (q, J = 7.0 Hz, 2H), 2.33 (t, J = 7.5 Hz, 2H), 1.62 (p, J = 7.5 Hz, 2H), 1.53 (p, J = 7.0 Hz, 2H), 1.32-1.20 (m, 22H). ^{13}C NMR (125 MHz, CDCl$_3$): δ 174.98, 155.04, 140.88, 135.48, 132.62 (q, J = 33 Hz), 123.14 (q, J = 271 Hz), 122.10, 119.54 (q, J = 4 Hz), 115.87 (q, J = 4 Hz), 51.68, 40.62, 34.29, 31.07, 30.05,

29.51, 29.49, 29.48, 29.47 (2C), 29.37, 29.32, 29.24, 29.20, 26.92, 25.05. HRMS (ESI) *m/z* [M+H]⁺ calcd for $C_{25}H_{38}O_3N_2F_3Cl$ 507.2596; found 507.2576.
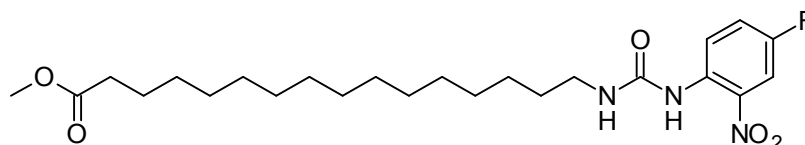
Methyl 16-[(4-fluoro-2-nitro-phenyl)carbamoylamino]hexadecanoate (7-Me).

White solid, yield = 48%. Mp = 96-98 °C. ¹H NMR (500 MHz, CDCl₃) δ 9.64 (br, 1H), 8.75 − 8.65 (m, 1H), 7.90 (dd, J = 8.5, 3.0 Hz, 1H), 7.36 (dd, J = 8.5, 3.0 Hz, 1H), 4.92 (br, 1H), 3.67 (s, 3H), 3.30 (q, J = 7.0 Hz, 2H), 2.31 (t, J = 7.0 Hz, 2H), 1.70 – 1.40 (m, 4H), 1.40 – 1.20 (m, 22H). ¹³C NMR (125MHz, CDCl₃) δ 177.09, 158.47 (d, J = 244 Hz), 156.70, 137.83 (d, J = 8 Hz), 136.46, 126.39 (d, J = 22 Hz), 125.98 (d, J = 7 Hz), 114.35 (d, J = 26 Hz), 54.12, 43.42, 36.79, 33.59, 32.51, 32.23 (3C), 32.19, 32.16, 32.06, 31.93, 31.89, 31.80, 29.51, 27.62. HRMS (ESI) *m/z* [M+H]⁺ calcd for $C_{24}H_{39}O_5N_3F$ 468.2868; found 468.2870.
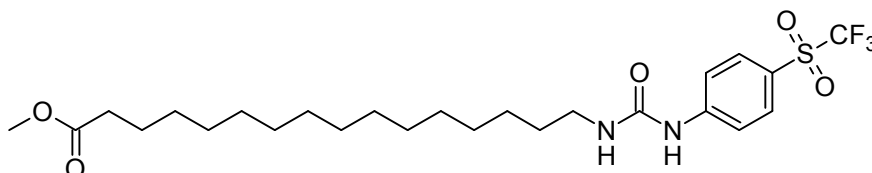
Methyl 16-({[4-(trifluoromethanesulfonyl)phenyl]carbamoyl}amino)hexadecanoate (9-Me).

Crude product triturated with methanol to yield a white solid, yield = 41%. Mp = 122.5-123.7 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.91 (AA'BB', 2H), 7.68 (AA'BB', 2H), 7.05 (s, 1H), 4.96 (br s, 1H), 3.69 (s, 3H), 3.29 (q, J = 7.0 Hz, 2H), 2.31 (br s, 2H), 1.60-1.40 (m, 4H), 1.40-1.15 (m, 22H). ¹³C NMR (125MHz, CDCl₃) δ 174.84, 153.82, 147.21, 132.41 (2C), 119.89 (q, J = 324.875 Hz), 118.24 (2C), 112.01, 51.58, 40.55, 34.20, 29.90, 29.54, 29.31 (3C), 29.28, 29.21,

29.18, 29.11 (2C), 29.09, 26.79, 24.95. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{25}H_{39}O_5N_2F_3$ 537.2605; found 537.2614.
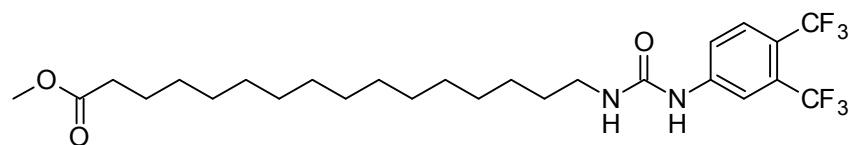
Methyl 16-[[3,4-bis(trifluoromethyl)phenyl]carbamoylamino]hexadecanoate (10-Me).

White solid, yield = 36%. Mp = 84-85 °C. ^{1}H NMR (500 MHz, DMSO-d$_6$) δ 9.23 (s, 1H), 8.16 (d, J = 2.0 Hz, 1H), 7.82 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 9.0 Hz, 1H), 6.42 (t, J = 6.5 Hz, 1H), 3.55 (s, 3H), 3.07 (q, J = 6.0 Hz, 2H), 2.25 (t, J = 7.5 Hz, 2H), 1.47 (p, J = 7.0 Hz, 2H), 1.42 (p, J = 6.5 Hz, 2H), 1.22-1.39 (m, 22H). ^{13}C NMR (125MHz, DMSO-d$_6$) δ 173.77, 154.99, 145.33, 129.70 (q, J = 6 Hz), 127.37 (q, J = 34 Hz), 123.71 (q, J = 270 Hz), 123.31 (q, J = 272 Hz), 120.24, 117.58 (q, J = 34 Hz), 116.36 (q, J = 6 Hz), 51.56, 33.69, 29.93, 29.47, 29.45, 29.44, 29.43, 29.40 (2C), 29.29, 29.14, 29.10, 28.88, 26.72, 24.86. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{26}H_{39}F_6N_2O_3$ 541.2859; found 541.2862.
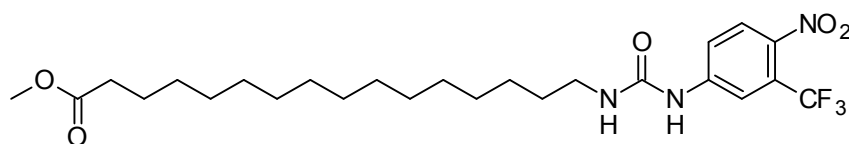
Methyl 16-[[4-nitro-3-(trifluoromethyl)phenyl]carbamoylamino]hexadecanoate (13-Me).

White solid, yield = 55%. Mp = 99-100 °C. ^{1}H NMR (500 MHz, DMSO-d$_6$) δ 9.45 (s, 1H), 8.15 (d, J = 2.5 Hz, 1H), 8.10 (d, J = 9.0 Hz, 1H), 7.72 (dd, J = 9.0, 2.5 Hz, 1H), 6.53 (t, J = 5.5 Hz, 1H), 3.55 (s, 3H), 3.07 (q, J = 7.0 Hz, 2H), 2.27 (t, J = 7.0 Hz, 2H), 1.48 (p, J = 7.5 Hz, 2H), 1.42 (p, J = 7.5 Hz, 2H), 1.50-1.30 (m, 22H). ^{13}C NMR (125MHz, DMSO-d$_6$) δ 173.78,

154.74, 146.32, 139.65, 128.35, 123.72 (q, J = 33 Hz), 122.66 (q, J = 271 Hz), 120.40, 115.77 (q, J = 6 Hz), 51.57, 33.70, 29.86, 29.47, 29.46, 29.45, 29.43, 29.40 (2C), 29.30, 29.14, 29.10, 28.88, 26.72, 24.86. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{25}H_{39}O_5N_3F_3$ 518.2836; found 518.2840.

General Procedure B: Ester hydrolysis

To a solution of the ester (0.3 mmol) in ethanol (20 mL) was added 1.5M NaOH (7 mL), and the resulting solution was stirred for 3 hours at 40 °C. 1M HCl was added until the pH reached 2.0. The precipitate was extracted into dichloromethane (3 x 30 mL) and the combined organic phases were washed with water (2 x 50mL), dried over sodium sulphate and evaporated under reduced pressure.
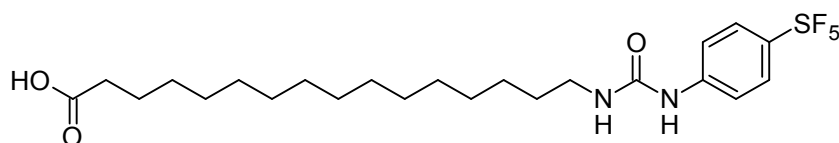
16-({[4-(pentafluoro-λ^6-sulfanyl)phenyl]carbamoyl}amino)hexadecanoic acid (2).

The crude product isolated after filtration was purified by DCVC using ethyl acetate/chloroform (10:90). White solid, yield = 80%. Mp = 101-102 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.82 (s, 1H), 7.58-7.52 (m, 4H), 6.25 (t, J = 5.5 Hz, 1H), 3.07 (q, J = 6.5 Hz, 2H), 2.17 (t, J = 7.5 Hz, 2H), 1.50-1.40 (m, 4H), 1.30-1.15 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 174.79, 155.47, 142.33, 140.69, 132.23 (2C), 122.41 (2C), 33.92, 30.02, 29.40, 29.39 (2C), 29.35 (2C), 29.26, 29.19, 29.10 (2C), 28.91, 26.71, 24.82. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{23}H_{38}O_3SN_2F_5$ 517.2518, found 517.2518. Anal. Calcd for $C_{23}H_{37}O_3SN_2F_3$: C 53.47, H 7.22, N 5.42. Found: C 53.09, H 7.07, N 5.30.
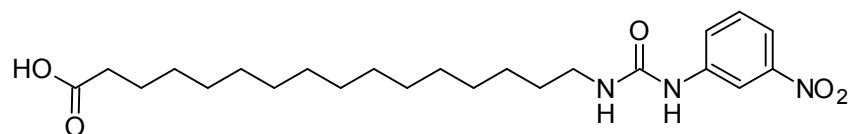
16-[(3-nitrophenyl)carbamoylamino]hexadecanoic acid (3).

White solid, yield = 86%. Mp = 104-105 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.94 (s, 1H), 7.96 (s, 1H), 7.49 (d, 7.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 7.18 (d, J = 7.5 Hz, 1H), 6.41 (br s, 1H), 3.06 (q, J = 6.5 Hz, 2H), 2.15 (t, J = 7.5 Hz, 2H), 1.50 - 1.36 (m, 4H), 1.30-1.20 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 175.01, 155.35, 148.57, 142.43, 130.30, 124.02, 115.75, 111.87, 34.20, 30.05, 29.47 (2C), 29.46 (2C), 29.43 (2C), 29.33, 29.19, 29.01, 26.78, 24.98. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{23}H_{38}N_3O_5$ 436.2806; found 436.2814. Anal. Calcd for $C_{23}H_{37}N_3O_5$: C 63.42, H 8.56, N 9.65. Found: C 63.80, H 8.75, N 9.26.
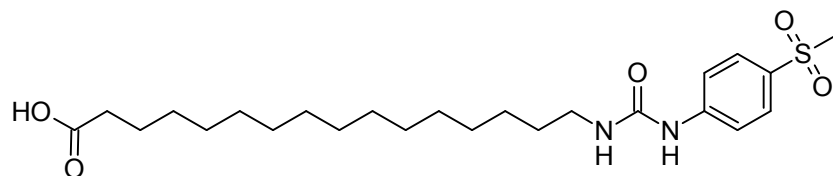
16-({[4-(methanesulfonyl)phenyl]carbamoyl}amino)hexadecanoic acid (4).

White solid, yield = 85%. Mp = 133-134 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.98 (s, 1H), 7.73 (AA'BB', 2H), 7.60 (AA'BB', 2H), 6.34 (s, 1H), 3.20-3.00 (m, 5H), 2.17 (br, 2H), 1.55-1.40 (m, 4H), 1.35-1.15 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 174.67, 154.78, 145.52, 132.18, 128.31 (2C), 117.06 (2C), 44.13, 33.83, 29.69, 29.15 (3C), 29.12 (2C), 29.03, 28.88 (2C), 28.86, 28.67, 26.47, 24.63. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{24}H_{41}O_5SN_2$ 469.2731; found 469.2727. Anal. Calcd for $C_{24}H_{40}N_2O_5S$: C 61.51, H 8.60, N 5.98. Found: C 61.37, H 8.80, N 5.72.
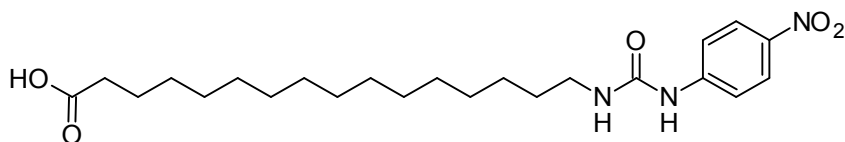
16-[(4-nitrophenyl)carbamoylamino]hexadecanoic acid (5).

White solid, yield = 90%. Mp = 115-116 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ11.76 (br, 1H), 8.88 (br, 1H), 8.06 (AA'BB', 2H), 7.71 (AA'BB', 2H), 3.03 (q, J = 6.0 Hz, 2H), 2.00 (t, J = 6.5 Hz, 2H), 1.46 (p, J = 7.0 Hz, 2H), 1.39 (p, J = 7.0 Hz, 2H), 1.30 – 1.20 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 177.48, 155.51, 149.16, 139.42, 125.08 (2C), 116.52 (2C), 37.27, 30.81, 29.39, 28.93, 28.78, 28.58, 28.49, 28.39, 28.22, 28.09 (2C), 27.72, 26.46, 25.92. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{23}H_{38}N_3O_5$ 436.2806; found 436.2809. Anal. Calcd for $C_{23}H_{37}N_3O_5$: C 63.42, H 8.56, N 9.65. Found: C 63.15, H 9.41, N 9.56.
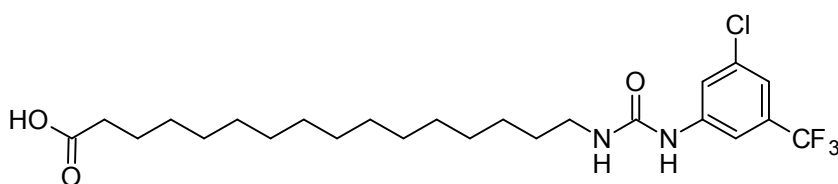
16-[[3-chloro-5-(trifluoromethyl)phenyl]carbamoylamino]hexadecanoic acid (6).

White solid, yield = 60%. Mp = 99-100°C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.95 (s, 1H), 9.00 (s, 1H), 7.75 (s, 2H), 7.27 (s, 1H), 6.39 (br, 1H), 3.06 (q, J=6.5 Hz, 2H), 2.17 (t, J = 7.0 Hz, 2H), 1.48-1.39 (m, 4H), 1.28-1.18 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 174.53, 154.73, 143.03, 134.08, 130.96 (q, J = 32 Hz), 123.38 (q, J = 271 Hz), 122.23, 116.71 (q, J = 4 Hz), 112.31 (q, J = 4 Hz), 33.69, 29.54, 29.06, 29.04 (2C), 29.01 (2C), 28.99, 28.92, 28.76, 28.73, 28.56, 26.30, 24.51. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{24}H_{37}O_3N_2F_3Cl$ 493.2439; found 493.2437. Anal. Calcd for $C_{24}H_{36}O_3N_2F_3Cl$: C 58.47, H 7.36, N 5.68. Found: C 58.72, H 7.52, N 5.47.
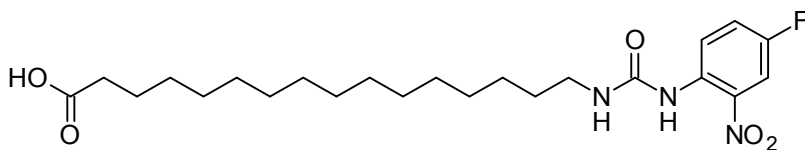
16-[(4-fluoro-2-nitro-phenyl)carbamoylamino]hexadecanoic acid (7).

White solid, yield = 87 %. Mp = 124-125 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.54 (br, 1H), 8.16 (d, J = 2.0 Hz, 1H), 8.10 (d, J = 8.5 Hz, 1H), 7.73 (dd, J = 8.5, 1.5 Hz, 1H), 6.63 (br, 1H), 3.05 (q, J = 6.5 Hz, 2H), 2.12 (t, J = 7.0 Hz, 2H), 1.45-1.39 (m, 4H), 1.30-1.10 (m, 22H). ^{13}C NMR (125MHz, DMSO-d_6) δ 178.04, 158.28 (d, J = 240 Hz), 157.40, 140.38, 127.36 (d, J = 7 Hz), 125.39 (d, J = 22 Hz), 114.63 (d, J = 28 Hz), 37.42, 32.49, 32.07 (6C), 31.98, 31.87, 31.85, 31.76, 29.46, 27.87. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{23}H_{37}O_5N_3F$ 454.2712; found 454.2717. Anal. Calcd for $C_{23}H_{36}O_5N_3F$: C 60.91, H 8.00, N 9.26. Found: C 60.50, H 7.81, N 9.27.
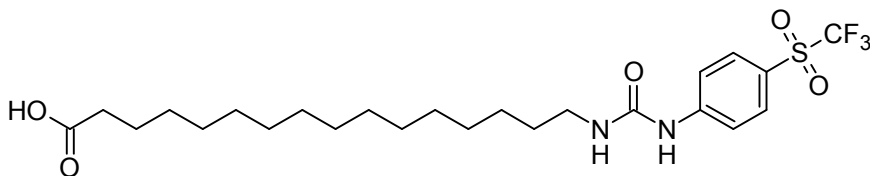
16-({[4-(trifluoromethanesulfonyl)phenyl]carbamoyl}amino)hexadecanoic acid (9).

White solid, yield = 72%. Mp = 95-97 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.45 (s, 1H), 7.91 (AA'BB', 2H), 7.77 (AA'BB', 2H), 6.56 (br, 1H), 3.09 (q, J = 6.5 Hz, 2H), 2.17 (t, J = 7.5 Hz, 2H), 1.55-1.40 (m, 4H), 1.35-1.15 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 175.02, 154.67, 149.71, 132.80 (2C), 120.14 (q, J = 324 Hz), 119.09, 118.15 (2C), 34.20, 29.86, 29.46 (3C), 29.44, 29.42, 29.33, 29.18 (2C), 29.17, 29.00, 26.74, 24.98. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{24}H_{38}O_5SN_2F_3$, 523.2448, found 523.2449. Anal. Calcd for $C_{24}H_{37}F_3N_2O_5S$: C 55.16, H 7.14, N 5.36. Found: C 55.04, H 6.88, N 5.30.
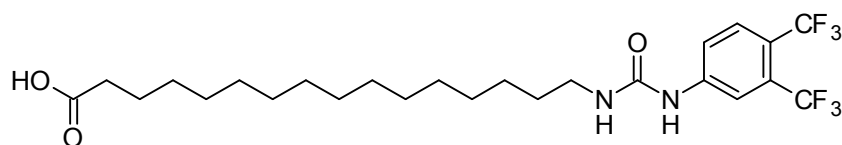
16-[[3,4-bis(trifluoromethyl)phenyl]carbamoylamino]hexadecanoic acid (10).

White solid, yield = 80%. Mp = 83-84 °C. ^{1}H NMR (500 MHz, CDCl$_3$) δ 9.29 (s, 1H), 8.16 (d, J = 2.0 Hz, 1H), 7.82 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 9.0 Hz, 1H), 6.47 (t, J = 6.0 Hz, 1H), 3.07 (q, J = 6.5 Hz, 2H), 2.15 (t, J = 7.0 Hz, 2H), 1.50-1.30 (m, 4H), 1.22-1.39 (m, 22H). ^{13}C NMR (125MHz, DMSO-d_6) δ 174.98, 155.02, 145.36, 129.72 (q, J = 6 Hz), 127.31 (q, J = 32 Hz), 123.72 (q, J = 270 Hz), 123.31 (q, J = 272 Hz), 120.24, 117.55 (q, J = 33 Hz), 116.34 (q, J = 7 Hz), 34.16, 29.92, 29.47, 29.45 (2C), 29.43, 29.42, 29.40, 29.30, 29.18, 29.15, 28.99, 26.73, 24.95. HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{25}$H$_{37}$F$_6$N$_2$O$_3$ 527.2703; found 257.2699. Anal. Calcd for C$_{25}$H$_{36}$F$_6$N$_2$O$_3$: C 57.02, H 6.89, N 5.32. Found: C 56.92, H 6.83, N 5.29.
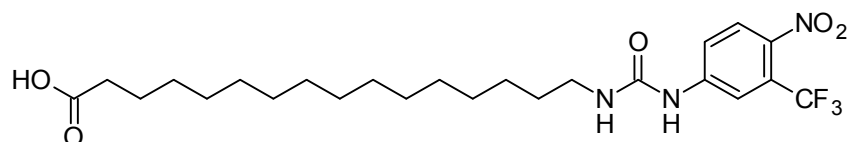
16-[[4-nitro-3-(trifluoromethyl)phenyl]carbamoylamino]hexadecanoic acid (13).

 White solid, yield = 41%. Mp = 106-107 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.54 (br, 1H), 8.16 (d, J = 2.0 Hz, 1H), 8.10 (d, J = 9.0 Hz, 1H), 7.74 (dd, *J* = 9.0, 2.0 Hz, 1H), 6.23 (br, 1H), 3.09 (q, *J* = 6.5 Hz, 2H), 2.16 (t, J = 7.0 Hz, 2H), 1.50 – 1.40 (m, 4H), 1.30 – 1.10 (m, 22H). ^{13}C NMR (125.5 MHz, DMSO-d_6): δ 174.63, 154.42, 146.02, 139.31, 128.04, 123.37 (q, J = 21 Hz), 122.38 (q, J = 283 Hz), 120.09, 115.44, 33.81, 29.54, 29.14 (3C), 29.10 (3C), 29.01, 28.85, 28.82, 28.66, 26.40, 24.62. HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{24}$H$_{37}$O$_5$N$_3$F$_3$ 504.2680,

found 504.2681. Anal. Calcd for $C_{24}H_{36}F_3N_2O_5$: C 57.24, H 7.21, N 8.34. Found: C 57.22, H 7.39, N 8.18.

Synthesis of 6-NNMe
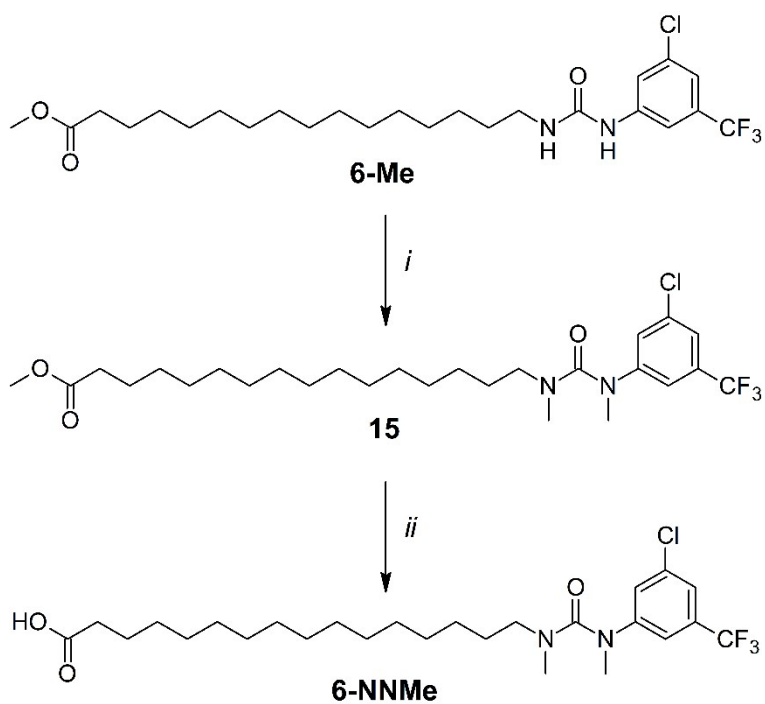
Scheme S2. Synthesis of **6-NNMe**. Reagents and conditions (*i*) NaH, DMF, 0°C, 10 min, then MeI, rt, 8 h; (*ii*) 1.5M NaOH, ethanol, rt, 3 h.
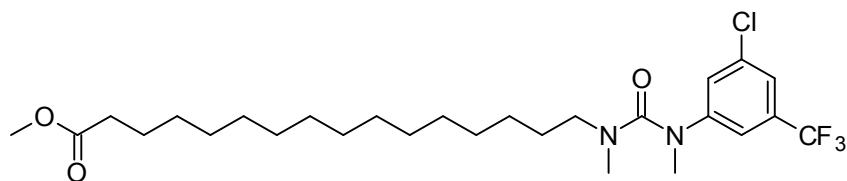
methyl 16-[{[3-chloro-5-(trifluoromethyl)phenyl](methyl)carbamoyl}(methyl)amino]hexadecanoate (15)

6-Me (0.150 g, 0.30 mmol) was dissolved in dry DMF (7 mL) under N_2 at 0°C. NaH (60% solution in mineral oil, 0.018 g, 0.74 mmol) was added and the reaction mixture was stirred at 0°C for 10 minutes. MeI (92 uL, 1.48 mmol) was then added and solution was stirred at room temperature for 8 hours. The reaction mixture was diluted in water (50 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layers were washed with water (2 x 100 mL), brine (1 x 100 mL) and dried on Na_2SO_4, and then concentrated under reduced pressure. The residue was purified on silica gel by stepwise gradient elutions with dichloromethane/ethyl acetate (100:0 to 80:20), yielding 0.150 g (95%) of an off-white solid. Mp 39-40 °C. ^{1}H NMR (500 MHz, CDCl$_3$): δ 7.27 (s, 1H), 7.18-7.17 (m, 1H), 7.14 (s, 1H), 3.66 (s, 3H), 3.22-3.19 (m, 5H), 2.70 (s, 3H), 2.30 (t, J = 7 Hz, 2H), 1.62 (p, J = 7 Hz, 2H), 1.49 (p, J = 7 Hz, 2H), 1.29-1.25 (m, 22 H). ^{13}C NMR (125 MHz, CDCl$_3$): δ 174.5, 160.7, 148.4, 135.8, 133.1, (q, J = 33 Hz), 124.5, 123.2 (q, J = 273 Hz), 119.9, 116.4, 51.5, 50.1, 38.62, 36.05, 34.25, 29.75 (3C), 29.71, 29.70, 29.63, 29.58, 29.45, 29.38, 29.28, 27.27, 27.00, 25.09. HRMS (ESI) *m/z* [M+H]$^+$ calcd for C$_{27}$H$_{43}$ClF$_3$N$_2$O$_3$, 535.2914; found, 535.2903.
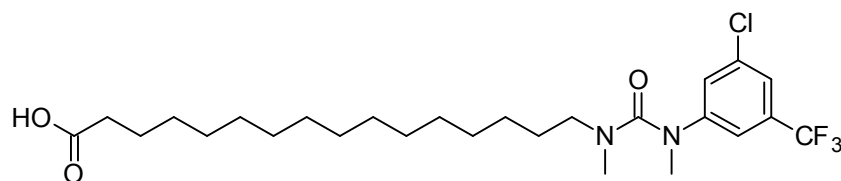
16-[{[3-chloro-5-(trifluoromethyl)phenyl](methyl)carbamoyl}(methyl)amino]hexadecanoic acid (6-NNMe)

Prepared from **15** according to General Procedure B. White solid, yield = 99%. Mp = 64-65 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.94 (s, 1H), 7.39 (s, 1H), 7.35 (s, 1H), 7.22 (s, 1H), 3.20 (t, J = 8.5 Hz, 2H), 3.12 (s, 3H), 2.70 (s, 3H), 2.17 (t, J = 7 Hz, 2H), 1,48-1.41 (m, 4H), 1.25-1.17 (m, 22H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 174.4, 159.8, 147.9, 134.6, 131.5 (q, J = 32 Hz), 123.2 (q, J = 273 Hz), 122.7, 117.8, 114.5, 48.96, 37.27, 35.21, 33.65, 29.00, 28.99 (3C), 28.92, 28.90, 28.75, 28.66, 28.55, 26.51, 26.19, 24.49. HRMS (ESI) m/z [M+H]$^+$ calcd for $C_{26}H_{41}ClF_3N_2O_3$, 521.2758; found, 521.2750. Purity by Q-NMR = 96.1%.

6. Experimental procedures – Crystallography

Single crystals of **6** and **6**-DMF solvate were obtained by vapour diffusion of H_2O and Et_2O, respectively, into DMF solutions of **6**. The crystals were mounted on a MITIGEN holder with paratone-N oil. Data were collected using a SuperNova-Duo, Atlas diffractometer equipped with an Oxford Cryosystems low-temperature device operating at $T = 100(2)$ K. The structure was solved with the olex2.solve 1.3[6] structure solution program using the Charge Flipping solution method and by using **Olex2**[7] as the graphical interface. The model was refined with version 2018/3 of ShelXL 2018/3[8] using Least Squares minimisation.

Compound	6	6-DMF
Formula	$C_{24}H_{36}ClF_3N_2O_3$	$C_{27}H_{43}ClF_3N_3O_4$
Dcalc./ g cm^{-3}	1.337	1.305
μ/mm^{-1}	1.824	1.656
Formula Weight	493.00	566.09
Colour	clear colourless	clear colourless
Size / mm^3	0.40×0.05×0.02	0.186×0.094×0.041
T / K	100(2)	100(2)
Crystal System	monoclinic	triclinic
Space Group	*P21/c*	*P-1*
a / Å	19.0452(4)	10.4481(3)
b / Å	7.53882(12)	13.0857(4)
c / Å	18.2425(4)	21.6967(8)
α / °	90	90.279(3)
β / °	110.706(2)	98.533(3)
γ / °	90	100.758(2)
V / Å^3	2450.04(9)	2880.37(16)
Z	4	4
Z'	1	1
Wavelength / Å	1.54184	1.54184
Radiation type	Cu Kα	Cu Kα
Θ_{min} / °	4.892	3.951
Θ_{max} / °	72.689	72.738
Measured Refl.	16382	20897
Independent Refl.	4788	11109
R_{int}	0.0323	0.0258
Parameters	382	784
Restraints	229	379
Largest Peak	0.293	0.27
Deepest Hole	-0.351	-0.35
GooF	1.066	1.027
wR$_2$ (all data)	0.1066	0.1141
wR$_2$	0.1019	0.1042
R$_1$ (all data)	0.0458	0.0549
R$_1$	0.0394	0.0406

7. Experimental procedures – Computational Methodology

Calculation of Aqueous pKa Values

To investigate the possible role of fatty acid aryl ureas in a mitochondrial uncoupling mechanism, we first calculated the pKa of the urea NH proton most proximal to the ring for each of the derivatives shown in Table 1 using a high accuracy thermochemistry method. The studied fatty acid aryl ureas are too large to be considered in their entirety without significant computational expense. Furthermore, the 16-carbon tail will likely have a minimal effect on pKa values at the urea NH proton proximal to the ring. To this end, model compounds were constructed by truncating the 16-carbon tail of the structures in Table 1 to a propyl moiety. The resulting structures are shown in Table S1. pKa calculations were conducted using an isodesmic proton exchange method, otherwise known as a relative pKa calculation. The G3(MP2)CC(+)[9,10] composite procedure was used to obtain ab initio gas phase reaction energies from geometries optimised using the M06-2X functional[11] and 6-31+G(d) basis set.[12-16] The G3(MP2)CC(+) composite procedure is a modification of the original G3(MP2)CC variant of Gaussian-n theory[9,10] in which calculations with the 6-31G(d) basis set have been replaced by the 6-31+G(d) basis set, allowing improved description of anionic species.[17] The G3(MP2)CC(+) procedure has demonstrated high accuracy for determination of pKa values over a range of studies and compound classes.[17-18] As stated above, ab initio gas-phase reaction energies were computed using the G3(MP2)CC(+) composite method, using geometries optimised at the M06-2X/6-31+G(d) level of theory. DFT geometry optimisations and MP2 calculations were carried out in Gaussian09, Revision E.01,[19] while CCSD(T) calculations were carried out with QChem 5.0[20] using the libxm tensor backend.[21] Frequency calculations were conducted at each DFT optimised geometry to ensure a minimum on the potential energy surface had been located. Gas and solvent phase optimised geometries are provided in Supporting Information. Gas phase free energies at 298.15 K were obtained by inclusion of

zero-point vibrational energy, thermal corrections and entropies calculated from the frequencies of the M06-2X/6-31+G(d) optimised geometry. Standard statistical mechanics formulae for an ideal gas were used, invoking the rigid-rotor/harmonic oscillator approximation.[22] Scale factors for the M06-2X functional were used to correct the frequencies.[23] The G3(MP2)CC(+) protocol includes spin orbit (SO) and high level correction (HLC) terms which can be neglected in this case as relative pKa calculations do not involve atomic species and the total number of valence alpha and beta electrons is conserved. Solvation free energies were obtained using the SMD continuum solvation model,[24] in which the free energy of solvation is obtained from the difference of electronic energies in the gas-phase and implicit solvent at each respective optimised geometry.[25] Proton exchange methods for computing pKa values rely on choice of a reference species similar to the target compound to maximise cancellation of errors. Triclocarban (TCC) and diphenylurea (DPU) were chosen as reference species with published experimental pKa values of 12.7[26] and 12.59[27] respectively. For the formula used to obtain pKa values from an isodesmic proton exchange reaction and a comprehensive overview of pKa calculation strategies, the reader is directed to Ho & Coote.[17] pKa values obtained using each reference species (TCC and DPU) varied by ~0.5 pKa units, well within desired error for the calculation of aqueous pKa values.[17] Values stated in the main text are for those obtained using TCC as the reference species. Values for TCC and DPU are presented in Table S1, while components used in their calculation are presented in Table S3.

Calculation of Free Energies of Carboxylate Complexation

In light of experimentally determined uncoupling by the studied fatty acid aryl ureas, reaction energies were computed for binding of a model carboxylate compound, to each of the model compounds presented in Table S1. Propanoate was used as a model compound for carboxylic acids in this work, and the same truncated model compounds were used for the fatty acid aryl ureas as in the pKa calculations. Gas phase reaction energies for complexation of propanoate

were computed at the M06-2X/6-31+G(d) level of theory, using the Boys-Bernadi counterpoise correction for basis set superposition error (BSSE).[28,29] Gas phase free energies were obtained by the same method as described above for the pKa calculations. Solvation free energies were obtained in a non-polar solvent, n-pentadecane and in water using the SMD continuum solvent model,[24] yielding reaction free energies in each of these two solvents. These are termed ΔG_{bind}propanoate (or ΔG_{bind}prop) with the appropriate solvent indicated with brackets eg ΔG_{bind}propanoate(water) (or ΔG_{bind}prop(water)). Resulting free energies in the studied solvents are presented in Table S1. Components used in their calculation are presented in Table S4.

Calculation of Model Compound lipophilicity

Gibbs Free Energies of solvation (ΔG_{Solv}) were calculated for transferring the model fatty acid aryl urea compounds from water to n-pentadecane, either in isolation or in complex with propanoate. These will be referred to as ΔG_{Solv}Monomer$_{(W-P)}$ and ΔG_{Solv}Complex$_{(W-P)}$ respectively. Each of these values was calculated by subtracting the ΔG_{Solv} in water from that in n-pentadecane. This provides a relative measure of the lipophilicity of each of the model compounds, either in isolation or in complex with propanoate. ΔG_{Solv}Monomer$_{(W-P)}$ and ΔG_{Solv}Complex$_{(W-P)}$ values are tabulated in Table S2. Components used in their calculation are presented in Table S4.

Molecular Dynamics Simulations

To examine the interaction of a prototypical fatty acid aryl urea compound with a model bilayer, molecular dynamics simulations were conducted. Compound **6** was chosen for simulations as it had the most complete experimentally determined SAR. Both the carboxylate and carboxylic acid protonation states were simulated, referred to as **6-D** and **6** for deprotonated and protonated compound **6**, respectively.

A 128 lipid united atom 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) bilayer was used as a model bilayer, to mimic the tethered DOPC bilayer setup on which these compounds were tested. As phosphocholine lipids make up ~ 40% of the mitochondrial inner membrane,[30] DOPC was chosen as a physiologically relevant model bilayer for both the simulation and tethered bilayer setup. DOPC parameters were obtained from Poger et al[31,32] and united atom parameters for compounds 6-D and 6 were obtained from the Automated Topology Builder (ATB).[33] As the uncouplers are large by ATB standards (>40 atoms), the ATB-QM1 parameterisation was used, involving optimisation at the AM1 semi-empirical level of theory and assignment of MOPAC charges.[33]

The 128 DOPC bilayer was obtained pre-equilibrated from the ATB, with the bilayer oriented in the x-y plane.[33] The size of the box was extended in the z-direction to 14.3 nm, and the system was resolvated in the larger rectangular box. 100mM of NaCl was added to the solvent. For each of the systems, namely **6-D** and **6**, 5 molecules of the target compound were placed randomly in the water layer such that they were closer than half the box length to the positive z-axis of the bilayer. For each of the systems, this placement process was conducted four times to obtain four replicates for each system, giving a total of 8 replicates.

All simulations were performed using the GROMACS 2018 simulation package[34-36] under periodic boundary conditions. The temperature of the system was maintained at 310 K by coupling to an external bath using the Bussi velocity rescaling thermostat[37] and a temperature coupling constant of 0.1 ps. The pressure of the system was maintained at 1 bar with semi-isotropic pressure coupling, using an iso-thermal compressibility of 4.5×10^{-5} bar^{-1} and a coupling constant of 5 ps. A Berendsen barostat[38] was used for equilibration to ensure

stabilization of the box volume, followed by a Parinello-Rahman barostat[39] for production simulation. A timestep of 2 fs was used for all simulations. The LINCS[40] algorithm to constrain the length of covalent bonds to hydrogen atoms. Nonbonded interactions were calculated using particle mesh Ewald (PME) method[41] and a Verlet scheme, with a single cutoff of 1.4 nm. Each of the 8 systems was energy minimized, prior to 50 ns of equilibration. A one sided, flat-bottom harmonic restraint with a force constant of 20 kJ/mol and active distance of 6 nm was placed between the z axis distance between the center of mass of each of uncoupler molecules and the center of mass of the DOPC bilayer to ensure the aryl urea uncouplers annealed to the upper leaflet of the bilayer rather than passing through the periodic boundary and annealing to both leaflets. Each replicate was then simulated for 1 μs. The flat bottom restraint did not exert any force on the system during production replicates, ie the **6** and **6-D** molecules successfully annealed to the upper leaflet of the bilayer during the equilibration phase.

The final frame of each of the 4 **6-D** simulation replicates was used to initiate a set of systems, containing 20 uncoupler molecules in total: the original 5 deprotonated **6-D** molecules and 15 protonated **6** molecules. The additional 15 **6** molecules were placed in the water solvent layer next to the upper leaflet, using the same methodology as described above. These four systems were also simulated for 1 μs, using the same simulation protocol as described above. In total, this gave 12 μs of simulation across all systems.

Analysis

Analysis was conducted using VMD[42] and MDTraj[43] python scripts.

Data availability

Gaussian archive files for all optimised geometries are attached as Supporting Information.

Additionally, these along with Gaussian logfiles are available on Github:

https://github.com/hmacdope/Fatty-Acid-Aryl-Urea-QC-data. Molecular dynamics

topologies employed in this work are available on FigShare at:

https://doi.org/10.6084/m9.figshare.12095223.v1

8. Experimental procedures – NMR studies

Concentration-dependent ^{1}H NMR studies

A suspension of compound **6** in CDCl$_3$ was treated with 1.0 equivalent of tetrabutylammonium hydroxide (TBAOH, ~40% in H$_2$O) and sonicated for 20 min to give a clear solution of **6-TBAOH** at 5 mM. The solution was diluted to various concentrations in CDCl$_3$ and subject to ^{1}H NMR measurements on a Bruker AVANCE III 400 NMR Spectrometer. The data was fitted to a monomer-dimer equilibrium model.[44] Due to the ambiguity of relative peak positions during the dilution experiment and the overlap of one of the aromatic CH peaks of **6** with the CHCl$_3$ peak at the lowest concentration tested, the average chemical shifts of the two aromatic CH peaks from 7.5 to 7.9 ppm [($\delta_{ArH1} + \delta_{ArH2}$)/2] were used for data fitting.

Diffusion NMR studies

Pulse field gradient diffusion NMR experiments were performed on a Bruker Avance III 600 MHz Cryo NMR at 298 K with uncalibrated gradient strengths. The data were analysed using Bruker TopSpin 4.0.9. To obtain the absolute diffusion coefficients, the diffusion coefficient of CHCl3 in CDCl3 was measured and compared with a literature value.[45] The ratio between the literature and experimental values of diffusion coefficient of CHCl3 was used to calibrate the data.

9. NMR Spectra of test compounds

^{1}H NMR spectrum of **2** (500 MHz, DMSO-d_6)
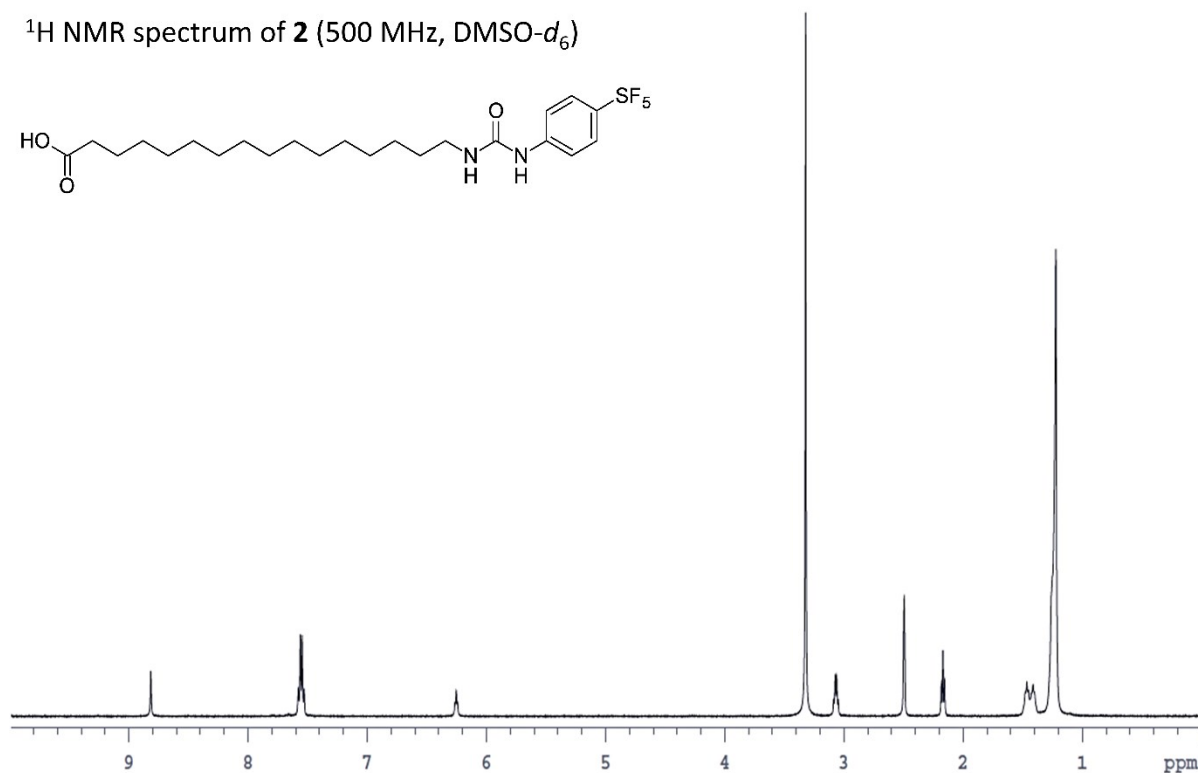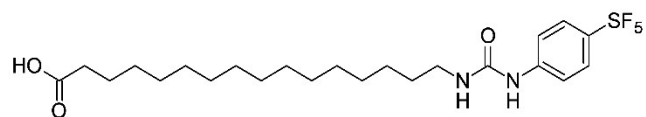
^{13}C NMR spectrum of **2** (125 MHz, DMSO-d_6)

^{1}H NMR spectrum of **3** (500 MHz, DMSO-d_6)

^{13}C NMR spectrum of **3** (125 MHz, DMSO-d_6)
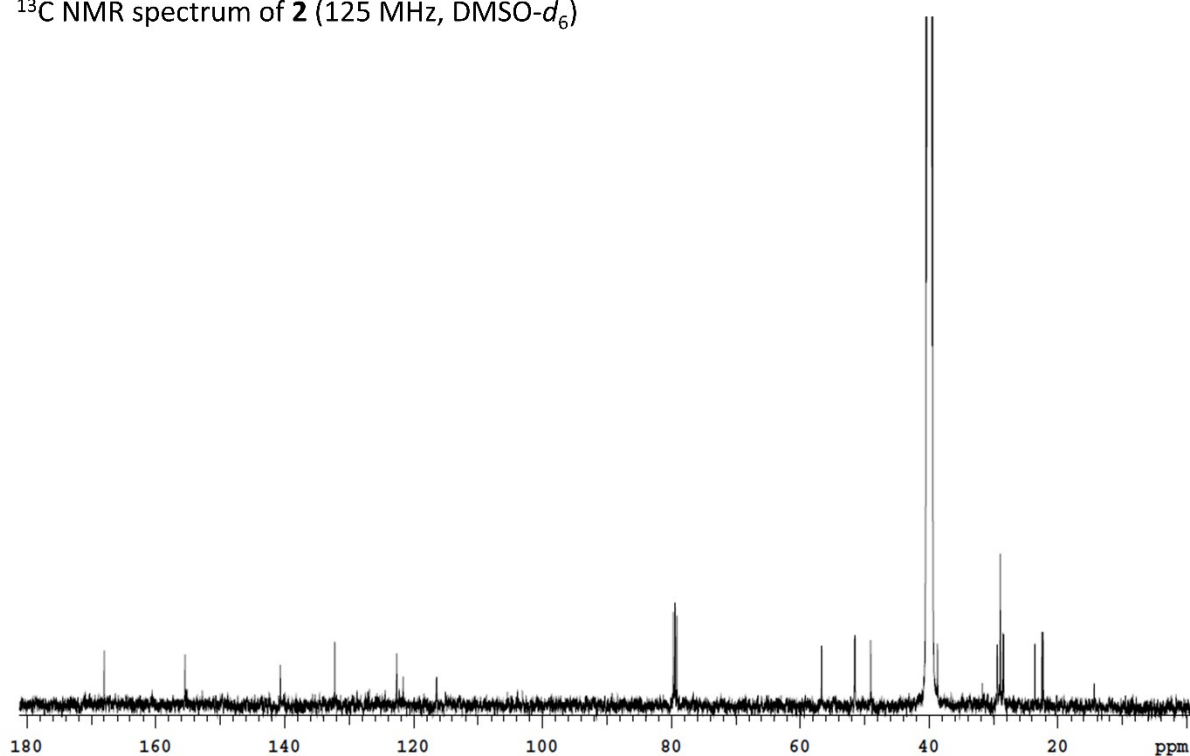
¹H NMR spectrum of **4** (500 MHz, DMSO-d_6)
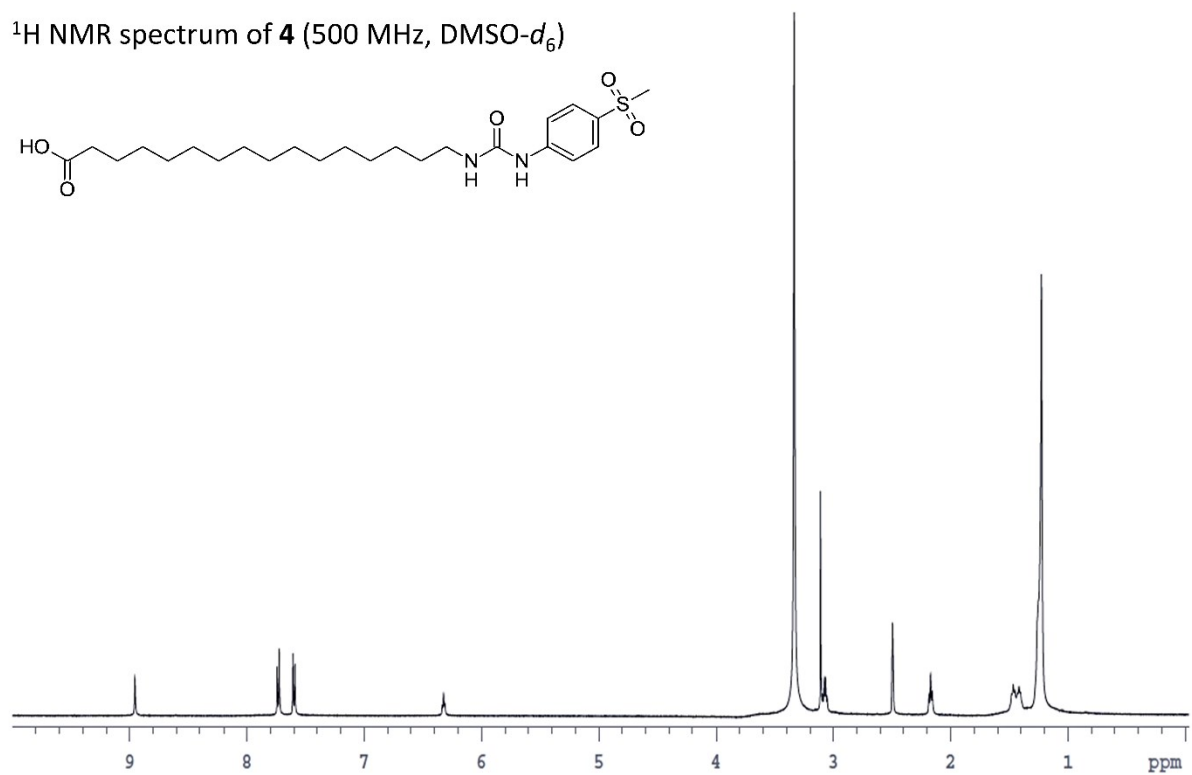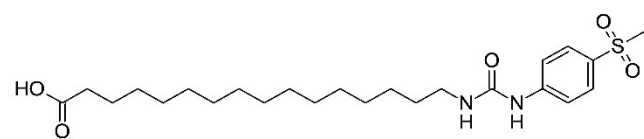
¹³C NMR spectrum of **4** (125 MHz, DMSO-d_6)
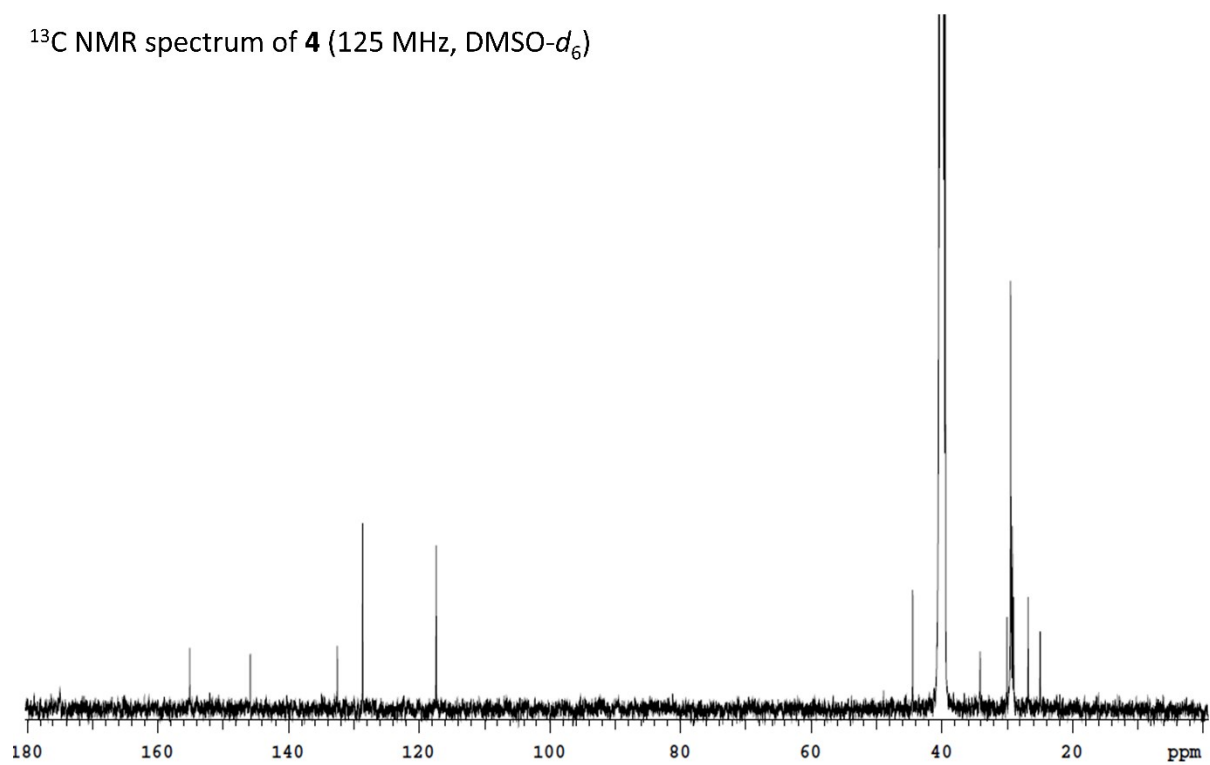
¹H NMR spectrum of **5** (500 MHz, DMSO-d_6)
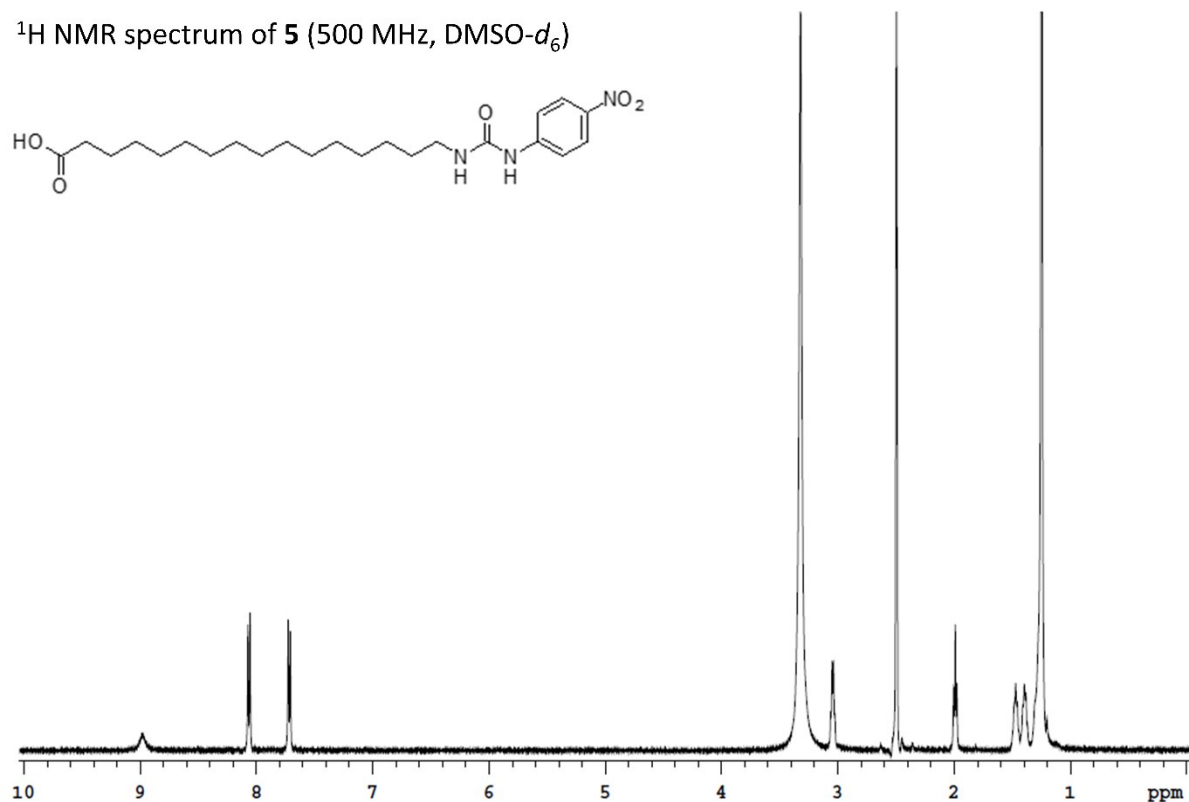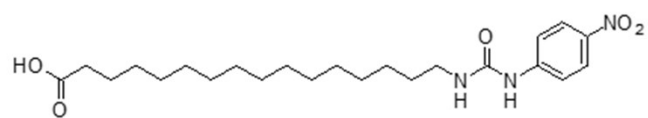
¹³C NMR spectrum of **5** (125 MHz, DMSO-d_6)
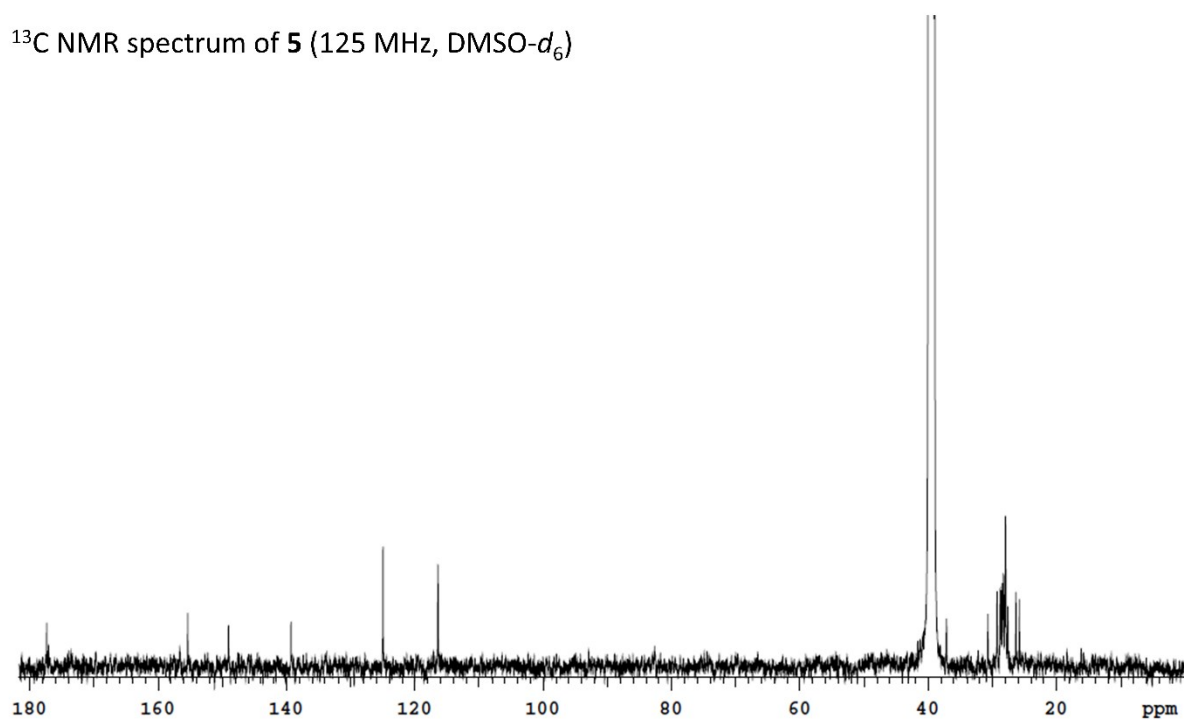
^{1}H NMR spectrum of **6** (500 MHz, DMSO-d_6)
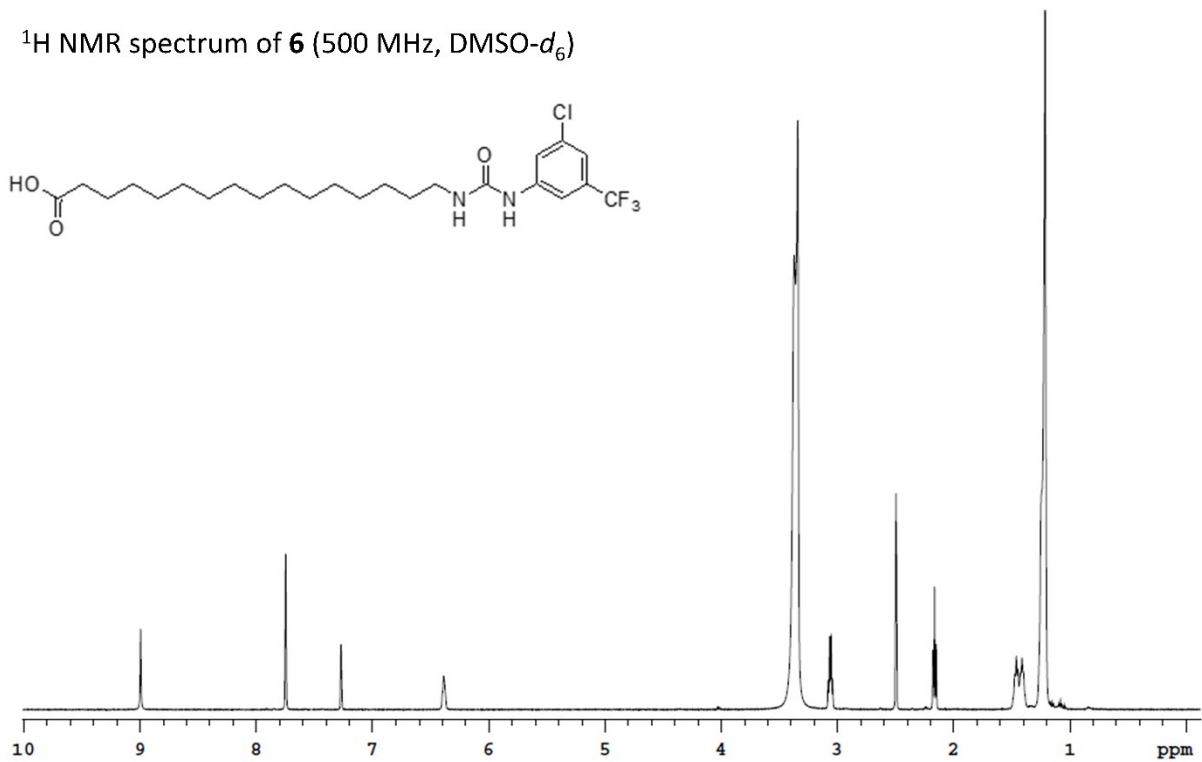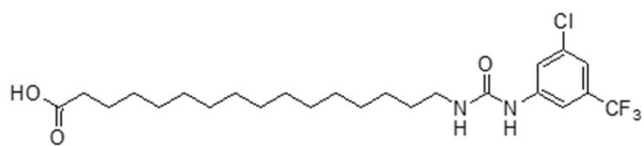
^{13}C NMR spectrum of **6** (125 MHz, DMSO-d_6)
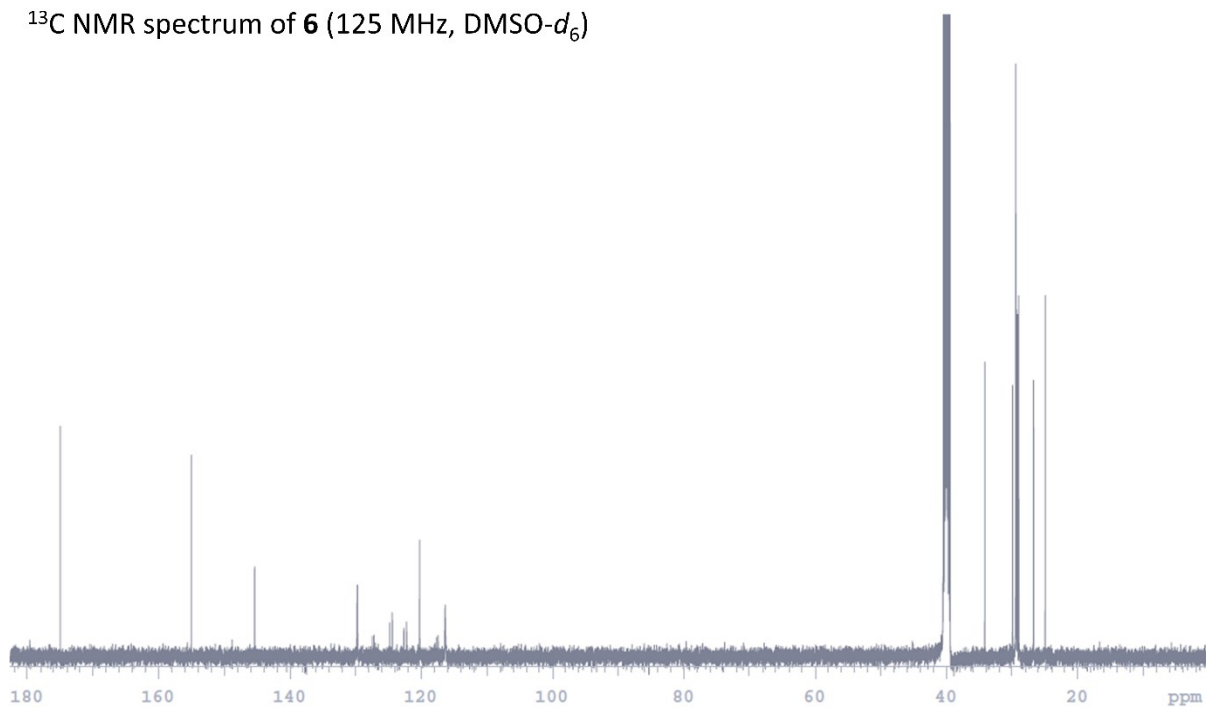
¹H NMR spectrum of **6-Me** (500 MHz, DMSO-d_6)
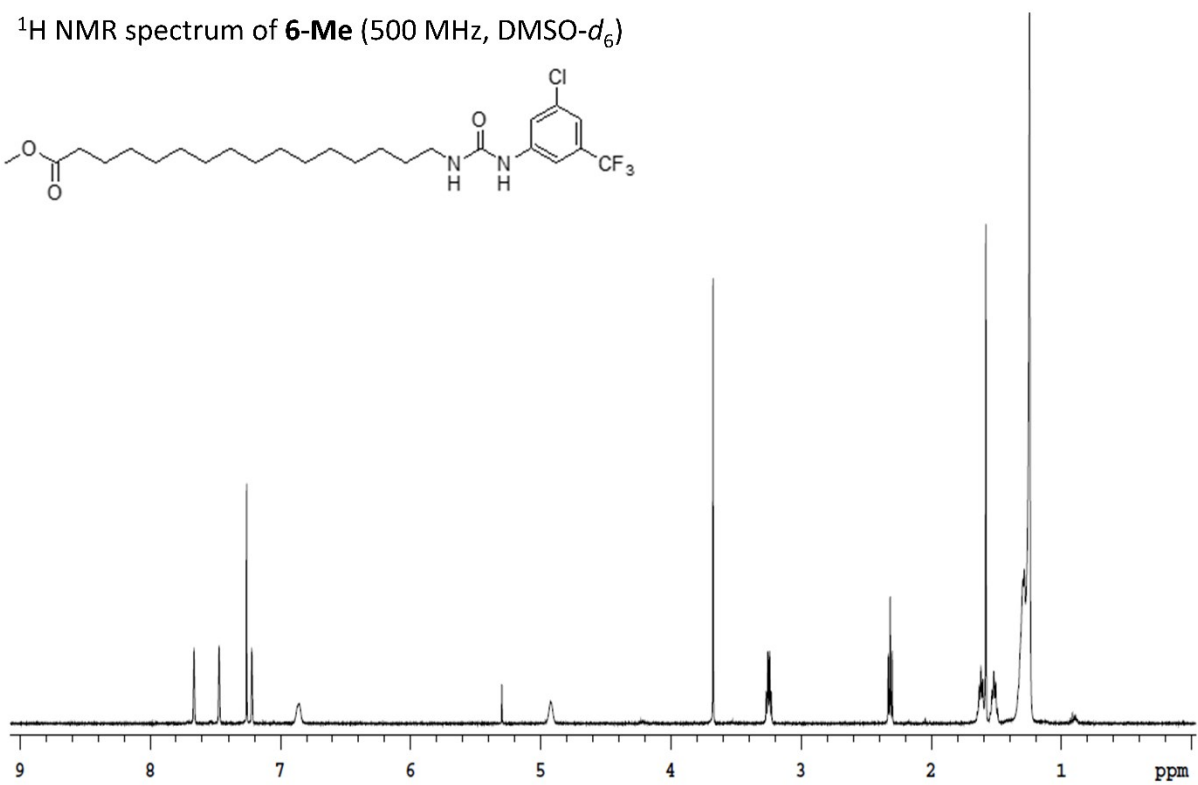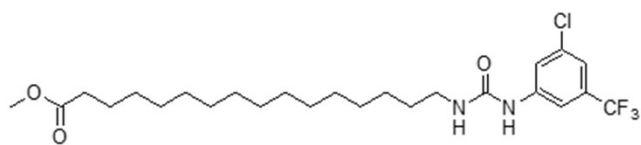
¹³C NMR spectrum of **6-Me** (125 MHz, DMSO-d_6)
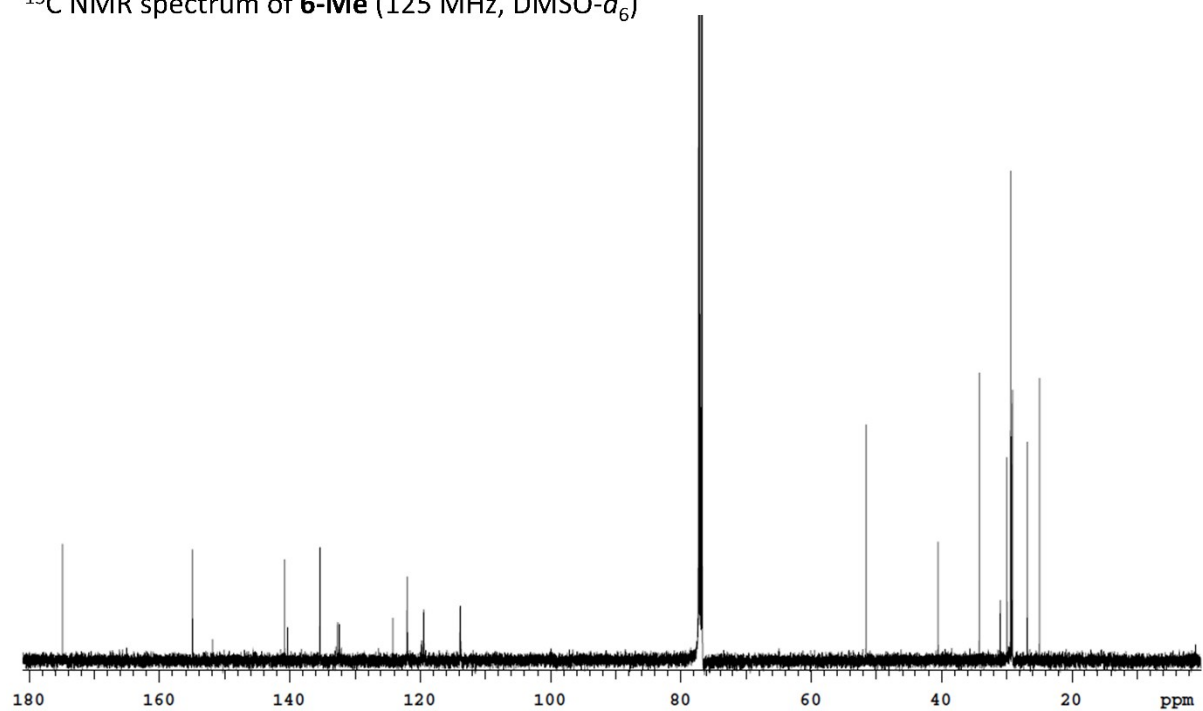
¹H NMR spectrum of **6-NNMe** (500 MHz, DMSO-*d*₆)
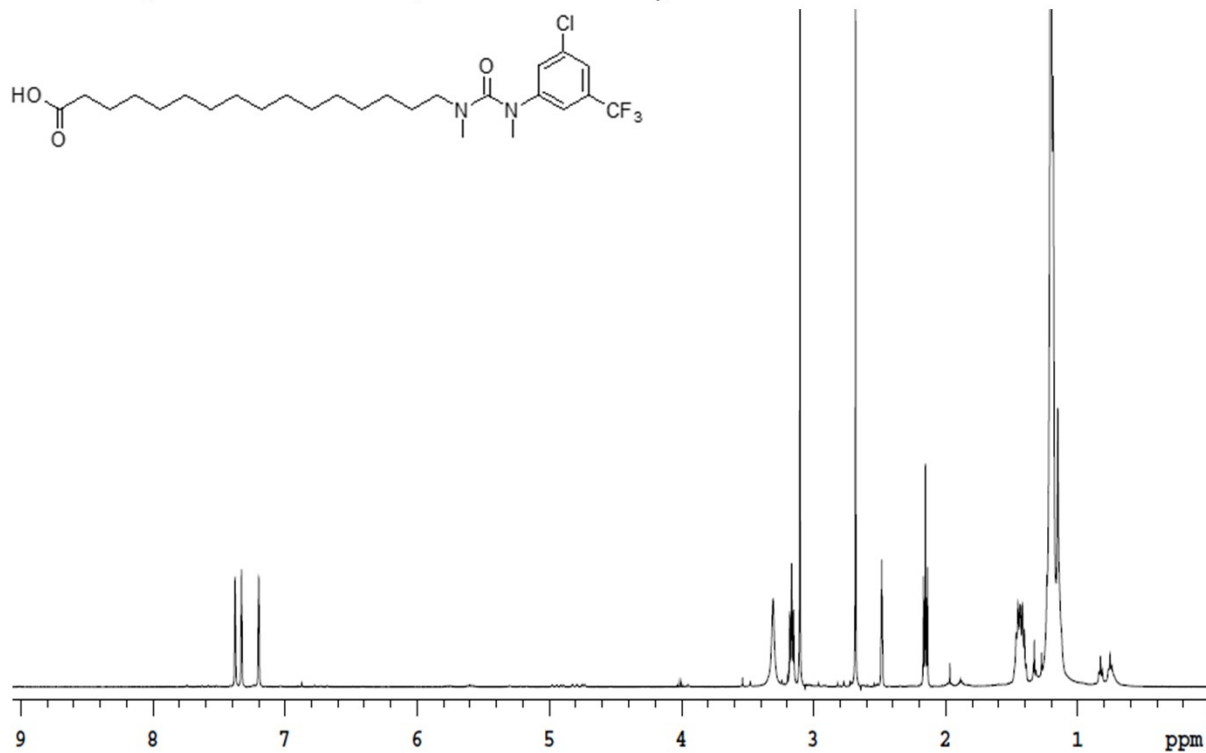
¹³C NMR spectrum of **6-NNMe** (125 MHz, DMSO-*d*₆)
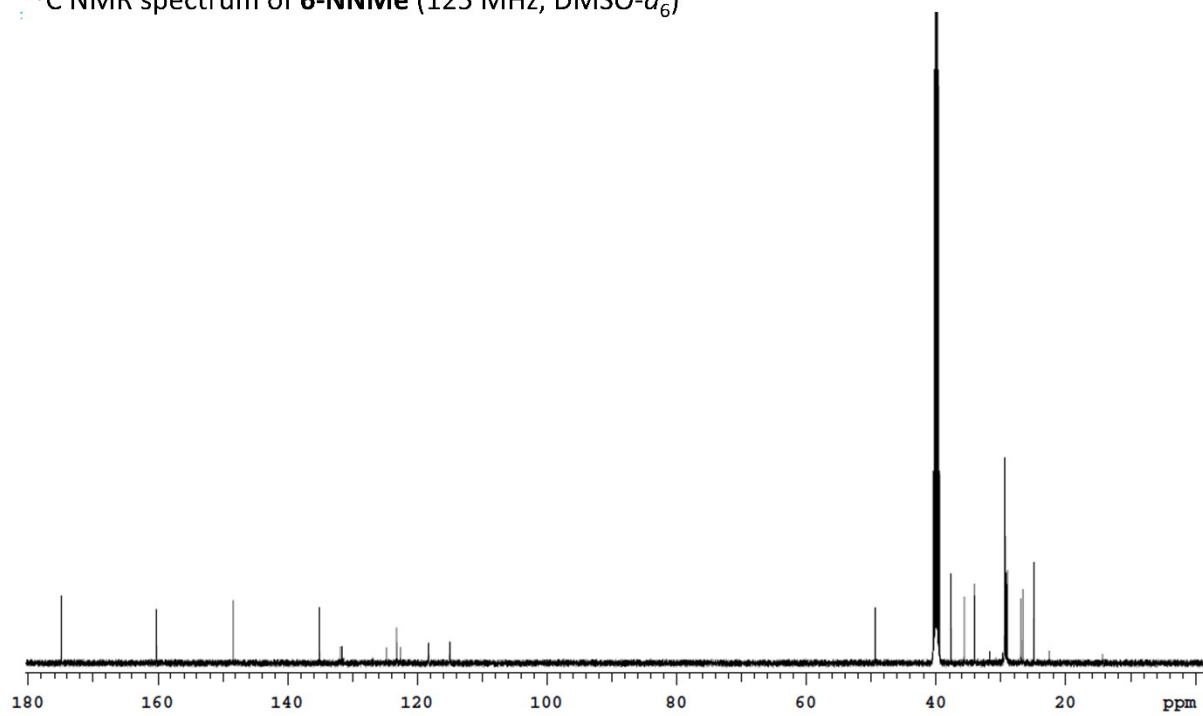
¹H NMR spectrum of **7** (500 MHz, DMSO-*d*₆)
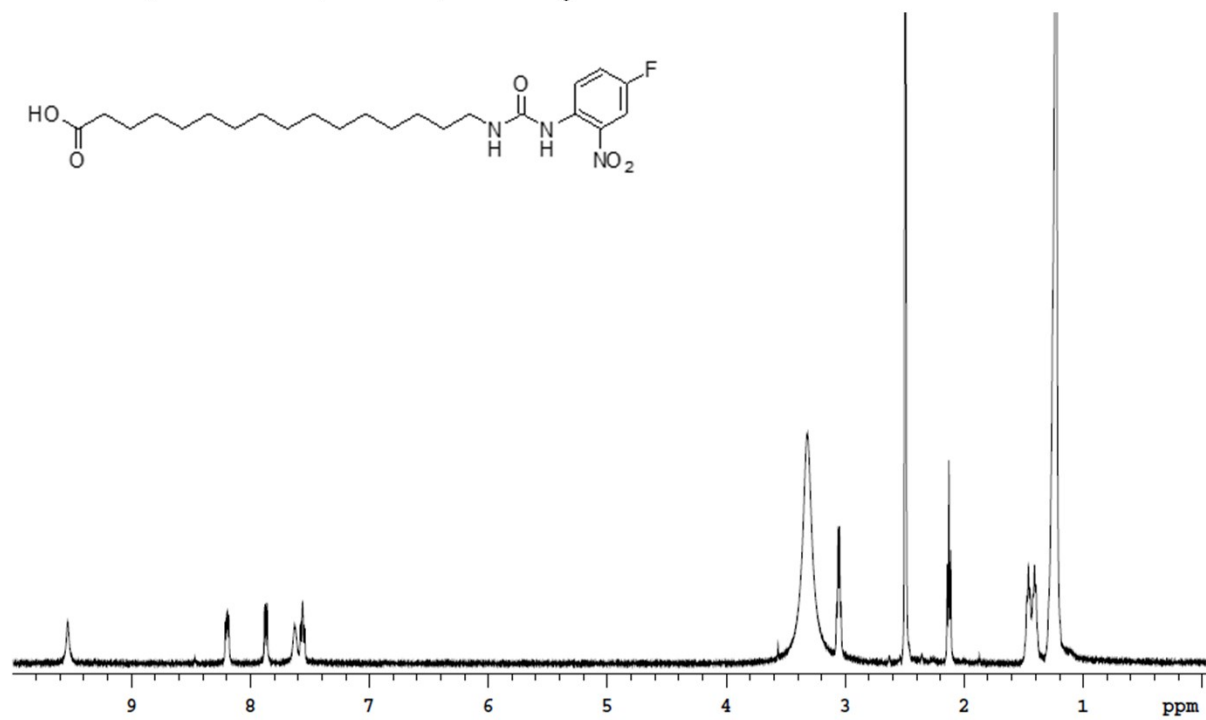
¹³C NMR spectrum of **7** (125 MHz, DMSO-*d*₆)
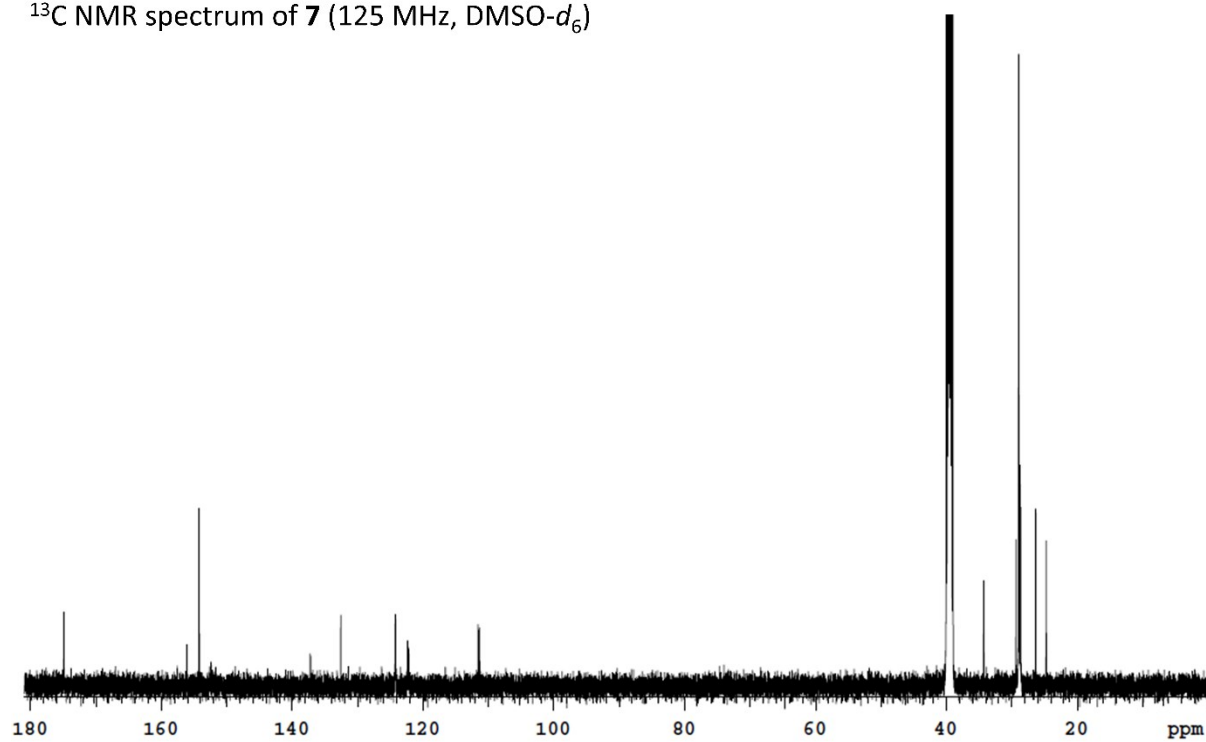
^{1}H NMR spectrum of **9** (500 MHz, DMSO-d_6)
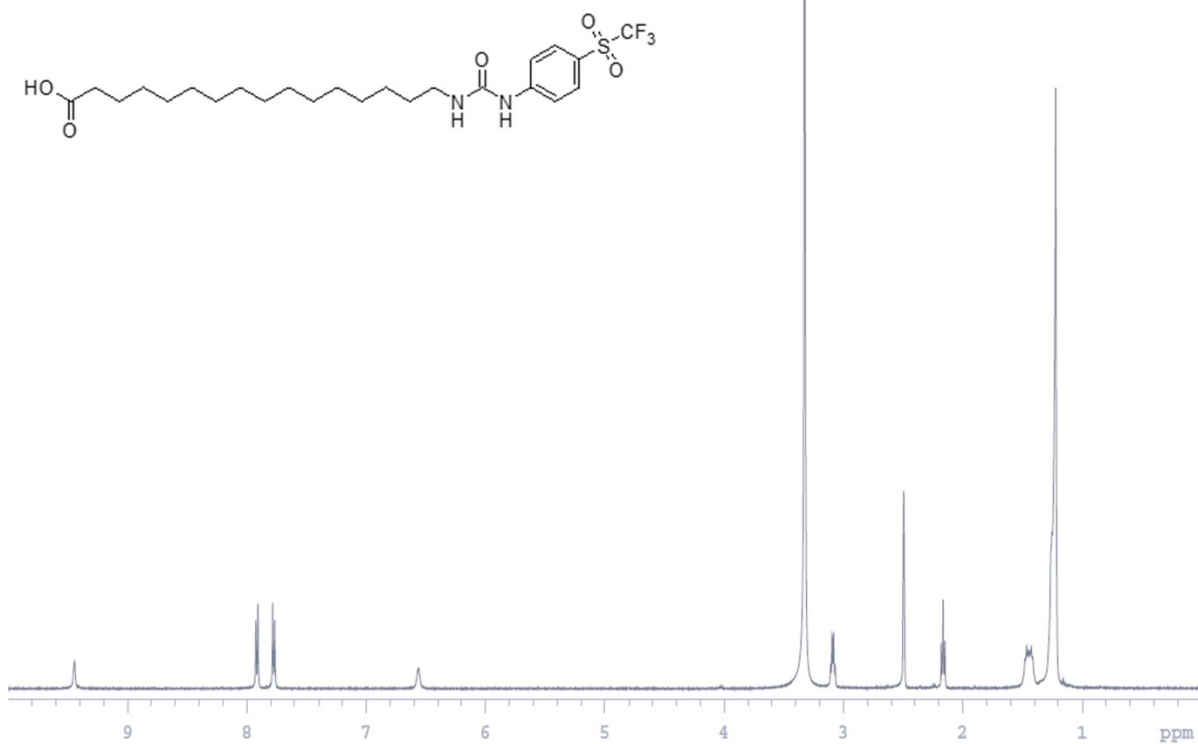
^{13}C NMR spectrum of **9** (125 MHz, DMSO-d_6)
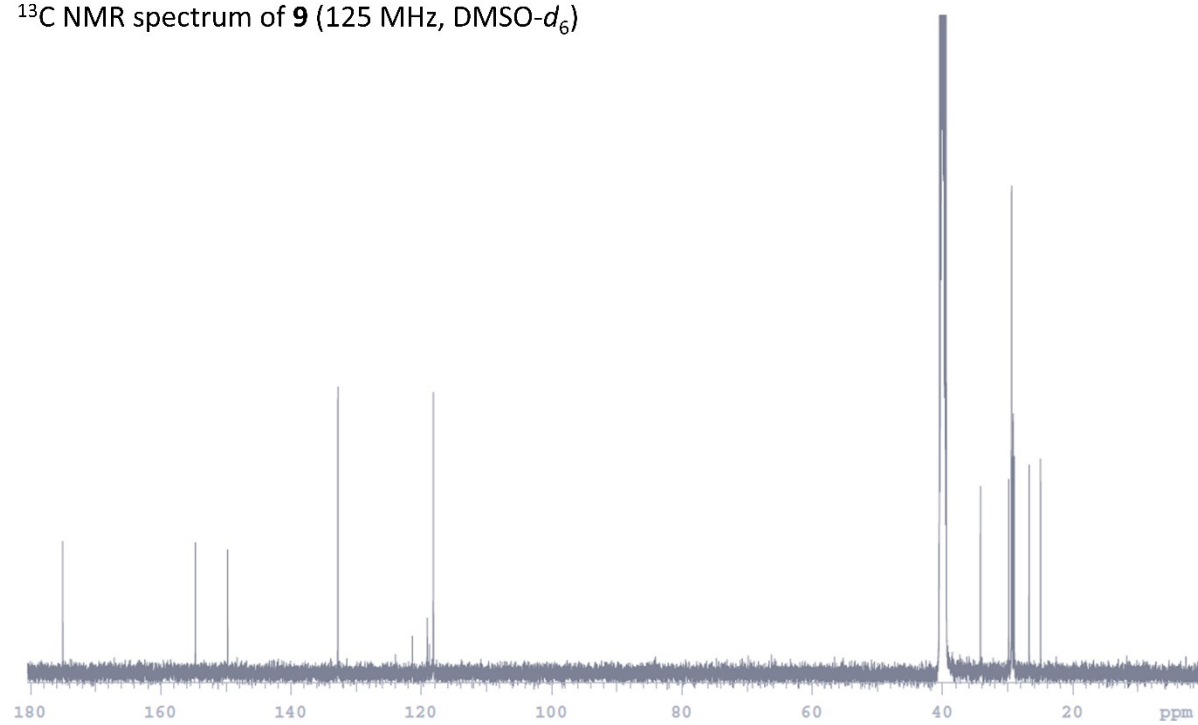
¹H NMR spectrum of **10** (500 MHz, DMSO-*d*₆)
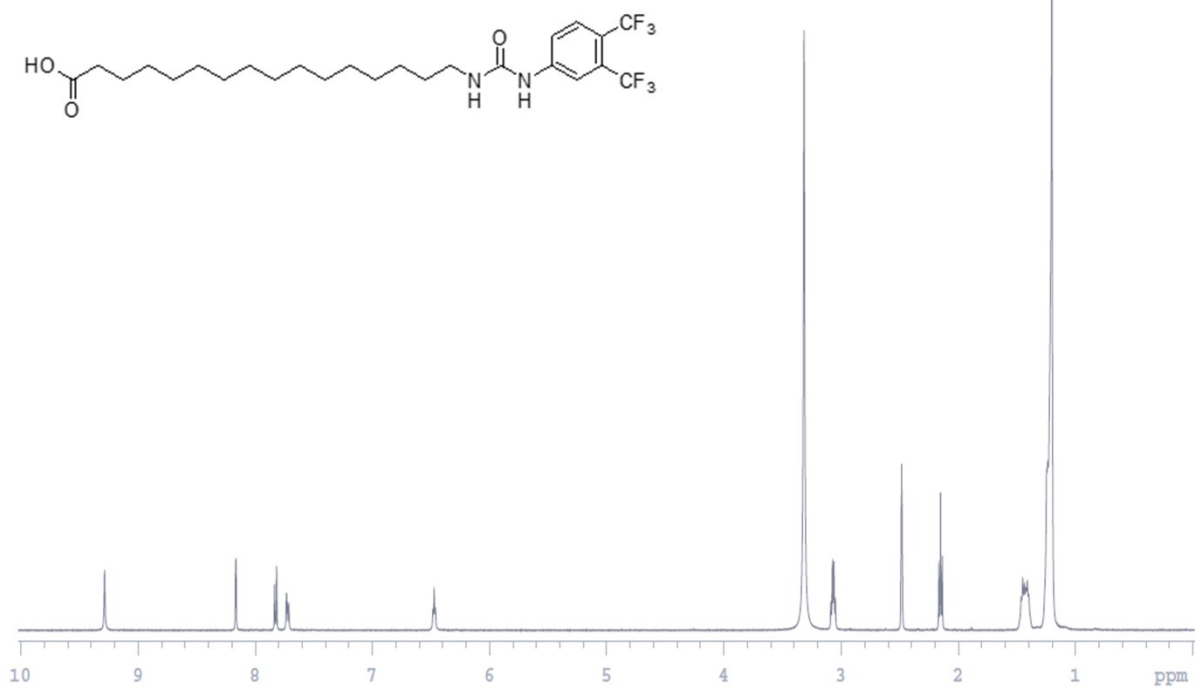
¹³C NMR spectrum of **10** (125 MHz, DMSO-*d*₆)
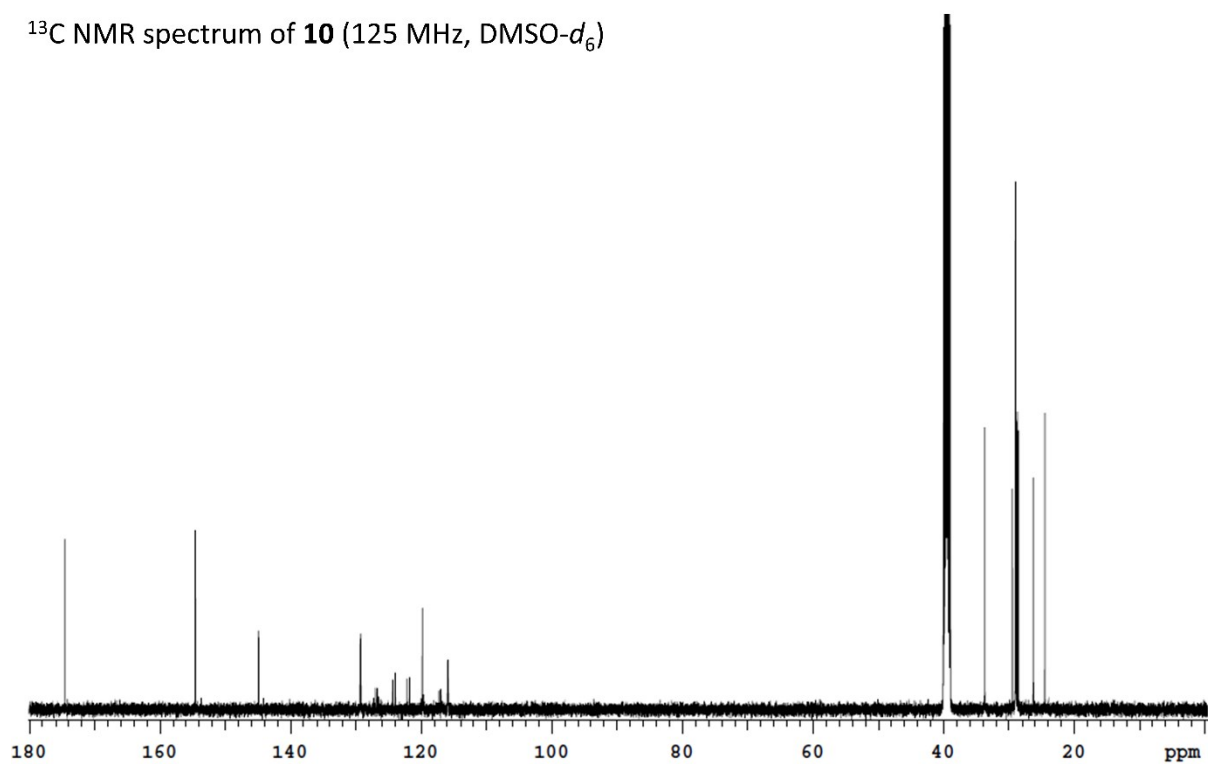
¹H NMR spectrum of **13** (500 MHz, DMSO-d_6)
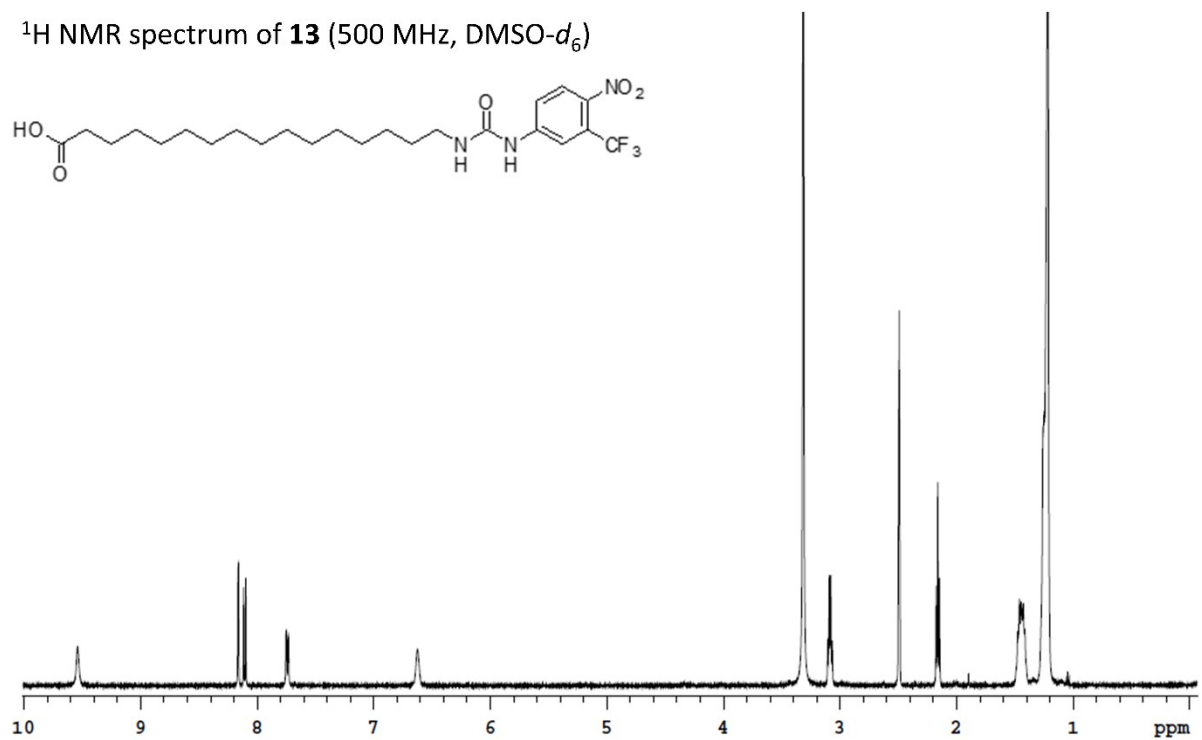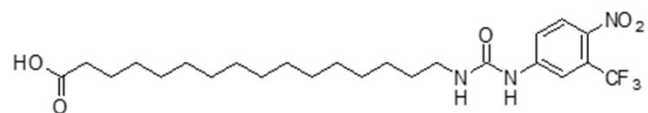
¹³C NMR spectrum of **13** (125 MHz, DMSO-d_6)
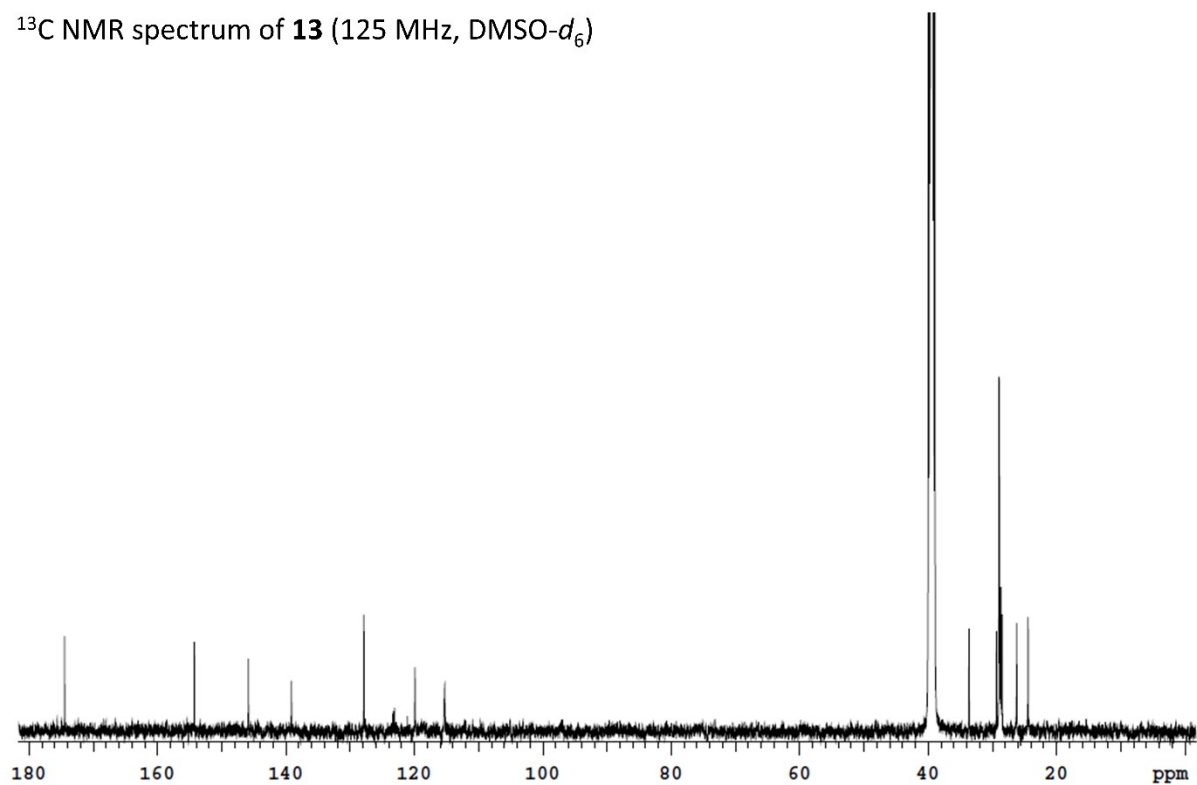
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10. Quantum Chemistry Data

Table S3. G3(MP2)CC(+) pKa calculations

Unless otherwise noted, all units are in Hartree

Species	S (J/mol K)	TC (kJ/mol)	ZPVE (kJ/mol)	RM06-2X/ 6-31+G(d)	RM06-2X/ 6-31+G(d) SMD	RMP2/ 6-31+G(d)	RMP2/ GTMP2L	RCCSD(T)/ 6-31+G(d)	G3(MP2) CC(+)	ΔGsolv (water)	G_{Soln} (water)
1	615.3144	51.3165	574.5681	-1370.53293	-1370.552902	-1367.74362	-1368.786984	-1367.925299	-1368.968663	-0.0199718	-1368.869689
1_Anion	606.2881	49.8935	539.857	-1369.994447	-1370.073169	-1367.208385	-1368.244312	-1367.385925	-1368.421852	-0.07872127	-1368.394853
2	623.1395	53.6822	607.1102	-1470.53108	-1470.550228	-1467.487194	-1468.7471	-1467.664085	-1468.923991	-0.01914863	-1468.762221
2_Anion	617.3279	52.5372	571.4207	-1469.995408	-1470.071728	-1466.954603	-1468.204039	-1467.127813	-1468.37725	-0.07632044	-1468.28602
3	569.5849	45.2255	593.6588	-778.4465485	-778.4707003	-776.4554898	-777.2651047	-776.6188365	-777.4284514	-0.024151819	-777.2739467
3_Anion	557.3928	43.7532	558.8179	-777.9071289	-777.9914678	-775.918748	-776.721367	-776.077736	-776.880355	-0.084338942	-776.7984839
4	610.8752	51.5753	683.9726	-1161.800096	-1161.838368	-1159.282955	-1160.222611	-1159.469902	-1160.409558	-0.03827191	-1160.237045
4_Anion	602.9291	50.1146	649.5807	-1161.263341	-1161.359823	-1158.747797	-1159.681141	-1158.93132	-1159.864664	-0.0964815	-1159.763114
5	560.7009	45.0902	594.2082	-778.4499459	-778.4742615	-776.4564581	-777.2663925	-776.6208069	-777.4307413	-0.0243156	-777.2752338
5_Anion	543.9791	43.2751	560.0956	-777.9200994	-777.9997638	-775.9278647	-776.7302199	-776.0885366	-776.8908918	-0.079664421	-776.8025184
6	631.1736	51.6668	574.1954	-1370.537252	-1370.556221	-1367.747506	-1368.791046	-1367.929202	-1368.972742	-0.018969	-1368.825008
6_Anion	619.0641	50.1385	539.5163	-1370.000659	-1370.078063	-1367.214187	-1368.250126	-1367.391637	-1368.427576	-0.077404	-1368.350693
7	579.5895	47.1046	573.5415	-877.6632646	-877.6784303	-875.4835236	-876.3927008	-875.6485735	-876.5577507	-0.015165664	-876.4023426
7_Anion	573.7579	46.132	538.0044	-877.1208194	-877.2034746	-874.9462513	-875.8449342	-875.1082666	-876.0069495	-0.082655196	-875.9322745
8	609.8229	51.1704	574.886	-1370.534934	-1370.554551	-1367.74505	-1368.788336	-1367.927007	-1368.970294	-0.01961694	-1368.82071
8_Anion	609.5418	49.9391	539.7257	-1369.999556	-1370.076983	-1367.212596	-1368.247918	-1367.390737	-1368.426059	-0.07742699	-1368.348114
9	662.2908	57.2287	625.6368	-1459.435642	-1459.463076	-1456.368086	-1457.602548	-1456.557237	-1457.791699	-0.02743367	-1457.634252
9_Anion	646.0618	55.5194	591.6146	-1458.910472	-1458.988285	-1455.844455	-1457.072263	-1456.030489	-1457.258298	-0.0778128	-1457.634252
10	658.7141	57.2782	612.3808	-1247.917843	-1247.937026	-1244.987608	-1246.292858	-1245.176862	-1246.482113	-0.01918249	-1246.321039
10_Anion	646.3597	55.7799	577.525	-1247.386108	-1247.459921	-1244.459394	-1245.755975	-1244.644616	-1245.941197	-0.07381305	-1245.847197
11	655.8584	57.2342	581.8994	-1930.09628	-1930.114621	-1926.518304	-1927.860578	-1926.704765	-1928.047039	-0.01834093	-1927.896426
11_Anion	649.0203	56.0506	546.3669	-1929.566076	-1929.638511	-1925.991443	-1927.323594	-1926.173448	-1927.505599	-0.07243483	-1927.422287
12	648.4863	54.3254	550.3939	-1830.100785	-1830.117557	-1826.780498	-1827.9034	-1826.97211	-1828.095012	-0.016772	-1827.9551
12_Anion	640.4742	53.4147	515.1865	-1829.564345	-1829.645898	-1826.245421	-1827.362389	-1826.433298	-1828.095012	-0.081553	-1827.487982
13	635.7661	54.5804	606.8602	-1115.391566	-1115.416102	-1112.725617	-1113.878334	-1112.906452	-1114.059169	-0.02453583	-1113.903972
13_Anion	623.4394	52.7356	572.9406	-1114.871496	-1114.944651	-1112.205525	-1113.350247	-1112.383024	-1113.527746	-0.07315462	-1113.43339
DPU	517.1455	39.3047	576.7359	-687.0717424	-687.0920097	-685.2422428	-685.9359181	-685.4105805	-686.1042558	-0.0202673	-685.9486123
DPU_Anion	497.9421	37.7225	540.391	-686.5491241	-686.6350162	-684.7014613	-685.3890619	-684.8653722	-686.1042558	-0.0858921	-685.4752191
TCC	613.3873	49.2944	502.1753	-2065.797791	-2065.82034	-2062.339685	-2063.279289	-2062.538943	-2063.478547	-0.02254886	-2063.360708
TCC_Anion	592.0961	47.9402	467.7675	-2065.274434	-2065.345463	-2061.817512	-2062.751501	-2062.012406	-2062.946395	-0.07102919	-2062.88824

Table S4. Calculation of Propanoate Binding and Lipophilicity Metrics

Unless otherwise noted, all units are in Hartree. If complexed to propanoate the tabulated values in the RM06-2X/6-31+G(d) (BSSE) column are BSSE corrected. For isolated compounds this column corresponds directly to the RM06-2X/6-31+G(d) energy.

Species	S (J/mol K)	TC (kJ/mol)	ZPVE (kJ/mol)	RM06-2X/ 6-31+G(d) (BSSE)	RM06-2X/ 6-31+G(d) SMD H$_2$O	RM06-2X/ 6-31+G(d) SMD n-pentadecane	ΔGsolv (water)	ΔGsolv (n-pentadecane)	G$_{Soln}$ (water)	G$_{Soln}$ (pentadecane)
Propanoate	318.92	17.3706	197.0105	-267.7291889	-267.8436842	-267.7772298	-0.1114764	-0.045022	-267.7952283	-267.7287739
1	615.3144	51.3165	574.5681	-1370.53293	-1370.552902	-1370.549327	-0.0199718	-0.016397	-1370.381371	-1370.377796
1_Propanoate	782.3849	69.5042	777.188	-1638.338392`	-1638.411338	-1638.380308	-0.0699276	-0.0388973	-1638.174678	-1638.143648
2	623.1395	53.6822	607.1102	-1470.53108	-1470.550228	-1470.54628	-0.0191486	-0.0152005	-1470.36629	-1470.362342
2_Propanoate	788.8887	71.9168	809.0003	-1738.337698	-1738.408755	-1738.377894	-0.0680379	-0.0371776	-1738.159798	-1738.128938
3	569.5849	45.2255	593.6588	-778.4465485	-778.4707003	-778.4653178	-0.0241518	-0.0187693	-778.289025	-778.2836426
3_Propanoate	737.1348	63.4003	796.1931	-1046.251802	-1046.329149	-1046.296126	-0.0743279	-0.0413056	-1046.082437	-1046.049414
4	610.8752	51.5753	683.9726	-1161.800096	-1161.838368	-1161.821218	-0.0382719	-0.0211217	-1161.624564	-1161.607414
4_Propanoate	778.5165	69.6409	886.7418	-1429.605579	-1429.696835	-1429.65171	-0.0882374	-0.0431117	-1429.417957	-1429.372832
5	560.7009	45.0902	594.2082	-778.4499459	-778.4742615	-778.4688472	-0.0243156	-0.0189013	-778.2914196	-778.2860053
5_Propanoate	717.1386	62.5499	797.4688	-1046.259195	-1046.333389	-1046.302573	-0.0711747	-0.0403588	-1046.084244	-1046.053428
6	631.1736	51.6668	574.1954	-1370.537252	-1370.556221	-1370.553427	-0.0189685	-0.0161745	-1370.386499	-1370.383705
6_Propanoate	790.6445	69.7335	776.4501	-1638.342739	-1638.414847	-1638.384199	-0.0690896	-0.0384413	-1638.179319	-1638.148671
7	579.5895	47.1046	573.5415	-877.6632646	-877.6784303	-877.6701264	-0.0151657	-0.0068618	-877.5048377	-877.4965338
7_Propanoate	732.955	64.9937	775.4275	-1145.454522	-1145.537408	-1145.499117	-0.0798675	-0.0415761	-1145.297524	-1145.259232
8	609.8229	51.1704	574.886	-1370.534934	-1370.554551	-1370.551301	-0.0196169	-0.0163669	-1370.382331	-1370.379081
8_Propanoate	777.6691	69.3816	776.9903	-1638.341614	-1638.413309	-1638.383266	-0.0686768	-0.0386334	-1638.176236	-1638.146193
9	662.2908	57.2287	625.6368	-1459.435642	-1459.463076	-1459.453273	-0.0274337	-0.0176312	-1459.275176	-1459.265374
9_Propanoate	826.7351	75.2772	828.0718	-1727.247043	-1727.322222	-1727.287876	-0.0721607	-0.0378144	-1727.069019	-1727.069019
10	658.7141	57.2782	612.3808	-1247.917843	-1247.937026	-1247.932808	-0.0191825	-0.0149648	-1247.753751	-1247.749533
10_Propanoate	821.8673	75.4018	814.5097	-1515.727052	-1515.795897	-1515.766247	-0.065826	-0.036176	-1515.547259	-1515.517609
11	655.8584	57.2342	581.8994	-1930.09628	-1930.114621	-1930.111759	-0.0183409	-0.0154791	-1929.942648	-1929.939786
11_Propanoate	813.1511	74.9624	784.4002	-2197.906486	-2197.97368	-2197.945167	-0.0641757	-0.0356629	-2197.735688	-2197.707176
12	648.4863	54.3254	550.3939	-1830.100785	-1830.117557	-1830.115812	-0.0167714	-0.0150265	-1829.957854	-1829.956109
12_Propanoate	818.4732	73.0388	750.0251	-2097.894541	-2097.976295	-2097.938445	-0.0787351	-0.0408859	-2097.752733	-2097.714883
13	635.7661	54.5804	606.8602	-1115.391566	-1115.416102	-1115.409889	-0.0245358	-0.0183232	-1115.233351	-1115.227138
13_Propanoate	812.7423	72.6425	809.0761	-1383.206184	-1383.275541	-1383.246982	-0.0663389	-0.0377801	-1383.028988	-1383.000429

Gaussian Archive Files

1_anion_water.M062X_6-31pGd_opt_water

1\1\GINC-R3758\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\27-Feb-2019\0\
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45\N,1.9185364151,1.7685829129,0.1936433513\C,3.1174304402,2.468548545
8,0.2831950309\O,3.0732346003,3.6645387003,0.6999285861\N,4.198913701,
1.7381928273,-0.0201964044\C,5.4440129495,2.3278394685,-0.0649227622\C
,5.7062533214,3.6695888682,-0.4305920072\C,6.5728040294,1.5154624603,0
.1808010863\C,7.8703640125,2.0012983439,0.0937413882\C,8.0967509468,3.
328829874,-0.2539437478\C,7.0060623989,4.1604883678,-0.5224902908\H,-2
.657698884,1.594703564,-0.3973144513\H,-1.8068191841,2.9849388411,-1.0
883732354\H,-2.0335804716,2.8667990333,0.6644260658\H,-0.3188667578,0.
9559428974,-1.031483443\H,-0.5452630469,0.8312364289,0.713561269\H,0.5
043595371,3.0620044318,1.0242450943\H,0.6919573187,3.2334756345,-0.722
1959859\H,1.9763013056,0.9490977885,-0.4018671295\H,4.8798217889,4.327
8425626,-0.6623222365\H,6.4135661475,0.4745708824,0.4487590053\H,8.713
7309456,1.3485588011,0.2982141179\Cl,9.7468559727,3.9062241156,-0.3460
560061\C,7.215642009,5.5935440364,-0.9257489193\F,6.0595428346,6.24295
21548,-1.1430224836\F,9.9341554449,5.7094439416,-2.0627450071\F,7.8764
737431,6.3024593092,0.0137547146\\Version=ES64L-G09RevE.01\State=1-A\H
F=-1370.0731685\RMSD=5.764e-09\RMSF=9.095e-06\Dipole=0.0301817,-0.7355
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1_water.M062X_6-31pGd_opt_water

1\1\GINC-R3741\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\27-Feb-2019\0\\# M
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4949760555,0.1359820335\C,0.5459946396,2.5119576818,-0.2055934555\N,1.
867250505,1.9528576485,0.0528612208\C,2.9871122186,2.6713508328,-0.174
062174\O,2.9503977216,3.8575858235,-0.5369271189\N,4.1665046975,1.985
1881227,0.0351253059\C,5.4730232011,2.4601588653,-0.1028456508\C,5.800
826279,3.8100603532,-0.2761091453\C,6.5072797756,1.5156366436,-0.03720
65254\C,7.8345175143,1.9019455587,-0.1461813046\C,8.1556526882,3.24319
27918,-0.3267667575\C,7.1362597153,4.1932777432,-0.3907706592\H,-2.698
0224932,1.326787448,0.1178737322\H,-2.0417522701,2.329728065,-1.185593
4516\H,-2.1040509548,2.9572990842,0.4704814881\H,-0.3753888052,0.58786
20479,-0.4606729402\H,-0.4384430857,1.2097006808,1.1908046277\H,0.4149
98265,3.4169651479,0.3979811533\H,0.4682293655,2.8045281316,-1.2600243
298\H,1.936940364,0.9674589784,0.2834534437\H,4.0881512136,0.997888441
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,0.4647996648,0.100738294\H,8.6229741991,1.1583061295,-0.0941844108\Cl
,9.8370630088,3.6893851195,-0.4652875873\C,7.4533683416,5.6529690339,-
0.5788273484\F,6.3487249905,6.4144530967,-0.6166907427\F,8.1186091916,
5.8861950739,-1.727513336\F,8.2212181382,6.1405961886,0.415423694\\Ver
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.0361921,-6.9603699,5.2681364,-2.0183325,-2.0343225\PG=C01 [X(C11H12Cl
1F3N2O1)]\\@

1_anion.M062X_6-31pGd_opt

1\1\GINC-R3782\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\27-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) m
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6\C,0.6240899407,2.2893357228,-0.4337909853\N,1.9049205506,1.791334124
9,0.0039180017\C,3.0617872932,2.5856724944,-0.1532610697\O,2.926546832
1,3.8184292203,-0.2594673726\N,4.1760569791,1.8250837293,-0.1417676423
\C,5.4118705819,2.3895999522,-0.2024853322\C,5.7437617792,3.7753823299
,-0.2607135294\C,6.5164516368,1.4956023918,-0.2036298148\C,7.830526128
3,1.9275069077,-0.2573959489\C,8.1221152153,3.2881020863,-0.3122998188
\C,7.0681080649,4.2060198165,-0.3132870741\H,-2.7043512472,1.787825195
7,0.5051468483\H,-2.0619590627,1.9472498006,-1.1378337967\H,-1.9390467
63,3.3013100146,-0.0078562399\H,-0.4969292851,0.6022655971,0.314014494
4\H,-0.3624105984,1.9498911962,1.4373984954\H,0.6565615536,3.376284601
7,-0.3143724769\H,0.4440845503,2.0903434148,-1.5074310015\H,2.09857382
,0.8123139018,-0.1676922062\H,4.9400449726,4.4984362495,-0.2655910144\
H,6.2927575777,0.4333001916,-0.1583615925\H,8.6476481438,1.2112677488,
-0.2560453323\Cl,9.8068418799,3.7848295876,-0.3780595038\C,7.346625749
7,5.6821934024,-0.371821707\F,6.2278964044,6.42639195,-0.3680733718\F,
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565e-09\RMSF=1.275e-06\Dipole=-0.2250419,-0.4775989,-0.1613016\Quadrup
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1.M062X_6-31pGd_opt

1\1\GINC-R3718\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\27-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) maxdi
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02060249,-0.0240079758\C,-0.5429143905,1.4923382681,0.1105817285\C,0.5
655679541,2.4874657783,-0.2071689609\N,1.872892206,1.8558202101,-0.071
8067082\C,2.9968520996,2.6475966299,-0.109349224\O,2.9498935416,3.8648
380839,-0.1160847102\N,4.1813751465,1.9201664846,-0.106434271\C,5.4874
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6838\C,6.5364316884,1.5211782723,0.0630119031\C,7.8576652566,1.9411742
67,0.0220745769\C,8.1582485447,3.2777412516,-0.2168317359\C,7.11888143
52,4.189105686,-0.4140953478\H,-2.7147920025,1.4116712985,0.2076565257
\H,-2.0906467037,2.2972241989,-1.0422625423\H,-2.0301418537,2.97921784
72,0.6593440632\H,-0.4700464089,0.630914136,-0.5681065784\H,-0.3978293
366,1.1102735155,1.1279793269\H,0.5371674955,3.3309517059,0.4877451983
\H,0.435628158,2.8992092059,-1.2182088599\H,1.9491634331,0.9130890974,
-0.4341078472\H,4.1077510669,0.9330023215,0.1008931075\H,4.9935104698,
4.4878714164,-0.5198244001\H,6.3194677656,0.4721620893,0.250682255\H,8
.6643388522,1.2326654297,0.1770699552\Cl,9.8281376784,3.7588369322,-0.
2597943325\C,7.411075842,5.6480748895,-0.6756822117\F,6.2864576725,6.3
609571409,-0.8354179655\F,8.1431281052,5.8180777815,-1.7895677907\F,8.
0911368843,6.2109870818,0.3366546157\\Version=ES64L-G09RevE.01\State=1
-A\HF=-1370.5329301\RMSD=3.506e-09\RMSF=1.227e-06\Dipole=-1.5885245,-2
.7672284,0.09641\Quadrupole=2.5521173,2.8576786,-5.4097959,2.539066,1.
8461054,-0.1723318\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

2_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3718\FOpt\RM062X\Gen\C10H12F5N2O1S1(1-)\ROOT\30-Oct-2018\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=h2o) maxdisk=2147483648\\4SF5_a1.M062X_6-31pGd_opt_water\\-1,
1\C,-2.0268012249,1.8787540089,-0.2185201531\C,-0.7159415916,1.4088752

293,0.4046916782\C,0.4774806024,2.1485622719,-0.1825040083\N,1.7200155
253,1.6713418954,0.4112879082\C,2.935743179,2.1482203429,-0.0509026733
\O,2.9450835986,3.2509480119,-0.6704264789\N,3.9775574955,1.3356565015
,0.2034071003\C,5.261617383,1.7960848323,0.0778675564\C,5.6810871952,3
.141666335,0.2569863139\C,6.2827679717,0.8410684409,-0.1644724456\C,7.
6199446994,1.1896665944,-0.2471212487\C,7.9787568133,2.5272712805,-0.0
759151587\C,7.0177122451,3.5032894678,0.1832654165\H,-2.881582573,1.34
80983439,0.2118118591\H,-2.0316750161,1.7035167298,-1.3001633971\H,-2.
1774285455,2.9512022903,-0.0511407378\H,-0.5906651141,0.3309261644,0.2
38431793\H,-0.7389020194,1.5652049218,1.4901405885\H,0.3777569016,3.22
1016458,0.0127708026\H,0.490525442,2.0195868401,-1.2755514133\H,1.7314
596283,0.6847956792,0.647465998\H,4.9468300018,3.9071557262,0.47572755
73\H,5.9966373634,-0.1991342856,-0.2914273434\H,8.3662529424,0.4263300
841,-0.4432147827\S,9.7024162485,2.9979491825,-0.1835731546\H,7.300278
4306,4.5405486642,0.3345350067\F,9.9654304586,2.1233739712,-1.52397445
53\F,11.2680169096,3.425409947,-0.281574976\F,9.3971170886,4.303219254
2,-1.0960941042\F,9.6400026525,3.9270820478,1.1445392944\F,10.20791530
59,1.747409168,0.7167776579\\Version=ES64L-G09RevE.01\State=1-A\HF=-14
70.0717283\RMSD=3.220e-09\RMSF=6.504e-06\Dipole=0.3967925,-0.9033423,0
.4574439\Quadrupole=-16.2649275,10.8383299,5.4265976,2.2003942,-2.3293
845,3.579997\PG=C01 [X(C10H12F5N2O1S1)]\\@

2_anion.M062X_6-31pGd_opt

1\1\GINC-R4171\FOpt\RM062X\Gen\C10H12F5N2O1S1(1-)\ROOT\31-Oct-2018\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2
147483648\\4SF5_a1.M062X_6-31pGd_opt\\-1,1\C,-2.0455909683,2.009040752
7,0.0349015857\C,-0.7079737747,1.3876257084,0.4327449064\C,0.460222365
3,1.9957872587,-0.3411346233\N,1.7185585468,1.394651108,0.024163797\C,
2.9106871921,2.1412092208,-0.035255058\O,2.8402147047,3.3820740099,-0.
0193123297\N,3.9881486635,1.3221250721,-0.0858549385\C,5.2479329161,1.
8158794023,-0.0744947826\C,5.6617896202,3.1825629259,0.0140521255\C,6.
2996901374,0.8519202469,-0.1564675307\C,7.6351878575,1.1958001584,-0.1
526072102\C,7.9889585574,2.5467090773,-0.0637855209\C,7.0030620186,3.5
308256758,0.0194170186\H,-2.8790078424,1.572991707,0.5962735987\H,-2.2
461473632,1.8599815712,-1.0328490611\H,-2.0426351583,3.0892410287,0.22
14658042\H,-0.7378842093,0.3027357098,0.2583337294\H,-0.522276381,1.52
64285961,1.5042872537\H,0.5501564564,3.0630070658,-0.118070654\H,0.259
0913289,1.9105393269,-1.4256329547\H,1.8634150638,0.4256937313,-0.2305
702342\H,4.9038343157,3.9512123644,0.0752608625\H,6.0054760778,-0.1915
929979,-0.2223104152\H,8.3996575787,0.4278450145,-0.216586561\S,9.7106
239383,3.0096585142,-0.0578713028\H,7.2830168601,4.5777808172,0.088212
4108\F,10.1001702017,2.0126311197,-1.2825013375\F,11.2884899773,3.4299
819874,-0.0528671122\F,9.507615022,4.2288107502,-1.1126185189\F,9.5441
65381,4.0639524901,1.1672046466\F,10.1367609154,1.8479905859,0.9975906
065\\Version=ES64L-G09RevE.01\State=1-A\HF=-1469.9954079\RMSD=2.988e-0
9\RMSF=4.692e-06\Dipole=0.2102839,-0.4492842,-0.1815086\Quadrupole=-27
.5011031,14.329375,13.1717281,-1.9880876,1.75653,1.258722\PG=C01 [X(C1
0H12F5N2O1S1)]\\@

2.M062X_6-31pGd_opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13F5N2O1S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=21474
83648\\4SF5.M062X_6-31pGd_opt\\0,1\C,-2.0948335042,1.9046393492,0.0044
342604\C,-0.7387005762,1.2091435064,0.0979128525\C,0.408084306,2.20365
44755,-0.0249872519\N,1.6878407,1.5158695525,0.0682705488\C,2.85177333
54,2.220609996,-0.034915754\O,2.8683270034,3.4287793658,-0.2037620392\
N,3.9992797709,1.4395905567,0.071456147\C,5.3292742418,1.8632288845,0.
0073631391\C,5.7138230818,3.1993799716,-0.1763848696\C,6.3187306185,0.
8755412601,0.1376630783\C,7.6646618585,1.201190052,0.0876681324\C,8.02
66286555,2.5310910273,-0.0950741354\C,7.0652418884,3.5245267145,-0.226
435952\H,-2.9135377655,1.1853756323,0.0927245266\H,-2.2037356321,2.422
8325913,-0.953942271\H,-2.2104659744,2.6459935776,0.8018584347\H,-0.65
27215837,0.4558511302,-0.6962839698\H,-0.6593480367,0.679465311,1.0565
080968\H,0.3465416167,2.9602827842,0.7662296943\H,0.3549141013,2.73501
8087,-0.9824559294\H,1.688479682,0.5155120816,0.2084528423\H,3.8730138
82,0.4459185867,0.2096761318\H,4.9621638561,3.9689113161,-0.2783096187
\H,6.0301970677,-0.1631051756,0.2802254097\H,8.41731823,0.4275780245,0
.1898297642\S,9.775366344,2.9694067766,-0.1619778373\H,7.358385244,4.5
588334301,-0.3686207991\F,10.1215643051,1.7341942428,-1.145352719\F,11
.3351324769,3.35722828,-0.2211755462\F,9.5624590014,3.9305039196,-1.44
15318488\F,9.5718424038,4.237262061,0.8165344846\F,10.1310894012,2.040
9426307,1.1124129979\\Version=ES64L-G09RevE.01\State=1-A\HF=-1470.5306
35\RMSD=4.697e-09\RMSF=3.326e-05\Dipole=-2.7126732,-1.98461,0.28297\Qu

adrupole=1.0205306,4.541292,-5.5618225,8.046695,-1.1271033,-1.450379\P
G=C01 [X(C10H13F5N2O1S1)]\\@

2.M062X_6-31pGd_opt_water

1\1\GINC-R3714\FOpt\RM062X\Gen\C10H13F5N2O1S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2147483648\\4SF5.M062X_6-31pGd_opt_water\\0,1\C,-2.0
874983117,1.8805065948,0.0189597345\C,-0.7268055172,1.1994554923,0.123
9606135\C,0.4020532443,2.1994084289,-0.0744248406\N,1.6939631322,1.533
8635482,0.0419683464\C,2.8454377421,2.2197985863,-0.1117044544\O,2.865
6735446,3.4215918137,-0.415035459\N,3.9911653428,1.4702449884,0.081135
3734\C,5.3181546514,1.8884149835,0.0080895559\C,5.7197028526,3.2267677
464,-0.1254226112\C,6.298606783,0.8840322528,0.0974702407\C,7.64687980
78,1.1957330538,0.050443926\C,8.0189649091,2.5306158907,-0.0872380303\
C,7.073177096,3.5440382396,-0.1734955657\H,-2.8985787841,1.1598611384,
0.1588681164\H,-2.21654674,2.3474651913,-0.9636798573\H,-2.1942821804,
2.6611738624,0.7801590987\H,-0.64396145,0.4066648505,-0.6293296882\H,-
0.6203347073,0.7249212149,1.1073436379\H,0.3313821637,3.0008536204,0.6
71352024\H,0.3257821824,2.6630733979,-1.0641110643\H,1.713432322,0.574
6490841,0.3711392352\H,3.8611701975,0.4774613767,0.2516164683\H,4.9887
376242,4.0191928392,-0.1873247487\H,5.5950265495,-0.1534685656,0.20523
86517\H,8.3845311347,0.403440359,0.1195510582\S,9.7671329868,2.9501620
068,-0.15193494\H,7.3673391676,4.5834012593,-0.2745409286\F,10.1065168
611,1.7627577044,-1.1979075374\F,11.3421278343,3.3263337872,-0.2101401
321\F,9.5706537518,3.9785036301,-1.3856027126\F,9.6062986077,4.1798385
542,0.8874065125\F,10.1428872017,1.9644930696,1.0751799774\\Version=ES
64L-G09RevE.01\State=1-A\HF=-1470.5502283\RMSD=6.128e-09\RMSF=7.732e-0
6\Dipole=-3.3558652,-3.1069071,0.7806074\Quadrupole=-1.3209659,7.06165
37,-5.7406879,12.5173808,-4.1283499,-1.5860141\PG=C01 [X(C10H13F5N2O1S
1)]\\@

4_anion.M062X_6-31pGd_opt

1\1\GINC-R4385\FOpt\RM062X\Gen\C11H15N2O3S1(1-)\ROOT\31-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214
7483648\\4SulfOxyMethyl_a1.M062X_6-31pGd_opt\\-1,1\C,-1.9466282003,1.8
87911438,-0.0700129613\C,-0.5770083084,1.342544214,-0.4704566581\C,0.5
517558051,1.9715696828,0.3443715412\N,1.8410836847,1.4414140184,-0.022
4696655\C,2.9959219593,2.2407054425,0.0695877141\O,2.86804271,3.476379
7031,0.0886694805\N,4.1102877756,1.4695663839,0.101742533\C,5.34634553
69,2.0159031433,0.134826174\C,5.6994350044,3.4047977513,0.1527848247\C
,6.4381847186,1.0904949224,0.1581022174\C,7.7559689783,1.4923411402,0.
1795824314\C,8.0606988533,2.862985995,0.1926495226\C,7.0243586744,3.80
53277453,0.1760052874\H,-2.7516378445,1.4376332205,-0.6608231314\H,-1.
9896595089,2.9736684953,-0.2146688242\H,-2.1551574404,1.6882403044,0.9
878837413\H,-0.3828923379,1.5312099105,-1.5328636577\H,-0.5602682224,0
.2514729781,-0.3381742098\H,0.3393839024,1.8357896089,1.4214178606\H,0
.5969425288,3.0494926572,0.1630068607\H,2.0290338056,0.4726107804,0.20
28087326\H,4.9063666503,4.1397824464,0.1521533574\H,6.1829767229,0.034
4657514,0.1602594887\H,8.563152474,0.7643182705,0.2052979859\S,9.72129
11872,3.3860642907,0.0764835\O,10.6131261483,2.3199236648,0.5574564107
\O,9.8602863436,4.7459629521,0.6173371486\H,7.2726276668,4.8642557812,
0.2000801561\C,10.0394546945,3.5291752095,-1.6878718902\H,9.8871967109
,2.5513143076,-2.1475694591\H,11.0768571305,3.8547592645,-1.79623575\H
,9.3529521963,4.2680285255,-2.1044507611\\Version=ES64L-G09RevE.01\Sta
te=1-A\HF=-1161.2633412\RMSD=7.646e-09\RMSF=4.784e-06\Dipole=-1.001672
3,-0.6685656,-1.2566563\Quadrupole=-28.54696,11.587586,16.959374,-3.40
21616,-13.7689258,-3.8074471\PG=C01 [X(C11H15N2O3S1)]\\@

4.M062X_6-31pGd_opt

1\1\GINC-R3717\FOpt\RM062X\Gen\C11H16N2O3S1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483
648\\4SulfOxyMethyl.M062X_6-31pGd_opt\\0,1\C,-2.004263388,1.8464310338
,-0.0619611429\C,-0.6364865026,1.173271879,-0.1508238027\C,0.491430347
4,2.1644063527,0.1050600288\N,1.7859964779,1.5005241731,0.010388262\C,
2.9256908545,2.2693583333,0.0027417071\O,2.9039951239,3.4856778398,-0.
0561231676\N,4.0946538437,1.5149515788,0.0320442189\C,5.4106605759,1.9
866672237,0.0576662473\C,5.7447546566,3.3304413867,0.2884984485\C,6.43
08061142,1.0385648995,-0.1264199383\C,7.7642466362,1.4151355017,-0.087
9587748\C,8.0827586951,2.7526253088,0.1344028277\C,7.0838751806,3.7024
376149,0.3284910275\H,-2.8095746333,1.1299437332,-0.0254841161\H,-2.09
32757984,2.6490466794,-0.8015645517\H,-2.1638570882,2.2849385298,0.928

8121993\H,-0.4976929599,0.7231664482,-1.1409418453\H,-0.582099623,0.35
65017316,0.5825208025\H,0.3699568775,2.6405506529,1.0884724605\H,0.478
7227364,2.9636249124,-0.6409158263\H,1.8432166431,0.5770077191,0.42231
31816\H,3.9962960489,0.5214934954,-0.1316070473\H,4.9642025641,4.06354
60007,0.4350274309\H,6.172380869,-0.0049657857,-0.2909688177\H,8.55678
81999,0.6823373587,-0.2081265147\S,9.7881599085,3.2506208111,0.1597084
041\O,10.5984677656,2.063190585,0.4320968977\O,9.9005993094,4.44923006
66,0.9897965512\H,7.3567033401,4.7339662248,0.5334050209\C,10.12212679
74,3.7447920648,-1.5287554839\H,9.9618936343,2.8881474885,-2.18503237\
H,11.1683710732,4.0584682241,-1.5517379059\H,9.4649239201,4.5758499335
,-1.7890544113\\Version=ES64L-G09RevE.01\State=1-A\HF=-1161.800096\RMS
D=5.841e-09\RMSF=8.042e-06\Dipole=-2.4401217,-1.6292881,-1.2398018\Qua
drupole=-4.2302542,4.6076668,-0.3774126,8.1990254,-15.3396003,-3.35054
94\PG=C01 [X(C11H16N2O3S1)]\\@

4.M062X_6-31pGd_opt_water

1\1\GINC-R3717\FOpt\RM062X\Gen\C11H16N2O3S1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2147483648\\4SulfOxyMethyl.M062X_6-31pGd_opt_water\\0,
1\C,-2.0090827246,1.7753965897,-0.0139678909\C,-0.6236195031,1.1420022
119,-0.0895583396\C,0.4666267849,2.186714157,0.0937141935\N,1.78251760
34,1.5658040467,0.0016176282\C,2.9072983041,2.2969312163,0.1484766621\
O,2.8814689615,3.5008316619,0.4418059523\N,4.0802721639,1.5890422342,-
0.0398578996\C,5.3923282378,2.0503270955,0.0337058381\C,5.7488514022,3
.3943456619,0.2363785129\C,6.4038718122,1.0831301448,-0.1208199396\C,7
.7401571886,1.4397419359,-0.0719761342\C,8.076997449,2.7780715458,0.13
75191508\C,7.0919023697,3.7506937914,0.2856618498\H,-2.7920095479,1.02
19890751,-0.1411197895\H,-2.1372893254,2.5310406663,-0.79678599\H,-2.1
641089363,2.2632786038,0.9546467258\H,-0.4908158232,0.6475374156,-1.05
98686592\H,-0.5194599433,0.3715641926,0.683951544\H,0.3666524498,2.668
769452,1.0723012931\H,0.3722790853,2.9686245235,-0.6701474329\H,1.8391
028178,0.6078194885,-0.3270360986\H,3.9835291075,0.5961913928,-0.23089
01851\H,4.9897709106,4.1531251738,0.354583452\H,6.1293323926,0.0433912
137,-0.2762423854\H,8.5104150361,0.6830502948,-0.1868484746\S,9.779273
2296,3.2518373349,0.1620831634\O,10.5813882382,2.0813011539,0.56720220
75\O,9.9103605622,4.4828812764,0.9651385233\H,7.3634255177,4.789965106
2,0.4462051552\C,10.189900076,3.6469324356,-1.5201109789\H,10.03197629
56,2.7562618857,-2.1316508822\H,11.2419794252,3.9444204197,-1.52857537
96\H,9.5491383824,4.468936602,-1.8455651922\\Version=ES64L-G09RevE.01\
State=1-A\HF=-1161.8383679\RMSD=4.572e-09\RMSF=7.413e-06\Dipole=-3.218
0021,-2.8364289,-2.9900456\Quadrupole=-6.9046103,6.610839,0.2937713,12
.486628,-16.9460975,-3.1831732\PG=C01 [X(C11H16N2O3S1)]\\@

4_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3718\FOpt\RM062X\Gen\C11H15N2O3S1(1-)\ROOT\30-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2147483648\\4SulfOxyMethyl_a1.M062X_6-31pGd_opt_wa
ter\\-1,1\C,-1.9546797156,1.706009016,0.22537293\C,-0.6191977491,1.353
3586973,-0.4224913892\C,0.5296595257,2.1209402848,0.2155478652\N,1.797
4165887,1.7543989626,-0.4024039038\C,2.9842606518,2.2591221079,0.09954
84434\O,2.9346080239,3.3075724542,0.8038976919\N,4.069242582,1.5249373
259,-0.2137248831\C,5.326500111,2.0418604319,-0.0647256636\C,5.6717511
344,3.4208967333,-0.1267358535\C,6.4002738667,1.1211337944,0.078027373
4\C,7.7164477583,1.5332819186,0.1729265248\C,8.012129397,2.9010560661,
0.1247232989\C,6.9896494683,3.8401232248,-0.0407988997\H,-2.7777741501
,1.1564582135,-0.2414476843\H,-2.1665145405,2.7766972027,0.1274536\H,-
1.9491360877,1.4609010605,1.2933387432\H,-0.6516488087,1.5778364394,-1
.4956904016\H,-0.4318083934,0.2759786916,-0.3255436229\H,0.5505797545,
1.9225184636,1.2979107508\H,0.3684270997,3.1964037096,0.089724388\H,1.
8610855034,0.7928218979,-0.7190969494\H,4.8924233341,4.1607226361,-0.2
618486174\H,6.1648345874,0.0612528921,0.1172590253\H,8.5111132439,0.80
16081298,0.2914489772\S,9.6839124353,3.4305695895,0.1727649309\O,10.47
37925457,2.4488371798,0.9464622078\O,9.7260982377,4.8379410576,0.62150
65261\H,7.2254537082,4.899340829,-0.1003705174\C,10.2706554253,3.38392
70571,-1.5051662501\H,10.1890548945,2.3576682674,-1.8694072697\H,11.31
36703285,3.7110119774,-1.4896594187\H,9.6581992391,4.0629236874,-2.101
8919523\\Version=ES64L-G09RevE.01\State=1-A\HF=-1161.3598227\RMSD=4.23
1e-09\RMSF=2.443e-06\Dipole=-0.5477146,-1.3257566,-2.9127505\Quadrupol
e=-13.5382401,6.0707191,7.467521,-0.9150713,-17.3961218,-6.2922403\PG=
C01 [X(C11H15N2O3S1)]\\@

8.M062X_6-31pGd_opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\01-Nov-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147
483648\\3Chloro4TFM.M062X_6-31pGd_opt\\0,1\C,-1.9565094212,1.814626811
8,-0.181558854\C,-0.5874716188,1.1471360095,-0.0715728372\C,0.53299707
31,2.1775467633,-0.0188852695\N,1.8294673454,1.5181930741,0.0830748055
\C,2.9693909695,2.2662743224,-0.0849748325\O,2.9513398032,3.4305802588
,-0.4416576465\N,4.137755468,1.5503650228,0.1597990633\C,5.4529166222,
2.0175392486,0.0944684381\C,5.782737842,3.3621239135,-0.118336894\C,6.
4791277022,1.0785603989,0.2709580441\C,7.8059660159,1.4739234579,0.237
7573699\C,8.1513423775,2.8088001731,0.0291871439\C,7.1210386503,3.7363
287784,-0.1463905957\H,-2.7566112053,1.0703399023,-0.2192192228\H,-2.0
217048368,2.4246438433,-1.0885961776\H,-2.1459478573,2.4687310968,0.67
61336085\H,-0.4192755117,0.4812344065,-0.9262111339\H,-0.5561875629,0.
5224546979,0.8321587158\H,0.38179686,2.8684103834,0.8227338003\H,0.544
7672715,2.7811221557,-0.9303576424\H,1.8741353076,0.7146229583,0.69772
32771\H,4.0435096833,0.5499670421,0.2759240191\H,5.0093984609,4.102490
02,-0.2665291767\H,6.2350273865,0.0325285559,0.4370557219\H,8.59031928
44,0.7380773414,0.375333781\Cl,7.474195244,5.4175784398,-0.4119541926\
C,9.6003375943,3.2120749746,-0.0027729808\F,9.9039350019,4.1049015048,
0.954245616\F,9.9535906643,3.7587257945,-1.1780024741\F,10.4062053861,
2.1504586494,0.1884865257\\Version=ES64L-G09RevE.01\State=1-A\HF=-1370
.5349342\RMSD=5.397e-09\RMSF=3.745e-06\Dipole=-2.1362019,-2.2848778,0.
6484399\Quadrupole=0.0676858,3.7511255,-3.8188112,3.8574915,-2.6584423
,-2.1657264\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

8.M062X_6-31pGd_opt_water

1\1\GINC-R3721\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\01-Nov-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,So
lvent=h2o) maxdisk=2147483648\\3Chloro4TFM.M062X_6-31pGd_opt_water\\0,
1\C,-1.9529072718,1.7850364894,-0.1521107346\C,-0.5769891008,1.1520883
555,0.0282790047\C,0.5263306866,2.1856109742,-0.1382417603\N,1.8334815
591,1.5667482074,0.0483967279\C,2.9664454673,2.28590839,-0.0834257173\
O,2.9590766261,3.4809694504,-0.4127416873\N,4.1305222423,1.5811895592,
0.1662286649\C,5.4430704985,2.0419692235,0.1081359436\C,5.79112872,3.3
922448447,-0.0453046487\C,6.4620975666,1.0836785871,0.2332606953\C,7.7
926479081,1.4621629972,0.2001303677\C,8.1536994645,2.8020135709,0.0405
90888\C,7.1329253097,3.7466889145,-0.0774179383\H,-2.7454252713,1.0401
039575,-0.0349776869\H,-2.0517352336,2.2292738271,-1.1486814305\H,-2.1
203154201,2.5754031,0.5878289497\H,-0.4334360101,0.3493176397,-0.70504
34972\H,-0.5005343947,0.6989463089,1.0244572492\H,0.3960697995,2.99710
65193,0.5882456943\H,0.4799084335,2.6288391368,-1.1390784577\H,1.87198
66718,0.6108011411,0.3849701229\H,4.0315992983,0.5877023744,0.35434155
78\H,5.0330190906,4.1564182313,-0.1340041578\H,6.2011588727,0.03665157
14,0.356401045\H,8.56392445,0.7057711744,0.2968667246\Cl,7.50526169,5.
4424274723,-0.2680941106\C,9.6008841939,3.1902630547,0.0021311099\F,9.
938313689,4.0421519515,0.9927850963\F,9.9459878663,3.7988437939,-1.151
8564575\F,10.4093925979,2.1240291817,0.1259484427\\Version=ES64L-G09Re
vE.01\State=1-A\HF=-1370.5545512\RMSD=7.957e-09\RMSF=2.551e-06\Dipole=
-2.6963403,-3.8839872,0.8325572\Quadrupole=-0.6090646,6.140591,-5.5315
265,7.4986795,-2.8790258,-1.7701773\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

8_anion.M062X_6-31pGd_opt

1\1\GINC-R3751\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\31-Oct-2018\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
2147483648\\3Chloro4TFM_a1.M062X_6-31pGd_opt\\-1,1\C,-1.9211533525,1.9
174764124,-0.0617557872\C,-0.5613363464,1.299205945,-0.3816712982\C,0.
5797330789,2.0228790406,0.3309677718\N,1.8602637904,1.4278486877,0.040
1669765\C,3.0248882178,2.2180352898,0.0129446538\O,2.9119183472,3.4450
429754,-0.1472516217\N,4.1307988613,1.4496356336,0.1583359673\C,5.3721
100809,1.9832996433,0.0955373423\C,5.7290609764,3.3486450375,-0.138924
5668\C,6.4622209695,1.082470764,0.280396383\C,7.776971114,1.4932917179
,0.2382426334\C,8.1188933665,2.8359069431,0.0069922401\C,7.0560511893,
3.7306457167,-0.176882686\H,-2.7352852022,1.3981483156,-0.578836207\H,
-1.9489910826,2.9710899846,-0.3629576867\H,-2.1278921799,1.8772067015,
1.0144436617\H,-0.368892426,1.3290963064,-1.4605549486\H,-0.5599320969
,0.2386543489,-0.0927006471\H,0.3707585231,2.046365341,1.4170065206\H,
0.6385802882,3.0627733024,-0.0037046448\H,2.0374230883,0.5004521577,0.
405138875\H,4.9473858559,4.0812967485,-0.2844509262\H,6.215623379,0.03
99403084,0.4580908378\H,8.5722711838,0.7687764278,0.3850291131\Cl,7.39
6174444,5.4346218675,-0.4723093549\C,9.5459366098,3.2547826702,-0.0331
37289\F,9.9249282814,3.7973517038,-1.2155755694\F,10.3845038272,2.2107
230995,0.1729850275\F,9.8735072132,4.1749369092,0.9062552294\\Version=

ES64L-G09RevE.01\State=1-A\HF=-1369.9995559\RMSD=7.534e-09\RMSF=4.340e
-06\Dipole=-0.3581807,-0.6868843,0.272637\Quadrupole=-19.7412802,7.841
8567,11.8994235,-5.0382061,-0.9941732,-0.6634683\PG=C01 [X(C11H11Cl1F3
N2O1)]\\@

1\1\GINC-R133\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\31-Oct-2018\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=h2o)\\3Chloro4TFM_a1.M062X_6-31pGd_opt_water\\-1,1\C,-1.91046
19917,1.8227346008,0.1611937628\C,-0.570722233,1.2852514556,-0.3326250
596\C,0.5837485316,2.1660061692,0.1225554215\N,1.8554633696,1.63087943
76,-0.3452338238\C,3.0421262488,2.2419582923,0.020556736\O,2.996974530
4,3.440049789,0.4203668676\N,4.1222013753,1.4432574516,-0.0841391038\C
,5.3858997686,1.9619288868,-0.0137176781\C,5.7528512878,3.3074471738,-
0.2892309769\C,6.4473756917,1.0701007377,0.285587325\C,7.7654539276,1.
4846815304,0.325894511\C,8.1155863161,2.8152792563,0.0630162223\C,7.07
85163065,3.7007989502,-0.2497797098\H,-2.7378909031,1.1888816601,-0.17
19528521\H,-2.0888680526,2.8356484233,-0.2170379079\H,-1.9372017159,1.
8633554635,1.2558832233\H,-0.5702552412,1.2270341325,-1.427945225\H,-0
.4178210321,0.2651631892,0.0431723143\H,0.5738173594,2.2501040264,1.22
00042152\H,0.4545867225,3.176765887,-0.2775282111\H,1.9095073747,0.618
9942672,-0.3904870131\H,4.995166238,4.0347412663,-0.5485153991\H,6.205
1458144,0.0311884944,0.4889415132\H,8.5442109445,0.7680334831,0.566823
0136\Cl,7.4324096299,5.3809343599,-0.6170517467\C,9.5430716294,3.24560
08874,0.1125511898\F,9.9951397238,3.7292775603,-1.0681495321\F,10.3661
889622,2.2314186603,0.4391167482\F,9.7742994164,4.2230845077,1.0195511
753\\Version=ES64L-G09RevE.01\State=1-A\HF=-1370.0769829\RMSD=6.088e-0
9\RMSF=6.111e-06\Dipole=-0.2250023,-1.3522572,-0.168897\Quadrupole=-9.
0276929,4.5529521,4.4747408,-0.7465206,1.9233299,-2.5239932\PG=C01 [X(
C11H11Cl1F3N2O1)]\\@

1\1\GINC-R4490\FOpt\RM062X\Gen\C11H10Cl2F3N2O1(1-)\ROOT\10-Jul-2018\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Nor
aman SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_dichloro_CF3
_a1.M062X.SMD.h2o.opt\\-1,1\C,-4.0937399789,3.4850692281,-1.0714905315
\C,-4.2006549607,2.4194643648,-0.1788781896\C,-3.0528800848,1.75256491
1,0.2132279719\C,-1.7518410116,2.0894642482,-0.2402626668\C,-1.7224797
986,3.1666942264,-1.1626783578\C,-2.8517063067,3.8616784596,-1.5712666
389\N,-0.6579925965,1.3507903215,0.1135923524\C,0.3655032753,1.9849935
147,0.6961586495\N,1.5521835257,1.2658284364,0.7396768772\O,0.34050130
78,3.1395900311,1.2146627529\C,2.5343070968,1.5668073097,1.7753888801\
C,3.71091757,0.6051158479,1.6952811667\C,4.7443543227,0.8950650078,2.7
795179422\H,1.4238450734,0.2748136413,0.5615150332\H,2.0810956777,1.51
16976493,2.7771298619\H,2.8891396677,2.5928788316,1.6387515328\H,4.174
3532921,0.6840490987,0.7042349653\H,3.3440770353,-0.4247352814,1.79664
34409\H,5.135059839,1.914516542,2.6846748104\H,5.5900590523,0.20362875
64,2.7148427477\H,4.3041043631,0.7957335586,3.778046448\H,-5.167818972
4,2.1187009558,0.2141159851\H,-2.7586704521,4.6754139356,-2.2828533213
\C,-5.3375542714,4.2080711657,-1.4748291528\F,-5.1121011328,5.15851016
47,-2.3975350377\F,-6.268800926,3.3768093095,-1.9927511639\F,-5.939401
0759,4.8205509244,-0.4297786986\Cl,-0.1991284686,3.6049085521,-1.89635
12424\Cl,-3.2236610619,0.4342962885,1.3455835829\\Version=ES64L-G09Rev
E.01\State=1-A\HF=-1829.6458983\RMSD=2.958e-09\RMSF=2.373e-06\Dipole=-
0.6051939,-0.7050399,-0.5499085\Quadrupole=-3.7740786,2.0020841,1.7719
944,-2.5041895,-2.9339209,-2.8744007\PG=C01 [X(C11H10Cl2F3N2O1)]\\@

1\1\GINC-R3771\FOpt\RM062X\Gen\C11H11Cl2F3N2O1\ROOT\10-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 maxdisk=2147483648\\aryl_urea_dichloro_CF3.M062X.opt\\0,1\C,-4.102067
2406,3.4964938621,-1.0116510989\C,-4.1881832392,2.2963878828,-0.311816
3197\C,-3.0214728883,1.6101242639,-0.0167946945\C,-1.758593676,2.07675
32369,-0.4168090302\C,-1.7179970922,3.270187356,-1.1522819433\C,-2.874
8969743,3.9887428376,-1.434613624\N,-0.5905621491,1.3613440121,-0.1313
400836\C,0.3933033967,1.9465020578,0.6982775681\N,1.4703050599,1.12572
41131,0.8895594068\O,0.269313819,3.046670427,1.1941120142\C,2.61447741
46,1.6145287809,1.6481988808\C,3.5462406832,0.4663436862,2.0139277475\
C,4.7540987215,0.956805829,2.8090990578\H,-0.7290152035,0.3678163463,0
.0176337884\H,1.6573645191,0.4407269505,0.1672776833\H,2.22250858209,2.
0977315983,2.5485942375\H,3.1556051717,2.3834187692,1.0787607796\H,3.8
888858962,-0.0346376214,1.0978882135\H,2.9854068152,-0.2767741485,2.59

\H,5.3349701728,1.6855533429,2.2337871682\H,5.4185310846,0.128
2451091,3.0692375277\H,4.4390391803,1.4400048224,3.7399644223\H,-5.146
7428617,1.9060830266,0.0147191213\H,-2.8082205867,4.9133650486,-1.9964
027429\C,-5.3757632216,4.2363626169,-1.3131299621\F,-5.1553088474,5.38
0496628,-1.9757357508\F,-6.2114593595,3.493525124,-2.0626989992\F,-6.0
456221302,4.5448042931,-0.1883530227\Cl,-0.2131578039,3.8497484863,-1.
7795847456\Cl,-3.1284844814,0.1205412621,0.8785847598\\Version=ES64L-G
09RevE.01\State=1-A\HF=-1830.1007854\RMSD=9.502e-09\RMSF=5.760e-06\Dip
ole=1.2868621,-1.5537144,-0.0445701\Quadrupole=3.4211721,0.4361818,-3.
857354,-3.8762883,-0.1015435,-2.3401996\PG=C01 [X(C11H11Cl2F3N2O1)]\\@

1\1\GINC-R4313\FOpt\RM062X\Gen\C11H10Cl2F3N2O1(1-)\ROOT\10-Jul-2018\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Nor
aman maxdisk=2147483648\\aryl_urea_dichloro_CF3_a1.M062X.opt\\-1,1\C,-
4.0881915047,3.4847035518,-1.1477936907\C,-4.2670922012,2.3908214461,-
0.2978147132\C,-3.1639125841,1.7350906233,0.2098719949\C,-1.8075788608
,2.1087808016,-0.0557026823\C,-1.701935425,3.2029039891,-0.975527107\C
,-2.794393275,3.8796686824,-1.4881391431\N,-0.8019080333,1.3864102139,
0.449429816\C,0.3093728466,1.987319624,0.9369344102\N,1.3874488743,1.0
901656922,1.0363736385\O,0.4398781462,3.1547176476,1.3249588649\C,2.44
78781135,1.3505734248,1.9811180835\C,3.7677527919,0.7268468924,1.53371
37582\C,4.8921892619,0.9834239976,2.5354265463\H,1.0858828197,0.127237
3086,0.9465690012\H,2.1982578305,0.9867772552,2.9952716727\H,2.5430894
342,2.4381368891,2.0488465745\H,4.02739999,1.135458991,0.550103077\H,3
.6342327695,-0.3557647788,1.3976151335\H,5.0542235832,2.0591813403,2.6
699055074\H,5.8379695856,0.5392347175,2.2066069708\H,4.6472586207,0.56
20744468,3.5177278775\H,-5.2631041248,2.0529976387,-0.0298528389\H,-2.
6327721655,4.698434178,-2.1820163463\C,-5.2649378519,4.2445581763,-1.6
42115357\F,-5.030036959,4.8702848824,-2.8169550076\F,-6.3513191497,3.4
600445396,-1.8318164511\F,-5.6766912458,5.2209498455,-0.7906811939\Cl,
-0.1344964572,3.6422866459,-1.6036845802\Cl,-3.4433948298,0.369651337,
1.265996184\\Version=ES64L-G09RevE.01\State=1-A\HF=-1829.5643446\RMSD=
6.370e-09\RMSF=1.213e-06\Dipole=0.071471,-0.4856177,-0.310418\Quadrupo
le=-10.7535696,5.5239315,5.2296382,2.9699964,-7.7293222,1.8388921\PG=C
01 [X(C11H10Cl2F3N2O1)]\\@

1\1\GINC-R3771\FOpt\RM062X\Gen\C11H11Cl2F3N2O1\ROOT\10-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_dichloro_CF3.M06
2X.SMD.h2o.opt\\0,1\C,-4.0977807217,3.4993409941,-1.0160881138\C,-4.15
95492663,2.3656666111,-0.2108722127\C,-2.9829805823,1.6907337813,0.075
6006447\C,-1.7435113545,2.1005592118,-0.4400087194\C,-1.734432149,3.23
32346194,-1.2652560628\C,-2.8945732609,3.9446343332,-1.548266367\N,-0.
5644725679,1.3941720136,-0.1650983682\C,0.4167200142,1.9607875547,0.64
43347632\N,1.4732647057,1.1684256105,0.8947308805\O,0.3134447017,3.113
9717649,1.0832477004\C,2.5577073217,1.601727645,1.7685065068\C,3.59749
35867,0.5001945138,1.9047166607\C,4.7367546623,0.930840559,2.822772771
5\H,-0.6299085217,0.3800625698,-0.1592141732\H,1.5154037845,0.24175291
05,0.4843261296\H,2.1483285151,1.8595857708,2.7522934984\H,3.018068246
6,2.5062893756,1.3546505615\H,3.9897085364,0.2495863934,0.9114814543\H
,3.1171094215,-0.4027624239,2.3010502347\H,5.2370323657,1.8243951559,2
.4335342299\H,5.485537761,0.1387110655,2.9155517655\H,4.3641497966,1.1
626955903,3.8265720078\H,-5.1032224923,2.0211629792,0.2012769021\H,-2.
8523900011,4.8205804385,-2.1862469485\C,-5.3790756334,4.2191189101,-1.
3254927657\F,-5.1778286458,5.3810072222,-1.9642695438\F,-6.1924787879,
3.4786198575,-2.1060546489\F,-6.080388849,4.497071604,-0.2098503194\Cl
,-0.2476304955,3.7491584066,-1.9979248076\Cl,-3.0454200905,0.302295061
9,1.1213763392\\Version=ES64L-G09RevE.01\State=1-A\HF=-1830.1175567\RM
SD=5.930e-09\RMSF=1.000e-05\Dipole=1.2433274,-2.7440607,-0.1444095\Qua
drupole=2.7160312,2.5957037,-5.3117349,-8.554226,0.7462797,-4.2646706\
PG=C01 [X(C11H11Cl2F3N2O1)]\\@

1\1\GINC-R3716\FOpt\RM062X\Gen\C11H13F3N2O3S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26843
54560\\4SulfOxyCf3.M062X_6-31pGd_opt\\0,1\C,-2.0010428586,1.8457922452
,-0.0802217512\C,-0.6280795585,1.1881093543,-0.199730912\C,0.490966029
7,2.1715336782,0.1173105902\N,1.7911286441,1.5222062396,-0.0032823291\
C,2.9251796531,2.2937181757,0.0193232059\O,2.9015059241,3.5108533237,0
.0178274491\N,4.1005460897,1.5424107228,0.0071138117\C,5.4113364331,2.
012427542,0.0606729887\C,5.7425655791,3.3610018192,0.2773447257\C,6.43

42840347,1.0581770941,-0.0921500446\C,7.7652610177,1.4299920546,-0.031
0973253\C,8.0771422241,2.772448547,0.184766214\C,7.0789643815,3.732583
1006,0.339631109\H,-2.7997741089,1.1353626376,-0.3098762045\H,-2.09188
46795,2.6891412553,-0.7726990896\H,-2.1693865933,2.2248341767,0.933325
1295\H,-0.4814448853,0.7954775369,-1.2128901096\H,-0.5713299435,0.3320
24479,0.4870890679\H,0.3608399052,2.5921329934,1.1244367314\H,0.478366
2693,3.0098810218,-0.5843934688\H,1.8513475808,0.5717711322,0.34065927
27\H,4.0043590024,0.5523619711,-0.1778058341\H,4.9602517835,4.09741663
48,0.392322073\H,6.1767146157,0.0142069758,-0.2528217913\H,8.558538358
1,0.6963002065,-0.1368037693\S,9.766966969,3.2587831967,0.2541742781\O
,10.5974129768,2.1023086784,0.5509458271\O,9.8898497575,4.5227285377,0.
9612589667\H,7.3514008765,4.7684492823,0.5190100027\C,10.1373533318,3.
6665644804,-1.5237031214\F,11.4021855692,4.0489420082,-1.6277020261\F
,9.9370507346,2.5949543986,-2.2878909408\F,9.343684886,4.6485984999,-1
.9425773257\\Version=ES64L-G09RevE.01\State=1-A\HF=-1459.435642\RMSD=3
.887e-09\RMSF=2.086e-06\Dipole=-3.1182809,-2.0747144,-0.3116659\Quadru
pole=-1.3693055,5.0674997,-3.6981942,8.4847527,-7.1167572,-1.851644\PG
=C01 [X(C11H13F3N2O3S1)]\\@

9_anion.M062X_6-31pGd_opt_water

1\1\GINC-R4423\FOpt\RM062X\Gen\C11H12F3N2O3S1(1-)\ROOT\30-Oct-2018\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=h2o) maxdisk=2684354560\\4SulfOxyCf3_a1.M062X_6-31pGd_opt_wat
er\\-1,1\C,-1.9389527813,1.8732122955,-0.13787557\C,-0.5881948127,1.25
68698097,0.2123523142\C,0.5578171545,2.1958329688,-0.1350741303\N,1.83
87027267,1.5818885765,0.1847583377\C,3.0197432882,2.2212976696,-0.1037
989546\O,2.9955419536,3.4559032319,-0.353500213\N,4.0986228227,1.39630
71054,-0.1217963365\C,5.3544606253,1.8903025352,-0.0307430016\C,5.7255
485971,3.1714622814,0.4878892354\C,6.4229221262,1.0236750142,-0.419883
0503\C,7.7439677324,1.3954832222,-0.3276139835\C,8.0627069811,2.666204
4736,0.187025499\C,7.047618019,3.549027905,0.5935106826\H,-2.759836249
1,1.1971494466,0.1197778385\H,-2.0048293359,2.0899004418,-1.2099237037
\H,-2.0929562509,2.8123939688,0.4052324754\H,-0.4578124839,0.311723022
3,-0.3304848022\H,-0.5494176463,1.0205281225,1.2827172466\H,0.45660827
03,3.1275834229,0.431159188\H,0.511621302,2.4594750431,-1.2020717605\H
,1.8767268782,0.5695798862,0.1463559755\H,4.9564358962,3.8539459834,0.
8245712091\H,6.1667432952,0.0396858531,-0.8013447114\H,8.5310160008,0.
7150381616,-0.6404522039\S,9.7073737616,3.1705471267,0.2589105006\O,10
.6209868208,2.0251759028,0.250615237\O,9.8963908163,4.2538319199,1.227
2146946\H,7.3034700408,4.522627006,1.0028789786\C,10.0337677678,3.9952
813229,-1.3753654872\F,11.2896489294,4.4319346339,-1.4035474763\F,9.85
11802624,3.131109217,-2.368926868\F,9.2106868911,5.0266224294,-1.53806
71596\\Version=ES64L-G09RevE.01\State=1-A\HF=-1458.9882849\RMSD=9.162e
-09\RMSF=8.404e-06\Dipole=-1.1123745,-0.8083526,-0.8647578\Quadrupole=
-19.4125568,10.313337,9.0992199,4.1094909,-8.4107552,0.9929282\PG=C01
[X(C11H12F3N2O3S1)]\\@

9_anion.M062X_6-31pGd_opt

1\1\GINC-R4385\FOpt\RM062X\Gen\C11H12F3N2O3S1(1-)\ROOT\31-Oct-2018\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2
684354560\\4SulfOxyCf3_a1.M062X_6-31pGd_opt\\-1,1\C,-1.4110125272,2.01
65556207,0.8115790793\C,0.0005665761,1.5316972596,0.4877601381\C,0.413
2576069,1.8893584764,-0.943339119\N,1.7558169893,1.4890985161,-1.29042
05233\C,2.8454060866,2.1739891446,-0.7433508617\O,2.6540037478,3.29258
60614,-0.240968523\N,3.9924732342,1.4507603009,-0.8771270373\C,5.17895
67636,1.9323987351,-0.4737262769\C,5.4640092876,3.2173071507,0.1065403
349\C,6.3025454429,1.0535900523,-0.6466218876\C,7.5799736584,1.4011740
447,-0.2858975528\C,7.8156628079,2.6691777385,0.2849074457\C,6.7475756
701,3.5669223024,0.4674035264\H,-1.7055851671,1.7559686901,1.833719254
\H,-2.1477341946,1.5753296061,0.1282061637\H,-1.4770804107,3.106122764
7,0.7118561631\H,0.066731653,0.4431650421,0.6205586138\H,0.7273257278,
1.9868482779,1.169620237\H,0.3525426405,2.9752349665,-1.0713583674\H,-
0.2824395541,1.429995356,-1.6590923005\H,1.9381402766,0.5075917823,-1.
4525666237\H,4.6465546491,3.9073814043,0.2612192876\H,6.0963026052,0.0
793259356,-1.0797853775\H,8.4095567909,0.7126013022,-0.4217097307\S,9.
4187741294,3.14453856,0.6803590835\O,10.2952633631,1.9862651689,0.8446
964955\O,9.4346280449,4.2494921359,1.6362554907\H,6.9459197159,4.53981
24493,0.9101541184\C,10.0782416587,3.9366216046,-0.8720470328\F,11.336
4925096,4.3419448903,-0.6775083365\F,10.0702425067,3.0716741957,-1.888
8510924\F,9.3451977708,4.9970704637,-1.2159377881\\Version=ES64L-G09Re
vE.01\State=1-A\HF=-1458.9104721\RMSD=3.109e-09\RMSF=3.924e-06\Dipole=
-0.4749481,-0.3462987,-0.5897039\Quadrupole=-26.8526346,15.2310702,11.
6215644,-1.2647544,-8.8568806,-1.1633887\PG=C01 [X(C11H12F3N2O3S1)]\\@

9.M062X_6-31pGd_opt_water

1\1\GINC-R3752\FOpt\RM062X\Gen\C11H13F3N2O3S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2684354560\\4SulfOxyCf3.M062X_6-31pGd_opt_water\\0,1
\C,-1.9975838106,1.7789303913,-0.0127286701\C,-0.610608386,1.151263683
4,-0.1041962688\C,0.4774723441,2.2028797606,0.0493724132\N,1.794425303
5,1.5849970306,-0.0507827099\C,2.9174085035,2.3162594073,0.0822768171\
O,2.8966739987,3.5343150794,0.3030423412\N,4.0931013522,1.5907393613,-
0.0484500269\C,5.4000302381,2.0427878792,0.0443302077\C,5.7584955071,3
.3777580913,0.3123992442\C,6.4105507279,1.076276379,-0.1451335991\C,7.
7449987777,1.4223041057,-0.0729218922\C,8.0792526846,2.7536305764,0.19
91308953\C,7.0980120613,3.7285375752,0.3869854927\H,-2.7785333445,1.02
03876371,-0.1196879738\H,-2.1422075045,2.5257564623,-0.8010975163\H,-2
.1395495067,2.2758914276,0.9532268312\H,-0.4905262078,0.6457302795,-1.
0702467072\H,-0.4900591744,0.3909721104,0.6771576258\H,0.3856701649,2.
7029034106,1.0203619322\H,0.3751603128,2.9694357671,-0.7278733862\H,1.
8499577573,0.5882236005,-0.2299295885\H,3.9920858528,0.5988920371,-0.2
445908711\H,5.0003113687,4.1312766154,0.4630955418\H,6.1327381882,0.04
59962874,-0.3476741677\H,8.5150201005,0.6710577701,-0.2188647192\S,9.7
600087543,3.216919327,0.2469202327\O,10.61391652,2.056993648,0.4945756
988\O,9.9418658674,4.4522209012,1.0066560192\H,7.3737280542,4.75774554
59,0.5964266491\C,10.1360187529,3.700341513,-1.5095086221\F,11.4070188
959,4.0757898479,-1.585240613\F,9.9318213922,2.6672029367,-2.317682829
4\F,9.3555844536,4.7090235543,-1.8777877806\\Version=ES64L-G09RevE.01\
State=1-A\HF=-1459.4630757\RMSD=5.273e-09\RMSF=4.772e-06\Dipole=-4.230
0964,-3.3556381,-1.2227587\Quadrupole=-4.6992877,8.7517511,-4.0524634,
14.6666191,-5.4570017,-1.2607973\PG=C01 [X(C11H13F3N2O3S1)]\\@

11.M062X_6-31pGd_opt

1\1\GINC-R3751\FOpt\RM062X\Gen\C10H12Cl1F5N2O1S1\ROOT\31-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26
84354560\\3SF55Chloro.M062X_6-31pGd_opt\\0,1\C,-1.8313614645,1.5664542
783,0.1428751125\C,-0.4028537498,1.0268055488,0.1286769734\C,0.6143487
873,2.1473274355,-0.042876205\N,1.9706831447,1.6107368696,-0.045657926
8\C,3.027619147,2.4831739217,0.0300145314\O,2.8914250719,3.6775959876,
0.2228544977\N,4.2668560775,1.8598484081,-0.1029688818\C,5.5241371208,
2.469933185,-0.0615582737\C,5.7055606952,3.8594474363,-0.0974141921\C,
6.6423085702,1.6277691458,-0.0070858381\C,7.919325697,2.1681053241,0.0
101822777\C,8.1346329797,3.5409016127,-0.0232017179\C,7.0046058648,4.3
453330402,-0.0768418135\H,-2.5572109911,0.758217505,0.2667817414\H,-2.
0648815813,2.0879160649,-0.7913844228\H,-1.9728520603,2.2746254262,0.9
659860407\H,-0.293371117,0.3014179341,-0.689652227\H,-0.1896963532,0.4
912770949,1.0613734188\H,0.5469220844,2.8590979363,0.7842412601\H,0.41
8112631,2.7084079686,-0.9674188508\H,2.1066143735,0.7409941318,-0.5463
3904\H,4.2755319665,0.8496892866,-0.052122342\H,4.8518674269,4.5211144
854,-0.12990053\H,6.5203752268,0.5487038092,0.0214740744\H,9.136705718
1,3.950934494,-0.0070436435\S,7.2408031133,6.1477680661,-0.1248846485\
F,6.1664904541,6.3244667561,-1.3123427275\F,8.4242111064,6.0251248554,
-1.2167205251\F,6.0819229495,6.3991032202,0.9630859962\Cl,9.2867865143
,1.0953068718,0.078779491\F,7.456737613,7.7380021819,-0.1694435944\F,8
.3393129835,6.0980797175,1.056871987\\Version=ES64L-G09RevE.01\State=1
-A\HF=-1930.0962802\RMSD=9.203e-09\RMSF=4.360e-06\Dipole=-1.5333625,-2
.7430307,-0.3073349\Quadrupole=5.4712852,0.3739384,-5.8452236,8.104772
8,2.1052901,1.5223336\PG=C01 [X(C10H12Cl1F5N2O1S1)]\\@

11.M062X_6-31pGd_opt_water

1\1\GINC-R4423\FOpt\RM062X\Gen\C10H12Cl1F5N2O1S1\ROOT\30-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,
Solvent=h2o) maxdisk=2684354560\\3SF55Chloro.M062X_6-31pGd_opt_water\\
0,1\C,-1.8209571608,1.5055211498,-0.0992953652\C,-0.3995589595,1.04436
21793,0.2063773557\C,0.606014931,2.1496847962,-0.0771310243\N,1.961462
4612,1.6884196919,0.2024038999\C,3.0185763471,2.5088997088,0.028973772
9\O,2.8916091967,3.7087202509,-0.2537421753\N,4.2521337789,1.907346418
,0.2071879382\C,5.5050587443,2.4973184623,0.0498424836\C,5.7153209616,
3.8822862059,0.0851691998\C,6.5997773549,1.6360907774,-0.1142414887\C,
7.8749639778,2.1607759862,-0.2454140831\C,8.1236743225,3.5297626936,-0
.2310856434\C,7.0144913939,4.3462112952,-0.0636217646\H,-2.5439992052,
0.7113806652,0.108786736\H,-1.9229848253,1.7873223216,-1.1530509514\H,
-2.0898674162,2.3753204489,0.5101639044\H,-0.1522667826,0.1655054662,-
0.4020959357\H,-0.3194097412,0.7437909335,1.2579469961\H,0.3924781311,
3.0225872754,0.5486916906\H,0.5318213906,2.4682432945,-1.1245702312\H,
2.1135650714,0.6923821486,0.3235944207\H,4.2590372376,0.8970042592,0.3

117395539\H,4.8857809958,4.5585884683,0.2312829502\H,6.4434189923,0.56
15502583,-0.1394139578\H,9.1289516275,3.9188695642,-0.3432799326\S,7.2
777563561,6.1406040159,-0.0252776541\F,6.0194245873,6.4312004182,-0.99
38085171\F,8.2548704217,6.106204752,-1.310949719\F,6.3260634874,6.3371
782545,1.2642476428\Cl,9.2186475731,1.0681259335,-0.4463806734\F,7.514
4914119,7.7388211916,0.0086959447\F,8.5613233373,6.0136007148,0.946594
6275\\Version=ES64L-G09RevE.01\State=1-A\HF=-1930.1146211\RMSD=4.435e-
09\RMSF=5.702e-06\Dipole=-1.752688,-4.3353976,0.4212078\Quadrupole=4.2
952473,3.555779,-7.8510263,12.8889754,-2.1346836,-1.286257\PG=C01 [X(C
10H12Cl1F5N2O1S1)]\\@

11_anion.M062X_6-31pGd_opt_water

1\1\GINC-R4407\FOpt\RM062X\Gen\C10H11Cl1F5N2O1S1(1-)\ROOT\30-Oct-2018\
0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(
SMD,Solvent=h2o) maxdisk=2684354560\\3SF55Chloro_a1.M062X_6-31pGd_opt_
water\\-1,1\C,-1.7685498408,1.5221527416,0.2592352266\C,-0.4008699954,
1.1828061519,-0.3254345024\C,0.6732813986,2.1329988775,0.1836644879\N,
1.9753040972,1.7811181138,-0.3685431467\C,3.1068768874,2.4689683736,0.
0373112219\O,2.9572537963,3.6154666808,0.5486398223\N,4.2554221349,1.7
953933019,-0.1595382021\C,5.460643938,2.4351723413,-0.0357491784\C,5.6
840075942,3.8267880606,-0.2068672127\C,6.6026056532,1.6335339885,0.206
2994077\C,7.8663416973,2.1915745477,0.2839879418\C,8.1040903913,3.5546
424916,0.1292366733\C,6.972721202,4.3242513531,-0.1198719101\H,-2.5385
194163,0.8400062101,-0.1139965995\H,-2.0653976827,2.5428581942,-0.0071
432102\H,-1.7564783083,1.4503582869,1.352571763\H,-0.4376785501,1.2326
490819,-1.4205535626\H,-0.127722668,0.1530763193,-0.060012624\H,0.6949
206281,2.1098605169,1.283934757\H,0.4275756969,3.1582672968,-0.1106995
807\H,2.1289708644,0.7878753917,-0.5070001802\H,4.8484174592,4.4793615
597,-0.4183983556\H,6.4713846666,0.5633024635,0.3315805752\H,9.1018383
344,3.9703713704,0.1980927372\S,7.2073876514,6.108838147,-0.3547307228
\F,6.2423471229,6.1601956406,-1.6516576259\F,8.4883465323,5.9037753694
,-1.3226369028\F,5.9524805162,6.4943805179,0.5894063208\Cl,9.235146540
2,1.1430906009,0.5947537526\F,7.4208362549,7.7012118673,-0.5643140065\
F,8.1987344037,6.2367341358,0.9184528359\\Version=ES64L-G09RevE.01\Sta
te=1-A\HF=-1929.6385112\RMSD=4.397e-09\RMSF=6.424e-06\Dipole=0.448088,
-0.5874985,-0.3277166\Quadrupole=-0.0081924,-3.6039748,3.6121672,2.541
5931,2.2081056,-0.3270603\PG=C01 [X(C10H11Cl1F5N2O1S1)]\\@

11_anion.M062X_6-31pGd_opt

1\1\GINC-R4407\FOpt\RM062X\Gen\C10H11Cl1F5N2O1S1(1-)\ROOT\30-Oct-2018\
0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdis
k=2684354560\\3SF55Chloro_a1.M062X_6-31pGd_opt\\-1,1\C,-1.7892818769,1
.6686475059,0.0973048239\C,-0.3748173225,1.2187639133,0.4585852742\C,0
.6865276347,1.9545733727,-0.3576043864\N,2.0207453024,1.5193827482,-0.
0271060773\C,3.0996395082,2.4193958459,-0.0718285931\O,2.866678892,3.6
394719104,-0.0242084946\N,4.2789536215,1.7582354198,-0.145074333\C,5.4
555438287,2.4268186475,-0.131100758\C,5.6607619738,3.8394570296,-0.027
983617\C,6.6323272792,1.6292533311,-0.2270169579\C,7.8898617748,2.1952
444403,-0.2207628687\C,8.1090763572,3.5668379729,-0.1209007029\C,6.951
1370033,4.335664174,-0.026937972\H,-2.5462781247,1.1420406345,0.688410
0086\H,-2.0023565804,1.4829905075,-0.9622753749\H,-1.9117238809,2.7434
788905,0.2742244529\H,-0.2773618259,0.1361377983,0.2954929324\H,-0.174
8987939,1.3937356175,1.5221769181\H,0.6509759099,3.0276109062,-0.14753
1845\H,0.4664123768,1.8294426745,-1.4341002603\H,2.2895069062,0.582299
3796,-0.299074063\H,4.7972916254,4.4858703871,0.0448308151\H,6.5081274
611,0.5545082542,-0.3045366832\H,9.1036852342,3.9913295962,-0.11775184
82\S,7.1665858081,6.136947535,0.1054614867\F,6.0233688663,6.4614318759
,-0.986872098\F,8.2920747125,6.180917747,-1.0666557947\F,6.0825746539,
6.2870364159,1.2920321377\Cl,9.2978106841,1.1416352884,-0.3432028285\F
,7.3775023097,7.7456004276,0.2231737671\F,8.3512186812,6.0063197523,1.
2108529397\\Version=ES64L-G09RevE.01\State=1-A\HF=-1929.5660763\RMSD=4
.533e-09\RMSF=4.147e-06\Dipole=0.0254648,-0.0182856,-0.1490213\Quadrup
ole=-9.6155157,-2.4767009,12.0922167,-2.6615162,1.4983354,0.3917027\PG
=C01 [X(C10H11Cl1F5N2O1S1)]\\@

DPU_anion.M062X.SMD.h2o.opt

1\1\GINC-R3745\FOpt\RM062X\Gen\C13H11N2O1(1-)\ROOT\21-Aug-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\diph_a1.M062X.SMD.h2o.opt\\
-1,1\C,-4.1740771105,2.1374006512,-0.074373422\C,-3.966840899,0.903498
2512,0.5458001574\C,-3.0876159998,2.7736309984,-0.6797644945\C,-1.8182
826112,2.1992808181,-0.659055739\C,-1.5874332904,0.9585623373,-0.02466
60137\C,-2.6996170373,0.3250703275,0.5665770833\N,-0.3679721118,0.2853

DPU_anion.M062X.opt

1\1\GINC-R3745\FOpt\RM062X\Gen\C13H11N2O1(1-)\ROOT\21-Aug-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
maxdisk=2147483648\\diph_a1.M062X.opt\\-1,1\C,-4.2541410926,2.03678234
20,0.0001086757\C,-3.9948324717,0.6617973815,0.0001106889\C,-3.16525347
91,2.9093112113,0.0000882662\C,-1.8499227769,2.4478269296,0.0000703372
\C,-1.5669392659,1.0554286909,0.0000721748\C,-2.6909111525,0.188192710
6,0.0000929443\N,-0.3349540516,0.4462326282,0.0000556993\C,0.792190938
4,1.1619699535,0.0000361444\O,1.0037165611,2.3879722837,0.0000318283\N
,1.9111326746,0.2720408961,0.0000280139\C,3.2590402921,0.5375729656,0.
0000141376\C,3.8106121369,1.8375015306,0.0000044039\C,5.1916233215,2.0
057480352,-0.0000092007\C,6.0705321513,0.9207647478,-0.0000139386\C,5.
5293052349,-0.3657418127,-0.0000045548\C,4.1536860015,-0.5560807984,0.
0000091934\H,-5.2738854995,2.4138319706,0.0001226265\H,-4.8209834644,-
0.0478972448,0.0001263761\H,-3.3397814553,3.9846489365,0.0000862038\H,
-1.0231676649,3.1455256195,0.0000547213\H,-2.4881858425,-0.8801113374,
0.0000944896\H,1.6250929801,-0.697905757,0.0000353051\H,3.1357634867,2
.6828462631,0.0000079962\H,5.5888541242,3.018793962,-0.0000163793\H,7.
1461922507,1.0727154941,-0.0000246561\H,6.1839088305,-1.2347847913,-0.
0000079322\H,3.7471272324,-1.5658228111,0.0000164351\\Version=ES64L-G0
9RevE.01\State=1-A\HF=-686.5491241\RMSD=5.830e-09\RMSF=2.718e-05\Dipol
e=1.2909176,-0.6741596,-0.0000105\Quadrupole=-19.2086273,12.4514524,6.
7571749,1.5900223,0.0003137,-0.0000384\PG=C01 [X(C13H11N2O1)]\\@

DPU.M062X

1\1\GINC-R3726\FOpt\RM062X\Gen\C13H12N2O1\ROOT\21-Aug-2018\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214748364
8\\diph.M062X\\0,1\C,-4.0552547451,1.6100548893,2.0400604329\C,-3.9146
099005,0.4579698094,1.2711531945\C,-2.9215574331,2.3513974264,2.357443
9922\C,-1.6551933627,1.9676329742,1.9249218816\C,-1.5213018508,0.81038
58747,1.149725389\C,-2.6601018715,0.0613568937,0.8291780996\N,-0.28906
94121,0.3251368081,0.6727932271\C,0.9443582175,0.9479299335,0.73842284
63\O,1.1286041188,2.0397973535,1.2406029593\N,1.9434225849,0.181842553
8,0.1652757413\C,3.3108227859,0.49769741,0.0567258841\C,3.8505663929,1
.7455674061,0.3877400555\C,5.2173532401,1.9569832291,0.2288990602\C,6.
0574764208,0.9586538295,-0.2539244443\C,5.5134816549,-0.279553466,-0.5
844016394\C,4.153328676,-0.5090825587,-0.4303501269\H,-5.0342761894,1.
9241591734,2.3861247614\H,-4.7836819591,-0.1380793483,1.0103609729\H,-
3.0148120773,3.2519073768,2.9569427521\H,-0.7822992407,2.5522672006,2.
1748147228\H,-2.5584629059,-0.8393454814,0.2273654641\H,-0.3557791401,
-0.5292691981,0.1380423201\H,1.707587557,-0.7566478554,-0.124612792\H,
3.2081677439,2.5268100206,0.7661208525\H,5.626456427,2.9282296752,0.49
02959451\H,7.120336129,1.141439284,-0.3715002227\H,6.1477654566,-1.074
8386329,-0.9635837333\H,3.7358826833,-1.4798831392,-0.6893075959\\Vers
ion=ES64L-G09RevE.01\State=1-A\HF=-687.0717424\RMSD=7.527e-09\RMSF=1.1
36e-06\Dipole=-0.2170388,-1.2861989,-0.5915888\Quadrupole=3.560782,2.3
947482,-5.9555302,0.895608,-1.4311447,5.2655488\PG=C01 [X(C13H12N2O1)]
\\@

DPU.smd.h2o

1\1\GINC-R3726\FOpt\RM062X\Gen\C13H12N2O1\ROOT\21-Aug-2018\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=h2o) maxdisk=2147483648\\diph.smd.h2o\\0,1\C,-3.9478017914,1.47578220
21,2.2791682321\C,-3.7822281311,0.2662902769,1.6060985591\C,-2.9023363
307,2.3957520395,2.2886044688\C,-1.6999950099,2.1255097762,1.638952008
6\C,-1.5318701906,0.9015682709,0.9823602014\C,-2.5831161048,-0.0227435

593,0.9657104999\N,-0.3603937714,0.561568054,0.276880823\C,0.913648289
2,0.9737900994,0.5833710282\O,1.1685563676,1.8004321137,1.4576412113\N
,1.872824084,0.3824106815,-0.2033806433\C,3.2643738188,0.5663076841,-0
.0798138586\C,3.8364083037,1.773013379,0.337372088\C,5.2228564272,1.88
94930284,0.4004095892\C,6.0502919181,0.8296220536,0.0368434979\C,5.475
3150793,-0.3637431973,-0.3969963297\C,4.0928235462,-0.4985201989,-0.45
14588849\H,-4.8812907172,1.6995250638,2.7850611577\H,-4.5869330778,-0.
4620051888,1.581990458\H,-3.0206468549,3.3472284271,2.798138954\H,-0.9
048407147,2.8580018828,1.6355755705\H,-2.4498000796,-0.9691765603,0.44
83497046\H,-0.4568848642,-0.2249121239,-0.3567848174\H,1.5932828524,-0
.4180584042,-0.7608885883\H,3.205212554,2.6107942296,0.6006744988\H,5.
6563670699,2.8295030547,0.7281788571\H,7.1292929124,0.9335343958,0.085
4894951\H,6.1030576627,-1.1994153704,-0.6904179334\H,3.6430007526,-1.4
310321101,-0.7817998477\\Version=ES64L-G09RevE.01\State=1-A\HF=-687.09
20097\RMSD=8.609e-09\RMSF=8.252e-06\Dipole=-0.46888,-1.8405548,-1.5218
801\Quadrupole=4.8619348,2.5194511,-7.3813859,1.2838995,-2.3038964,6.4
049269\PG=C01 [X(C13H12N2O1)]\\@

10_anion.M062X_6-31pGd_opt

1\1\GINC-R4490\FOpt\RM062X\Gen\C12H11F6N2O1(1-)\ROOT\31-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268
4354560\\34TFM_a1.M062X_6-31pGd_opt\\-1,1\C,-1.8624178357,1.970199117,
-0.1307311292\C,-0.4890999674,1.3383561445,-0.3508283115\C,0.617570300
6,2.1065324226,0.3700878655\N,1.9113751292,1.5012681828,0.1769034878\C
,3.0704216987,2.2913500444,0.0905569379\O,2.9563064181,3.4970414922,-0
.1859752089\N,4.1789131227,1.5460475898,0.3238660967\C,5.4171791225,2.
0774039597,0.2231742137\C,5.7764408536,3.4115330864,-0.152954121\C,6.5
095077022,1.2146440759,0.5168972519\C,7.8228526593,1.6331895623,0.4539
841122\C,8.1613687162,2.9444193948,0.0929516461\C,7.0999022804,3.81946
07779,-0.2186843585\H,-2.6514558186,1.4191406885,-0.6537556046\H,-1.87
65444417,3.0043099849,-0.4939723694\H,-2.118902634,1.9920417532,0.9352
699944\H,-0.246832434,1.3060682081,-1.4195044285\H,-0.5000763149,0.296
5844628,-0.0004878607\H,0.3589155781,2.192756126,1.4417891861\H,0.6916
206014,3.1247384647,-0.0232863526\H,2.0849642994,0.6083224548,0.620273
6287\H,4.9828824316,4.1056725031,-0.3905168714\H,6.2709300551,0.193739
9995,0.8010770352\H,8.6168754499,0.9325932489,0.6937746622\C,7.3491908
836,5.2582296929,-0.5976983736\C,9.6076419544,3.3069243043,0.017915880
2\F,9.8937817736,4.5205915693,0.5348338045\F,10.108361392,3.3152728939
,-1.243659188\F,10.3823060422,2.4248938378,0.6963792852\F,6.2865804828
,5.8315762958,-1.1899377938\F,8.3780077729,5.3988077465,-1.4607685337\
F,7.6399827259,6.0329699146,0.4715554172\\Version=ES64L-G09RevE.01\Sta
te=1-A\HF=-1247.3861076\RMSD=2.988e-09\RMSF=1.678e-05\Dipole=-0.152904
4,-0.4779047,0.2562211\Quadrupole=-18.8059814,6.4764512,12.3295302,-5.
6565606,-0.5539205,-0.0325575\PG=C01 [X(C12H11F6N2O1)]\\@

10.M062X_6-31pGd_opt

1\1\GINC-R3925\FOpt\RM062X\Gen\C12H12F6N2O1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354
560\\34TFM.M062X_6-31pGd_opt\\0,1\C,-1.9142136395,1.8711942098,-0.0275
844978\C,-0.5417488004,1.216713799,0.1131114462\C,0.5809773684,2.21545
97893,-0.1356781701\N,1.8804491043,1.5683066565,0.0039888146\C,3.00978
28851,2.3477908737,0.041503696\O,2.9775159911,3.5638645288,0.087170474
\N,4.1893512042,1.6052101934,0.0563023624\C,5.4969805011,2.0935978519,
0.0825155847\C,5.8212567678,3.4442076695,-0.1110518889\C,6.5300867167,
1.1733125295,0.2863752566\C,7.8522954874,1.5892683813,0.3019080976\C,8
.1867817461,2.9288560103,0.1161105135\C,7.1510078933,3.850738753,-0.09
83903419\H,-2.7155744354,1.1498014753,0.1538387042\H,-2.0534246679,2.2
82487243,-1.0329565964\H,-2.0313685835,2.6910431882,0.6887605946\H,-0.
4584587075,0.3841326756,-0.5994702719\H,-0.4243333885,0.7912777056,1.1
167790788\H,0.5419403555,3.0293300585,0.59322875\H,0.4795579367,2.6696
572443,-1.131483024\H,1.9588769189,0.6355686214,-0.382533685\H,4.09837
32928,0.6111740735,0.2206890705\H,5.0338426688,4.1675364793,-0.2666320
837\H,6.2991949496,0.1215039288,0.4363196711\H,8.6382140384,0.86134785
8,0.4683179924\C,7.4095718742,5.3323001891,-0.2904360365\C,9.651524078
9,3.2964436152,0.1252015534\F,9.8967178293,4.4236407267,0.8063022357\F
,10.1438679761,3.4582195932,-1.1148004293\F,10.3872557431,2.3260308127
,0.7015603525\F,6.3498709059,5.9499580785,-0.835089734\F,8.4525225566,
5.5612473923,-1.1011368576\F,7.6588154723,5.9476777947,0.8764893682\\V
ersion=ES64L-G09RevE.01\State=1-A\HF=-1247.9178435\RMSD=7.521e-09\RMSF
=4.946e-06\Dipole=-2.2138725,-2.8311815,-0.0711439\Quadrupole=1.094665
8,3.8342639,-4.9289297,5.3666069,2.0775385,0.1281928\PG=C01 [X(C12H12F
6N2O1)]\\@

10_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3743\FOpt\RM062X\Gen\C12H11F6N2O1(1-)\ROOT\30-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2684354560\\34TFM_a1.M062X_6-31pGd_opt_water\\-1,1
\C,-1.8638987153,1.8791190512,0.1634242953\C,-0.5154596909,1.318515945
4,-0.2783224777\C,0.627679068,2.2387590968,0.1241037201\N,1.9083089538
,1.6812763673,-0.2903598941\C,3.0863917179,2.3254112726,0.0454761955\O
,3.0312036189,3.5504275536,0.3512155163\N,4.170689325,1.5256141984,0.0
193409691\C,5.4302234462,2.0539190672,0.0785657559\C,5.8036790982,3.37
44859959,-0.2938500352\C,6.4877514743,1.1986854003,0.4676075585\C,7.80
21860186,1.6289683541,0.5155901899\C,8.1523889505,2.9374570237,0.16886
5529\C,7.1238702885,3.7989045367,-0.2567952664\H,-2.6833939368,1.21623
8081,-0.1305510669\H,-2.0463074109,2.8606948882,-0.2883725546\H,-1.901
3763873,1.9982662099,1.2520618676\H,-0.5036385479,1.182549064,-1.36667
04774\H,-0.3586034666,0.329091415,0.170689544\H,0.6051448095,2.4014298
408,1.2124994781\H,0.4958836898,3.2170464016,-0.3491145697\H,1.9700255
81,0.6693499212,-0.2560022823\H,5.0389913111,4.0601351388,-0.631494102
2\H,6.2500005971,0.1746463512,0.7409983086\H,8.5743324474,0.9356390223
,0.8334285633\C,7.3916472096,5.2272528824,-0.6622242311\C,9.5969433127
,3.325155481,0.2328597612\F,9.7952885325,4.5612798694,0.7373275561\F,1
0.2112504088,3.3112133328,-0.9744434033\F,10.3078777245,2.4848637567,1
.0103944047\F,6.3828016949,5.7545468736,-1.3774144225\F,8.4972040306,5
.3537125496,-1.4218280628\F,7.5594648464,6.0420250572,0.4015156331\\Ve
rsion=ES64L-G09RevE.01\State=1-A\HF=-1247.4599207\RMSD=5.094e-09\RMSF=
5.620e-06\Dipole=0.0335243,-1.2566623,-0.0777881\Quadrupole=-8.9732547
,3.6019509,5.3713038,-1.2792175,1.9572414,-1.9975859\PG=C01 [X(C12H11F
6N2O1)]\\@

10.M062X_6-31pGd_opt_water

1\1\GINC-R3724\FOpt\RM062X\Gen\C12H12F6N2O1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2684354560\\34TFM.M062X_6-31pGd_opt_water\\0,1\C,-1.91
64674437,1.8389407388,-0.028454318\C,-0.5315246213,1.2079429317,0.0708
834571\C,0.559553151,2.2636376158,-0.0204958431\N,1.8743572729,1.63943
37213,0.064468453\C,3.0006099857,2.3785808433,0.0230195177\O,2.9806994
912,3.6156699054,-0.0539617999\N,4.1739849385,1.6461560428,0.079727023
1\C,5.4824181469,2.1197701026,0.0836385362\C,5.8337568497,3.4533587525
,-0.1770356434\C,6.5006470703,1.1925949115,0.3415585774\C,7.8282736645
,1.5876625998,0.3532928955\C,8.1867643983,2.9135530543,0.1102352973\C,
7.1693048376,3.8393506887,-0.1657997277\H,-2.6993126372,1.0779492332,0
.0408047274\H,-2.0397641319,2.3643610142,-0.9818238528\H,-2.0761748699
,2.5621607122,0.7788014659\H,-0.3943868466,0.4761575421,-0.7347908\H,-
0.4319176263,0.6675770258,1.0201041847\H,0.4518192078,2.9895637076,0.7
933282054\H,0.4755306871,2.8128360689,-0.9660361181\H,1.9296848836,0.6
270407672,0.0925526458\H,4.0796450368,0.6427678163,0.2084205123\H,5.06
57666153,4.1807338227,-0.3928782925\H,6.2459259521,0.1551104155,0.5383
997047\H,8.5954978787,0.8499616229,0.5610050992\C,7.4529799749,5.29921
53949,-0.4346264798\C,9.6501402263,3.2617742499,0.1246090455\F,9.90482
99676,4.4322557116,0.7393887998\F,10.1760764169,3.3555498026,-1.114996
0047\F,10.3756065196,2.3297324503,0.7674839835\F,6.4164731532,5.913569
6542,-1.027179149\F,8.5141141855,5.4770892135,-1.2418237021\F,7.702507
6646,5.9868418657,0.6974095993\\Version=ES64L-G09RevE.01\State=1-A\HF=
-1247.937026\RMSD=4.094e-09\RMSF=5.886e-06\Dipole=-2.7981014,-4.472614
5,0.4009785\Quadrupole=-0.3475347,6.8620942,-6.5145595,9.765534,0.2654
655,-1.7842593\PG=C01 [X(C12H12F6N2O1)]\\@

6.M062X.opt

1\1\GINC-R4416\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\12-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 maxdisk=2147483648\\aryl_urea_Cl_CF3.M062X.opt\\0,1\C,-4.2219699984,3
.0921246846,-0.7877862884\C,-4.0860658285,1.7210908982,-0.594821155\C,
-2.9206125605,1.1692311931,-0.0883323545\C,-1.8376399534,1.9975987313,
0.2435210443\C,-1.9485226508,3.380033916,0.0595955416\C,-3.1375662396,
3.893914998,-0.4526744958\H,-5.1379710026,3.5111662118,-1.1866389109\N
,-0.6844809784,1.3686914757,0.7256437899\C,0.4525478734,1.9801669072,1
.2448969887\N,1.422272427,1.0856900858,1.6291910956\O,0.5725351375,3.1
850372104,1.3755688755\C,2.7152587543,1.5963802709,2.0691798224\C,3.54
47831769,0.4820712492,2.6937989154\C,4.9045272736,0.9933818727,3.16447
3032\H,-2.8538695307,0.0929563222,0.0451160945\H,-1.1262277945,4.03440
2607,0.3163437809\H,-0.7540370686,0.3660021024,0.8384310167\H,1.430764
4765,0.1757216212,1.1847624924\H,2.5224912071,2.3882236922,2.797877339
2\H,3.2569741948,2.0559763393,1.2302380227\H,3.6903518926,-0.323801297

7,1.960787145\H,2.9881053282,0.0520780117,3.5348303083\H,5.4797650977,
1.408345654,2.3300298723\H,5.4950635542,0.1894626435,3.6122965998\H,4.
7867336757,1.7821757665,3.91481177\Cl,-5.4108235508,0.6667124053,-1.00
11954293\C,-3.2363338903,5.3887637593,-0.6121811063\F,-3.2919853725,6.
0093421806,0.5799395755\F,-4.3306088736,5.7558521014,-1.2989301101\F,-
2.1715687763,5.8909663863,-1.2597732725\\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-1370.5372523\RMSD=3.304e-09\RMSF=3.794e-06\Dipole=1.2919467,
-2.3044984,0.3422649\Quadrupole=4.2697816,-0.6453867,-3.6243949,-6.920
8459,2.1221183,-1.89227\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

6_anion.M062X.opt

1\1\GINC-R4500\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\12-Jul-2018\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
2147483648\\aryl_urea_Cl_CF3_a1.M062X\\-1,1\C,-4.2078193452,3.07544780
8,-0.7209122552\C,-4.019496298,1.6989914778,-0.6279649118\C,-2.8327729
47,1.1292365573,-0.2174438211\C,-1.7073705434,1.9291698184,0.138340554
5\C,-1.8921819107,3.341371638,0.0463565829\C,-3.1107646388,3.864853761
3,-0.3687568555\H,-5.150907828,3.5016074546,-1.0400861253\N,-0.5990960
968,1.2503760372,0.5285329506\C,0.5342150294,1.9039972167,0.8669852225
\N,1.5216369123,1.0021104107,1.314129151\O,0.7988488656,3.1191988494,0
.8532068721\C,2.9121661521,1.3839135138,1.2961515377\C,3.7096958683,0.
6816481781,2.3933726828\C,5.18659633,1.0714853777,2.3684038495\H,-2.72
66995432,0.0514021099,-0.1521429913\H,-1.0688360315,3.9929258671,0.307
4204484\H,1.3021765559,0.0470003491,1.0596571124\H,2.9378184423,2.4678
64996,1.4416188284\H,3.3867272695,1.1805094874,0.3175356547\H,3.612678
1088,-0.4071896007,2.2776327742\H,3.2611819209,0.9337490768,3.36150251
03\H,5.6465980446,0.8076766306,1.4085177697\H,5.7528934208,0.569476414
6,3.1604333952\H,5.3048216781,2.1528775343,2.5036020498\Cl,-5.37041937
44,0.6430262389,-1.0483709736\C,-3.2337352973,5.3526258951,-0.51381429
69\F,-2.5447473632,6.0360237999,0.4185922408\F,-4.5155414055,5.7816286
527,-0.4317978606\F,-2.7792159756,5.7949244496,-1.7114120966\\Version=
ES64L-G09RevE.01\State=1-A\HF=-1370.0006588\RMSD=7.805e-09\RMSF=4.309e
-06\Dipole=0.3426461,-0.3168947,-0.0363242\Quadrupole=-8.9295447,0.811
654,8.1178907,-0.7313494,-7.6829357,1.7799217\PG=C01 [X(C11H11Cl1F3N2O
1)]\\@

6_anion.M062X.SMD.h2o.opt

1\1\GINC-R3718\FOpt\RM062X\Gen\C11H11Cl1F3N2O1(1-)\ROOT\10-Jul-2018\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Nor
aman SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_Cl_CF3_a1.M0
62X.SMD.h2o.opt\\-1,1\C,-4.1723372843,3.028692707,-0.8533404248\C,-3.9
675619341,1.6562629014,-0.7325508152\C,-2.8071170616,1.1152153207,-0.2
101269603\C,-1.7457418136,1.9450025395,0.2329151119\C,-1.9494042561,3.
3413671118,0.121875994\C,-3.1348810107,3.8433128968,-0.4074996966\H,-5
.088855596,3.4324640419,-1.2668717574\N,-0.6582040729,1.3184854922,0.7
927221325\C,0.5299554007,1.9425242459,0.84939317\N,1.4654139386,1.3010
341001,1.6492095872\O,0.880665997,3.0086786153,0.2649757165\C,2.886293
9036,1.5556258005,1.4488838154\C,3.7240248839,0.6746942322,2.364471933
2\C,5.2165216126,0.9165371972,2.1604960669\H,-2.694938181,0.0380483618
,-0.1316437723\H,-1.1842253575,4.0277008558,0.4631024707\H,1.230282865
4,0.3350326678,1.8514160893\H,3.0925882623,2.6089939635,1.6635154973\H
,3.1745680366,1.377706082,0.401416159\H,3.48800155,-0.3792743981,2.167
5646873\H,3.4503593003,0.8749628688,3.4076349393\H,5.5119473945,0.6971
665964,1.1283399085\H,5.8140472499,0.282886282,2.8230011627\H,5.475681
5953,1.9606084953,2.3694145649\Cl,-5.2393100975,0.5712246345,-1.266674
955\C,-3.270978409,5.3349463347,-0.4953284036\F,-3.0955631722,5.934679
9189,0.7021641424\F,-4.4727223623,5.7307050062,-0.9500453343\F,-2.3500
613817,5.882645128,-1.3191410297\\Version=ES64L-G09RevE.01\State=1-A\H
F=-1370.0780633\RMSD=3.772e-09\RMSF=5.176e-06\Dipole=-0.202,-0.8007281
,0.3197621\Quadrupole=-1.7659361,-1.6069133,3.3728494,-5.6919629,0.669
9411,0.2219294\PG=C01 [X(C11H11Cl1F3N2O1)]\\@

6.M062X.SMD.h2o.opt

1\1\GINC-R4493\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\12-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_Cl_CF3.M062X.SMD
.h2o.opt\\0,1\C,-4.2320811711,3.0839767232,-0.7844623646\C,-4.07831401
28,1.7174108925,-0.5669855614\C,-2.908898396,1.174906289,-0.0640005041
\C,-1.8236724454,2.0149367873,0.2411808117\C,-1.9463457573,3.392129601
8,0.027279577\C,-3.1459110193,3.8924734279,-0.4768194566\H,-5.15727554
81,3.4901184544,-1.1765097098\N,-0.6710785918,1.394347711,0.7254464162
\C,0.452369458,1.9951716602,1.2603693081\N,1.413783624,1.1383877891,1.
6628358232\O,0.5706696418,3.2243843827,1.3741823224\C,2.6816203312,1.6

286887429,2.19065385\C,3.5699342316,0.4643256051,2.6010242534\C,4.9070
343393,0.9593185171,3.1428098439\H,-2.8258113422,0.1036013792,0.095503
0662\H,-1.1254105081,4.0614644742,0.2442169958\H,-0.702152769,0.379348
4436,0.748913823\H,1.3167037726,0.1445368523,1.4857012287\H,2.48410639
11,2.2741567615,3.053484901\H,3.1862948242,2.2386733194,1.4312063663\H
,3.7350476291,-0.1875714495,1.7341991586\H,3.0536691776,-0.1329220353,
3.3622998882\H,5.4455425173,1.5396905788,2.3855819243\H,5.5437201394,0
.1212186764,3.4410628537\H,4.7610286382,1.6008019777,4.0188634651\Cl,-
5.4098333129,0.6505022566,-0.9381760578\C,-3.2323487267,5.3774890399,-
0.6875112472\F,-3.061579394,6.0597168368,0.463859427\F,-4.4116237021,5
.7659137405,-1.1973381966\F,-2.2772980187,5.8225825634,-1.5298722058\\
Version=ES64L-G09RevE.01\State=1-A\HF=-1370.5562207\RMSD=3.023e-09\RMS
F=2.834e-06\Dipole=1.43011,-3.6477761,0.5085546\Quadrupole=3.3949249,1
.1399976,-4.5349225,-10.9746854,2.7850249,-4.2831915\PG=C01 [X(C11H12C
l1F3N2O1)]\\@

TCC.M062X_6-31pGd_opt

1\1\GINC-R125\FOpt\RM062X\Gen\C13H9Cl3N2O1\ROOT\08-Oct-2018\0\\# M062X
/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)\\triclofen.M062X
_6-31pGd_opt\\0,1\C,-0.9957927212,2.4699123093,-0.0324389034\C,-0.6509
784201,1.131179623,-0.2223383942\C,0.6812032046,0.7402802654,-0.169523
4791\C,1.6929026453,1.6735574678,0.0771380114\C,1.3520978436,3.0181255
12,0.0269815170\C,0.0156552106,3.3948566766,0.2110123207\Cl,-1.8566086
364,-0.0757497906,-0.5306518862\Cl,-2.6446957385,2.999346261,-0.092783
1822\N,3.0072109875,1.1791953514,0.1321393957\C,4.175810027,1.91859473
19,0.2148400127\O,4.2030321959,3.1345362627,0.2448827775\N,5.302240373
4,1.1207076117,0.258448785\H,0.9199271033,-0.3084205719,-0.3243330968\
H,2.1193395087,3.7552081632,0.4567177356\H,-0.2543777223,4.4354618946,
0.3583931393\H,3.0891211786,0.1798336341,0.0027739994\H,5.1702660266,0
.1214323374,0.3376470832\C,6.6437588855,1.5426020152,0.3427749305\C,7.
0522239227,2.8741506579,0.2058287633\C,8.4065439935,3.1898525635,0.287
203809\C,9.35123112,2.1935344769,0.5001449791\C,8.9564605537,0.8666070
956,0.6351361043\C,7.6071173395,0.5489326976,0.557570018\Cl,11.0424439
677,2.6053975729,0.5989994887\H,6.3216079277,3.653733306,0.0436595214\
H,8.7254397584,4.221773133,0.1826879562\H,9.6960307808,0.0905441888,0.
8016318392\H,7.3004286837,-0.4891254469,0.6664231009\\Version=ES64L-G0
9RevE.01\State=1-A\HF=-2065.7977912\RMSD=6.783e-09\RMSF=2.281e-06\Dipo
le=0.3955098,-1.4106802,0.0598324\Quadrupole=-17.6222381,15.8408808,1.
7813573,-6.2514299,-1.2729907,-0.4829184\PG=C01 [X(C13H9Cl3N2O1)]\\@

TCC_anion.M062X_6-31pGd_opt

1\1\GINC-R119\FOpt\RM062X\Gen\C13H8Cl3N2O1(1-)\ROOT\08-Oct-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)\\triclofen_a
2cl.M062X_6-31pGd_opt\\-1,1\C,-0.9705460908,2.4569196774,-0.072868112\
C,-0.6075818623,1.1086812086,-0.0851527372\C,0.7222464258,0.732683179,
-0.0160190627\C,1.7726273276,1.682402604,0.0697817823\C,1.3821358082,3
.0496202621,0.080926859\C,0.0423743721,3.4092319935,0.0107902753\Cl,-1
.8304798783,-0.1431390434,-0.1886628879\Cl,-2.6402769806,2.9712577544,
-0.1586978467\N,3.0372826264,1.1656476796,0.1314602605\C,4.1042943359,
1.9692613718,0.2145961815\O,4.2097127429,3.2064327134,0.2517190848\N,5
.2852497297,1.1736716394,0.2637961394\H,0.9872340987,-0.3193973419,-0.
0266846189\H,2.1459468717,3.8122199386,0.1450925322\H,-0.2353668696,4.
4599590424,0.0206466901\H,5.083686443,0.183398629,0.2271889259\C,6.603
0655156,1.5546310939,0.3513479951\C,7.0365602389,2.8961184624,0.410718
4963\C,8.3928177789,3.1920516388,0.4983776496\C,9.3402517611,2.1747535
903,0.528805644\C,8.9396984504,0.8449643567,0.4716521581\C,7.587201999
5,0.543834028,0.384105357\Cl,11.0503885873,2.5673709046,0.6398266479\H
,6.2946286173,3.68285231,0.3866447068\H,8.7146818718,4.2284238891,0.54
34879275\H,9.6790579985,0.0500027154,0.4953624764\H,7.2768380803,-0.49
77442969,0.3395274758\\Version=ES64L-G09RevE.01\State=1-A\HF=-2065.274
4337\RMSD=7.283e-09\RMSF=1.865e-05\Dipole=0.9923403,-0.5030691,0.04597
07\Quadrupole=-47.5449442,25.9728366,21.5721076,-7.9542639,-4.2953092,
-0.3654248\PG=C01 [X(C13H8Cl3N2O1)]\\@

TCC.M062X_6-31pGd_opt_water

1\1\GINC-R158\FOpt\RM062X\Gen\C13H9Cl3N2O1\ROOT\08-Oct-2018\0\\# M062X
/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solven
t=h2o)\\triclofen.M062X_6-31pGd_opt_water\\0,1\C,-0.9494326515,2.51775
22406,0.0355259904\C,-0.6079013857,1.2622127917,-0.4682687761\C,0.7098
780051,0.8250295765,-0.4346473072\C,1.7084877187,1.6358631402,0.115447
9304\C,1.3661136684,2.889113667,0.6381570899\C,0.0455523971,3.31939651
33,0.5866423784\Cl,-1.8121115233,0.2151945317,-1.1591749631\Cl,-2.5892
624609,3.0948088023,-0.0007612356\N,3.00939259,1.1107475457,0.15135756

4\C,4.1757694026,1.8385501519,0.2015574316\O,4.2051424989,3.0690972829
,0.2374669034\N,5.2999253746,1.0537028785,0.2064366693\H,0.9607832471,
-0.152216536,-0.837451386\H,2.1157209272,3.5229639169,1.0907429494\H,-
0.2187441593,4.2911563933,0.9914839762\H,3.0845548998,0.1175842797,-0.
0502300021\H,5.17334465,0.0571741919,0.3563546509\C,6.6287479027,1.509
9609112,0.2961058753\C,7.0473431113,2.7466379431,-0.2070840614\C,8.386
597084,3.118839224,-0.110167326\C,9.3030269592,2.2513797909,0.47210503
42\C,8.9067504873,1.0099664939,0.9591720215\C,7.5680863817,0.646398273
1,0.872811597\Cl,10.9851526157,2.7234751013,0.5877240063\H,6.341549431
4,3.4155367289,-0.6817740018\H,8.7094727014,4.0793263491,-0.4993155891
\H,9.6288422735,0.3351554197,1.4074621607\H,7.246857853,-0.3187476033,
1.2561204196\\Version=ES64L-G09RevE.01\State=1-A\HF=-2065.82034\RMSD=8
.425e-09\RMSF=1.196e-05\Dipole=0.5557551,-2.5875843,0.2552049\Quadrupo
le=-24.9784433,19.0266247,5.9518186,-8.546733,-2.4125217,-1.7399105\PG
=C01 [X(C13H9Cl3N2O1)]\\@

TCC_anion.M062X_6-31pGd_opt_water

1\1\GINC-R123\FOpt\RM062X\Gen\C13H8Cl3N2O1(1-)\ROOT\08-Oct-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,So
lvent=h2o)\\\triclofen_a2cl.M062X_6-31pGd_opt_water\\-1,1\C,-0.94135955
29,2.4653911748,-0.0013830959\C,-0.5739447145,1.2061139876,-0.47549245
98\C,0.7445615752,0.7771852952,-0.4027418517\C,1.7580815972,1.59267901
69,0.1421612536\C,1.3635422664,2.8618496393,0.6261832643\C,0.042261519
7,3.2822339841,0.5537348716\Cl,-1.7609720327,0.1327874055,-1.173581618
5\Cl,-2.588987618,3.0310342762,-0.0762354259\N,3.0267364631,1.05186776
9,0.2382001774\C,4.0915928037,1.8536081053,0.1729489561\O,4.1481219406
,3.0757143371,-0.1297265732\N,5.2792047397,1.1642786382,0.4501309039\H
,1.0041680066,-0.2095407039,-0.774189721\H,2.0975485679,3.5157580154,1
.080897338\H,-0.23809412,4.2581852677,0.9394775504\H,5.1459712976,0.18
6332798,0.6796760964\C,6.6011248034,1.5922440229,0.3971579737\C,7.0166
891123,2.8925259931,0.0633967469\C,8.3736485005,3.2138743032,0.0427184
388\C,9.3248392818,2.2512427846,0.3523962877\C,8.9381655436,0.95606492
03,0.6864545535\C,7.5882075894,0.6359691814,0.7065897775\Cl,11.0286449
635,2.6669336881,0.3224609932\H,6.2889133803,3.6522464343,-0.180918982
8\H,8.6801865256,4.222496518,-0.2179072033\H,9.6806346422,0.2019572792
,0.9287390364\H,7.2842449177,-0.3749241316,0.9666227126\\Version=ES64L
-G09RevE.01\State=1-A\HF=-2065.345463\RMSD=7.221e-09\RMSF=6.865e-06\Di
pole=1.2025205,-0.8381855,0.6957866\Quadrupole=-34.2347576,20.0296787,
14.2050789,-10.3783831,-2.7113801,-0.3123602\PG=C01 [X(C13H8Cl3N2O1)]\
\@

3.M062X_6-31pGd_opt

1\1\GINC-R3711\FOpt\RM062X\Gen\C10H13N3O3\ROOT\05-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214748364
8\\3Nitro.M062X_6-31pGd_opt\\0,1\C,11.976345989,0.0061280099,-7.425520
7149\C,10.8599533005,-0.2924077031,-6.4272884814\C,10.5728612723,0.908
0702491,-5.5349502823\N,9.5095481378,0.5967348862,-4.5866521223\C,9.25
30092586,1.4844080597,-3.5681185861\O,9.952752698,2.4537198739,-3.3394
170983\N,8.1350171797,1.1430021223,-2.8121527081\C,7.6333355535,1.8305
06074,-1.6997216586\C,8.0070456154,3.1400457179,-1.3765148363\C,6.6863
913503,1.1702845688,-0.9025678979\C,6.1170359542,1.7948255666,0.200292
6271\C,6.4784965145,3.0946293002,0.5419748871\C,7.4160242875,3.7239169
032,-0.2643959348\H,12.1769164426,-0.8587165088,-8.0638275071\H,12.905
4839288,0.2637654957,-6.9064944111\H,11.1317909462,-1.1477822545,-5.79
74928625\H,9.947339418,-0.5730046714,-6.9716982387\H,10.3074211527,1.7
851039085,-6.1422505364\H,11.4592970175,1.177666817,-4.9545682245\H,8.
7290288318,0.0656375877,-4.9536922562\H,8.7385016168,3.6814458108,-1.9
596330923\H,6.3946268677,0.1526370683,-1.1522600875\H,5.3875463395,1.2
608258081,0.8005345069\N,7.8096120773,5.1086270685,0.0756222932\H,6.05
76182961,3.6087303978,1.3966338025\O,8.6108307305,5.6654731589,-0.6502
661505\O,7.3020524464,5.6082646417,1.0648925181\H,11.7105991917,0.8479
597051,-8.0736411785\H,7.771797585,2.0075823377,-2.9390657686\\Version
=ES64L-G09RevE.01\State=1-A\HF=-778.4465485\RMSD=5.446e-09\RMSF=3.616e
-06\Dipole=-0.9115699,-3.0607712,-1.4438158\Quadrupole=2.5712875,-6.69
18327,4.1205452,2.2393257,-4.2671613,-3.3203394\PG=C01 [X(C10H13N3O3)]
\\@

3.M062X_6-31pGd_opt_water

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13N3O3\ROOT\05-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=h2o) maxdisk=2147483648\\3Nitro.M062X_6-31pGd_opt_water\\0,1\C,11.958
3662522,-0.0398805739,-7.4267135578\C,10.7522815818,-0.2281169012,-6.5
123191543\C,10.665179954,0.8886003743,-5.4829591982\N,9.5112063584,0.6

865335269,-4.6151687795\C,9.237628695,1.5397411494,-3.6057799257\O,9.8
92789743,2.576605003,-3.4186311158\N,8.1711914219,1.170894275,-2.80966
48645\C,7.6579542565,1.8504793734,-1.7021361925\C,7.9662163512,3.17882
03266,-1.3952138614\C,6.7579391537,1.1496515703,-0.8803144671\C,6.1806
444095,1.7532018149,0.229101436\C,6.4828829829,3.0723550146,0.56008911
84\C,7.3712003108,3.7405161619,-0.2703208518\H,12.0176881047,-0.842921
909,-8.172437787\H,12.8903647103,-0.0421590674,-6.8508852079\H,10.822
3478404,-1.1922777084,-5.9936625521\H,9.8299782281,-0.2451620512,-7.10
55760172\H,10.5724272987,1.8578454845,-5.9855736369\H,11.5801635397,0.
9165315714,-4.8785712962\H,8.9906309808,-0.1799058751,-4.6996858865\H,
8.6379868926,3.7592609009,-2.0089785181\H,6.5151154162,0.1182575982,-1
.1229258904\H,5.4909959841,1.1879936407,0.8471252331\N,7.7038298848,5.
1340095056,0.0465781156\H,6.0489832865,3.5570355363,1.4256926132\O,8.5
202131906,5.7137359645,-0.6540116658\O,7.1486108854,5.6592067101,1.000
871033\H,11.8965588424,0.9121190607,-7.9653109286\H,7.7669034439,0.255
1095229,-2.9800502023\\Version=ES64L-G09RevE.01\State=1-A\HF=-778.4707
003\RMSD=4.352e-09\RMSF=4.333e-06\Dipole=-1.3828861,-5.0146593,-1.5740
941\Quadrupole=2.0411232,-5.8243226,3.7831994,2.5324333,-5.5294194,-3.
8730558\PG=C01 [X(C10H13N3O3)]\\@

3_anion.M062X_6-31pGd_opt

1\1\GINC-R3718\FOpt\RM062X\Gen\C10H12N3O3(1-)\ROOT\05-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=21474
83648\\3Nitro_a1.M062X_6-31pGd_opt\\-1,1\C,11.9291909684,0.1126843228,
-7.4447969266\C,10.6259036237,-0.0063046518,-6.6566253178\C,10.7336830
377,0.6242179617,-5.2694452404\N,9.5064967348,0.4942040249,-4.52290803
94\C,9.1649685559,1.4650467924,-3.5547969746\O,9.6674964826,2.59912017
54,-3.646623548\N,8.2886674523,0.9662574119,-2.6581799756\C,7.76385076
44,1.7519806438,-1.6798901892\C,7.9930906661,3.1411527463,-1.450794116
\C,6.869492532,1.1156290896,-0.7727643849\C,6.2521526242,1.7847863352,
0.2730607317\C,6.4792260962,3.1438513716,0.494066205\C,7.3521971354,3.
7711160417,-0.3918359537\H,11.8441852596,-0.3345653492,-8.441240716\H,
12.7522085255,-0.388591653,-6.9213257494\H,10.3490607749,-1.0656033081
,-6.5575956523\H,9.8045984599,0.4817439163,-7.1944757685\H,10.93286698
46,1.6966507577,-5.3534267916\H,11.5951810618,0.1789864897,-4.73618184
65\H,9.2509902639,-0.4381144622,-4.2213860665\H,8.6622672708,3.6903449
41,-2.0979084067\H,6.6838621694,0.0574553193,-0.9369689586\H,5.5783824
149,1.242217985,0.9326313061\N,7.6096927756,5.2088261838,-0.1828579944
\H,6.0131793706,3.6940109224,1.3006821725\O,8.3601714278,5.7886082953,
-0.9490777385\O,7.0535927083,5.7640287341,0.7592891459\H,12.211743859,
1.1643389624,-7.5706732058\\Version=ES64L-G09RevE.01\State=1-A\HF=-777
.9071289\RMSD=5.460e-09\RMSF=4.540e-06\Dipole=0.2985516,-1.7539744,-0.
7297253\Quadrupole=7.8078705,-5.9568538,-1.8510167,2.5833081,6.4491636
,-12.2956674\PG=C01 [X(C10H12N3O3)]\\@

3_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3719\FOpt\RM062X\Gen\C10H12N3O3(1-)\ROOT\05-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2147483648\\3Nitro_a1.M062X_6-31pGd_opt_water\\-1,1\
C,12.0336117707,-0.0871582733,-7.2876790829\C,10.6566352053,-0.0385358
776,-6.6324143625\C,10.6618021592,0.8399513395,-5.3897147894\N,9.34241
16148,0.8627019248,-4.7695917893\C,9.1644564605,1.5262231235,-3.560196
1299\O,9.9888295921,2.439164217,-3.2579484342\N,8.116550472,1.08849222
46,-2.8475901106\C,7.6936873027,1.7862954978,-1.7373562319\C,7.8441692
111,3.1761531297,-1.5284205829\C,6.970053655,1.0753695396,-0.748931608
9\C,6.4449901642,1.6907150627,0.3812023837\C,6.6048472028,3.0593325986
,0.5918283385\C,7.3039133028,3.7576218484,-0.3872739425\H,12.024402546
6,-0.7178241666,-8.1819110076\H,12.7822164516,-0.4925184734,-6.5977241
556\H,10.3397479877,-1.0529230803,-6.3566861615\H,9.915743088,0.346438
1525,-7.3438132064\H,10.9438463766,1.8614632473,-5.6637694847\H,11.423
1343424,0.4738511218,-4.6836629816\H,8.8450635243,-0.0208797522,-4.812
5090093\H,8.3567184851,3.7892282916,-2.2559710299\H,6.8284082992,0.007
6611962,-0.8939571037\H,5.9048891097,1.0973503642,1.112910227\N,7.4770
853168,5.2023523233,-0.2098297866\H,6.2109767825,3.5559519702,1.469469
1806\O,8.1499999194,5.8204172054,-1.0238472008\O,6.9400702087,5.741769
5681,0.7495689574\H,12.3601394484,0.9154156766,-7.5862308944\\Version=
ES64L-G09RevE.01\State=1-A\HF=-777.9914678\RMSD=4.559e-09\RMSF=6.478e-
06\Dipole=-0.4003463,-2.5660174,-0.6573291\Quadrupole=3.0141413,-8.940
824,5.9266827,1.2519374,-1.2743831,-8.9505715\PG=C01 [X(C10H12N3O3)]\\
@

5.M062X.opt

1\1\GINC-R4420\FOpt\RM062X\Gen\C10H13N3O3\ROOT\16-Jul-2018\0\\# M062X/

Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman maxd
isk=2147483648\\aryl_urea_nitro.M062X.opt\\0,1\C,-4.128982565,3.513988
4707,-1.183629988\C,-4.1394367067,2.1380556781,-0.980631752\C,-3.03562
00123,1.5473000123,-0.3915244311\C,-1.9239638653,2.3167845953,-0.00403
83317\C,-1.9358355191,3.7051896614,-0.2166303245\C,-3.0439732604,4.296
7312443,-0.8091844109\N,-0.8494364913,1.6312121575,0.5641581443\C,0.30
8824824,2.1728409354,1.1171399472\N,1.1888002006,1.2206407743,1.569444
1465\O,0.5144614668,3.3685438184,1.2209619949\C,2.4936961304,1.6435313
258,2.0637768724\C,3.2051943681,0.4848117514,2.7501874186\C,4.57461540
56,0.9040119455,3.2800831193\H,-3.0294983004,0.4724187398,-0.228228290
2\H,-1.0897004552,4.3048941219,0.0866659614\H,-0.9915740742,0.63770443
47,0.6915892694\H,1.1445721653,0.2963064929,1.1582438455\H,2.326574727
2,2.4641925997,2.7666049834\H,3.1082105742,2.0417376927,1.2439385006\H
,3.3258784696,-0.3454201641,2.0402325705\H,2.5771055313,0.1158543846,3
.5696552029\H,5.2198538338,1.2570295116,2.4686710726\H,5.0801740532,0.
0683053998,3.7714896634\H,4.4795597748,1.7152069562,4.0094514898\H,-5.
0003564541,1.5529591911,-1.2818353504\H,-3.0719931253,5.3664144182,-0.
9817447106\N,-5.2917156323,4.1494177591,-1.8063943022\O,-5.2575694001,
5.3567293852,-1.9739154499\O,-6.2275656631,3.4325567062,-2.1221368611\
\Version=ES64L-G09RevE.01\State=1-A\HF=-778.4499459\RMSD=6.870e-09\RMS
F=4.894e-06\Dipole=2.2256844,-2.5208187,1.018129\Quadrupole=-6.8461647
,7.6056811,-0.7595163,2.5829747,-6.6148256,1.6003784\PG=C01 [X(C10H13N
3O3)]\\@

5_anion.M062X.opt

1\1\GINC-R3711\FOpt\RM062X\Gen\C10H12N3O3(1-)\ROOT\30-Aug-2018\0\\# M0
62X/Gen 6D NoSymm SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdis
k=2147483648\\aryl_urea_nitro_a1.M062X\\-1,1\C,-3.7540222684,3.4086087
145,-1.4146779001\C,-4.0269121793,2.2269029926,-0.7030579476\C,-3.0701
70325,1.7062955296,0.1326612\C,-1.7840616804,2.3167479993,0.3183477455
\C,-1.5478413017,3.5224536499,-0.427182976\C,-2.5116960833,4.043133205
6,-1.2650489939\N,-0.9540569382,1.6907491084,1.1717796427\C,0.30306622
37,2.1527683468,1.4131186699\N,0.9457740951,1.3725796882,2.3825881803\
O,0.9148001194,3.1176140037,0.926968275\C,2.3808238203,1.4449816074,2.
5172343104\C,3.1554714036,0.7874047437,1.3708161128\C,4.6656076263,0.9
340454123,1.5459747072\H,-3.2619597194,0.7956189531,0.6926480375\H,-0.
5929114994,4.0175581392,-0.3199984363\H,0.4944336301,0.4813895258,2.54
13711031\H,2.664408628,0.9829087817,3.4731356723\H,2.6510237946,2.5050
472975,2.567636122\H,2.8313719763,1.2567720661,0.4354549024\H,2.882430
6718,-0.2752573739,1.3139327838\H,4.9497748475,1.992386839,1.572160009
3\H,5.2178457889,0.4597893833,0.7276209426\H,5.0014387575,0.476803301,
2.485485703\H,-4.9910702929,1.7456029963,-0.8258852505\H,-2.3213170277
,4.9544667894,-1.8222494569\N,-4.7401012747,3.9589431223,-2.2855383358
\O,-4.482501612,4.9973105439,-2.9006672732\O,-5.8246091808,3.379144633
7,-2.3985175493\\Version=ES64L-G09RevE.01\HF=-777.9200944\RMSD=7.270e-
09\RMSF=6.608e-06\Dipole=2.1984504,-1.5092109,1.1978451\Quadrupole=-13
.3477929,-6.732677,20.0804699,33.0076316,-22.9467941,12.0709478\PG=C01
 [X(C10H12N3O3)]\\@

5_anion.M062X.SMD.h2o.opt

1\1\GINC-R4490\FOpt\RM062X\Gen\C10H12N3O3(1-)\ROOT\10-Jul-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_nitro_a1.M062X.SM
D.h2o.opt\\-1,1\C,-4.071868236,3.5110849816,-1.214073499\C,-4.23675964
59,2.2641711875,-0.5794159616\C,-3.1566784168,1.6624049215,0.013648448
6\C,-1.8537142146,2.2621054413,0.0268476884\C,-1.7290645109,3.52688722
47,-0.6415254423\C,-2.8077072835,4.1272880321,-1.2463515847\N,-0.86172
92426,1.5580564651,0.5990200544\C,0.3287482074,2.1477219878,0.91519704
03\N,1.3628170606,1.2646691152,1.0464239995\O,0.5351783985,3.368887891
8,1.1339607576\C,2.6144032348,1.6463065059,1.6825403235\C,3.55558136,0
.4539019503,1.7705077752\C,4.8698887736,0.8322293887,2.4460683428\H,-3
.2753840082,0.6991904404,0.5009104678\H,-0.7622032183,4.0103296115,-0.
688874571\H,1.1168857311,0.2817588528,1.0480448758\H,2.4239252041,2.04
58406777,2.688927714\H,3.0838827817,2.44780165,1.10162134\H,3.74903230
61,0.0712339098,0.7609349608\H,3.0658926536,-0.3518744398,2.3321388039
\H,5.3812232899,1.6259562896,1.8900602314\H,5.5451476055,-0.0267834107
,2.503646552\H,4.6965051922,1.1935587622,3.4658275383\H,-5.2112431704,
1.7887849372,-0.5610343112\H,-2.6850923106,5.0763165842,-1.7571016974\
N,-5.1754458012,4.1402028164,-1.8268965955\O,-5.0241209333,5.242683880
7,-2.3746435443\O,-6.2830608067,3.5820543446,-1.8102997074\\Version=ES
64L-G09RevE.01\State=1-A\HF=-777.9997638\RMSD=5.676e-09\RMSF=3.949e-06
\Dipole=3.6575166,-2.7069051,1.235842\Quadrupole=-16.8065732,9.9398896
,6.8666837,9.6313496,-18.145095,3.4751132\PG=C01 [X(C10H12N3O3)]\\@

5.M062X.SMD.h2o.opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13N3O3\ROOT\16-Jul-2018\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman SCRF
=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_nitro.M062X.SMD.h2o.o
pt\\0,1\C,-4.125916005,3.4998430573,-1.206437773\C,-4.128771902,2.1259
278664,-0.9605600196\C,-3.0246350367,1.5584023043,-0.3576118826\C,-1.9
119464806,2.3456821077,0.0059553437\C,-1.9313341496,3.7288291274,-0.25
5360463\C,-3.0400976655,4.2997898532,-0.8608799511\N,-0.8512055527,1.6
766772167,0.5976971031\C,0.3193607839,2.2062546602,1.119767672\N,1.173
9391185,1.2886176225,1.613403176\O,0.5597848137,3.4207456825,1.1436391
442\C,2.4679646225,1.6830276002,2.1574539036\C,3.2188585319,0.46395184
31,2.6707726964\C,4.5824900658,0.8559491883,3.230461217\H,-3.010563251
9,0.4907358273,-0.1583851458\H,-1.0886115892,4.349875342,0.00839646\H,
-0.9664323857,0.6704535873,0.6781382897\H,0.9718771744,0.2991123058,1.
5175175017\H,2.310784151,2.4001941662,2.9706984173\H,3.0542511821,2.18
86527433,1.3804177611\H,3.3428834259,-0.2554520755,1.8519236849\H,2.62
09760398,-0.0281878136,3.447317251\H,5.2007183719,1.3287852149,2.45946
7659\H,5.1200131976,-0.0210156903,3.6029294341\H,4.4763612625,1.564290
3173,4.0594634011\H,-4.9808383039,1.5153116349,-1.2357679338\H,-3.0564
117285,5.3641711626,-1.0648929006\N,-5.2783902402,4.1058908085,-1.8367
558933\O,-5.2670118799,5.3139073691,-2.0490752659\O,-6.2277905702,3.38
95269707,-2.1373528872\\Version=ES64L-G09RevE.01\State=1-A\HF=-778.474
2615\RMSD=9.912e-09\RMSF=9.398e-06\Dipole=2.8426373,-4.0499692,1.68655
44\Quadrupole=-11.9526653,11.6593844,0.2932808,2.84577,-9.5921794,0.48
90728\PG=C01 [X(C10H13N3O3)]\\@

7.M062X_6-31pGd_opt_water

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H12F1N3O3\ROOT\04-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2147483648\\2Nitro4Fluro.M062X_6-31pGd_opt_water\\0,1\
C,-1.0125306187,2.0137799716,0.4981301908\C,0.2883085143,1.5904330624,
-0.1761984722\C,1.4720450154,2.3592671422,0.3899427657\N,2.7064605185,
1.9467995501,-0.2684328883\C,3.8908800932,2.4781745051,0.0827193511\O,
4.0030068211,3.3507302217,0.9516121919\N,4.9767417829,1.9392966714,-0.
6074013019\C,6.2919326308,2.3478020477,-0.516269283\C,7.3809896947,1.5
023087074,-0.8593377436\C,6.6159073498,3.6492842771,-0.0945225818\C,7.
9365242334,4.0345700765,-0.0261704793\C,9.0112985207,3.2146015975,-0.3
561888216\C,8.7101110433,1.9373123361,-0.7777311948\H,-1.8634146095,1.
4605264493,0.0900180407\H,-1.2013657893,3.0824629355,0.3482287602\H,0.
2260604467,1.7678729534,-1.2568328218\H,0.4538579866,0.5157357782,-0.0
327294416\H,1.560508879,2.1793367972,1.4676325626\H,1.3277503484,3.436
3028519,0.2457206468\H,2.6585426065,1.2459060521,-1.0007246647\H,5.839
4383038,4.3570915007,0.1587305259\F,8.1973697765,5.2930073839,0.369617
4246\N,7.1922880824,0.1403816708,-1.3056271005\H,10.0304803066,3.57691
92168,-0.2918303895\O,8.1619395458,-0.6056476948,-1.3423685523\O,6.068
8515175,-0.2352975144,-1.6413168232\H,-0.9735596895,1.8259329859,1.576
7222469\H,4.8109539025,1.08320985,-1.1265749631\H,9.5018827865,1.25426
86167,-1.060057184\\Version=ES64L-G09RevE.01\State=1-A\HF=-877.6784303
\RMSD=3.571e-09\RMSF=6.704e-06\Dipole=-1.1593172,-0.1071962,-0.9661862
\Quadrupole=18.9485783,-14.3365663,-4.612012,9.4325059,3.1287428,-6.74
0761\PG=C01 [X(C10H12F1N3O3)]\\@

7.M062X_6-31pGd_opt

1\1\GINC-R3812\FOpt\RM062X\Gen\C10H12F1N3O3\ROOT\04-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483
648\\2Nitro4FluroNside.M062X_6-31pGd_opt\\0,1\C,-1.0352678055,2.036279
399,0.4335330475\C,0.318954075,1.4442677246,0.049933106\C,1.4302717083
,2.4809518289,0.1538324012\N,2.7106141557,1.8952699927,-0.2171995475\C
,3.8708598619,2.5614737557,0.0526486769\O,3.9042813274,3.6007264633,0.
6892938521\N,4.9972788279,1.9068629247,-0.4557861809\C,6.312317588,2.3
181790852,-0.3910800272\C,7.3644533904,1.5406724905,-0.9512319958\C,6.
6777887645,3.530571848,0.2249560082\C,8.0036734159,3.9049305708,0.2589
34644\C,9.0412181228,3.1515251359,-0.2846028517\C,8.6978265154,1.96182
86222,-0.8908801088\H,-1.8284371654,1.2876699411,0.3567820672\H,-1.298
8014596,2.8735236115,-0.2213985301\H,0.272340478,1.0574717064,-0.97739
77919\H,0.5601221078,0.5956410796,0.7011145145\H,1.5200381887,2.849420
0718,1.179210141\H,1.2068977087,3.3486737469,-0.4825534905\H,2.706764
9081,1.162758537,-0.9153294545\H,5.9240694621,4.1623674563,0.672677997
5\F,8.3107997157,5.0652093172,0.8537883752\N,7.1400764495,0.2665364015
,-1.6220770058\H,10.0656374367,3.4983385991,-0.2247386039\O,8.09902786
65,-0.3207647954,-2.0843715113\O,5.9917389557,-0.1756668701,-1.7009136
117\H,-1.0219289235,2.4076542079,1.4635753727\H,4.8668511064,1.0035652

741,-0.8977444736\H,9.4537932168,1.3264318737,-1.3347258921\\Version=E
S64L-G09RevE.01\State=1-A\HF=-877.6632646\RMSD=8.727e-09\RMSF=2.068e-0
6\Dipole=-0.8554689,-0.1352166,-0.1707841\Quadrupole=14.6916499,-10.80
73033,-3.8843466,5.7497949,2.2093733,-6.0460769\PG=C01 [X(C10H12F1N3O3
)]\\@

7_anion.M062X_6-31pGd_opt

1\1\GINC-R3749\FOpt\RM062X\Gen\C10H11F1N3O3(1-)\ROOT\04-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214
7483648\\2Nitro4Fluro_a1.M062X_6-31pGd_opt\\-1,1\C,-1.0000577334,2.158
1915215,0.3375271011\C,0.3075739978,1.8606696857,-0.3939738059\C,1.525
5980725,2.0594959717,0.5066177851\N,2.7579586163,1.7569959228,-0.17670
1699\C,3.9332814157,2.4644323145,0.1056076968\O,3.8590720145,3.5622860
331,0.6809056655\N,5.0174622717,1.7721453816,-0.3317602773\C,6.2452914
907,2.3021772288,-0.3160128072\C,7.3670852839,1.5053086394,-0.73519578
69\C,6.5894927948,3.659792894,0.0067552267\C,7.8771318087,4.106177014,
-0.1325864375\C,8.9478068746,3.3294887493,-0.5844279563\C,8.6561234023
,2.012426525,-0.8941766534\H,-1.8698052802,2.0193579858,-0.3136199131\
H,-1.014591894,3.1916612225,0.7028932782\H,0.4152332612,2.5108051608,-
1.2701232734\H,0.2953550155,0.8281617486,-0.7698618623\H,1.4038157915,
1.4495676918,1.4205217894\H,1.5960358031,3.1033253106,0.826591663\H,2.
9399487396,0.7924385633,-0.4249756654\H,5.8127988484,4.3277910878,0.35
33686315\F,8.1455348532,5.4028057047,0.1841620625\N,7.2206136801,0.090
8763437,-1.0333798203\H,9.943847198,3.7473647683,-0.6696095971\O,7.930
7544406,-0.380340714,-1.9279862619\O,6.449940282,-0.5861670176,-0.3761
821124\H,-1.1229929365,1.4999762164,1.2059399097\H,9.4289118873,1.3407
68046,-1.2516668979\\Version=ES64L-G09RevE.01\State=1-A\HF=-877.120819
4\RMSD=4.782e-09\RMSF=2.206e-06\Dipole=-1.1640417,0.2528189,0.1206121\
Quadrupole=-0.2033485,-7.2667265,7.470075,5.4109432,4.3200221,-6.97333
61\PG=C01 [X(C10H11F1N3O3)]\\@

7_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H11F1N3O3(1-)\ROOT\04-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2147483648\\2Nitro4Fluro_a1.M062X_6-31pGd_opt_wate
r\\-1,1\C,-0.9807498847,2.1795186527,0.37861841\C,0.3215567742,1.89533
06841,-0.363023762\C,1.5320044244,2.2718608089,0.4785768405\N,2.763933
4411,1.9904782993,-0.2431542957\C,3.9884292139,2.2156645463,0.31445958
2\O,4.0695352927,2.8821936149,1.3785274814\N,5.020652407,1.6102857081,
-0.3398802905\C,6.2410623546,2.1581657112,-0.3395953229\C,7.4171319076
,1.4295797192,-0.7408831357\C,6.479193385,3.5501759128,-0.0749952891\C
,7.7234528121,4.0906745533,-0.2188769855\C,8.862723642,3.3751197671,-0
.6202450567\C,8.679415388,2.0415353658,-0.8882814091\H,-1.8483944641,1
.909812671,-0.2309947853\H,-1.0633159633,3.242727647,0.6304859108\H,0.
3476108704,2.4579113049,-1.3042398817\H,0.3792048456,0.8305396863,-0.6
226011827\H,1.5122141285,1.7206905085,1.4295707899\H,1.4965559896,3.33
89623467,0.7232758082\H,2.726064247,1.3019593976,-0.9857225355\H,5.654
5488182,4.1909542486,0.2106754842\F,7.8778167612,5.4122177073,0.029935
1575\N,7.3804049775,0.0312389869,-1.0174805018\H,9.8275807317,3.861257
7428,-0.7021170955\O,8.3195362061,-0.4765953484,-1.6519615455\O,6.4450
05149,-0.6622293034,-0.6183073343\H,-1.0334860652,1.607641997,1.311714
9838\H,9.5195326098,1.4304870634,-1.1948093389\\Version=ES64L-G09RevE.
01\State=1-A\HF=-877.2034746\RMSD=3.845e-09\RMSF=1.552e-05\Dipole=-1.8
320792,1.592814,-0.9160417\Quadrupole=13.393776,-13.2289243,-0.1648517
,10.8442798,6.916411,-8.0526493\PG=C01 [X(C10H11F1N3O3)]\\@

13.M062X_6-31pGd_opt_water

1\1\GINC-R4385\FOpt\RM062X\Gen\C11H12F3N3O3\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2684354560\\3TMF4Nitro.M062X_6-31pGd_opt_water\\0,1\C,
-1.9658583651,1.7695463288,-0.0806185923\C,-0.5748401399,1.1463961009,
-0.0305590128\C,0.5063299695,2.216108136,-0.0490110062\N,1.8263642127,
1.5984374705,-0.0000821539\C,2.9454696501,2.3446251474,-0.0058065997\O
,2.9248691756,3.5811891951,-0.0534855861\N,4.124626415,1.6091318544,0.
0466079608\C,5.4266422861,2.0726650522,0.0544016583\C,5.7725297188,3.4
370215379,-0.0002268114\C,6.4509666772,1.1159961964,0.1197849502\C,7.7
722455996,1.5126936927,0.1305456401\C,8.1086522995,2.8643317224,0.0767
05958\C,7.0990477618,3.843902737,0.0101327904\H,-2.7407901678,0.997521
9055,-0.0674054174\H,-2.0964904253,2.3635387404,-0.9918183894\H,-2.131
0648006,2.4285530951,0.7787918005\H,-0.4328059774,0.4754882938,-0.8866
41676\H,-0.4671247412,0.5406127915,0.8775174936\H,0.3889532993,2.88838
78603,0.8087869112\H,0.4237131695,2.8226806228,-0.9582852559\H,1.88682
29705,0.5864361641,0.0399825723\H,4.0270808005,0.5981791982,0.08690422

13.M062X_6-31pGd_opt

1\1\GINC-R4500\FOpt\RM062X\Gen\C11H12F3N3O3\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354
560\\3TMF4Nitro.M062X_6-31pGd_opt\\0,1\C,-1.9742617108,1.8081430099,-0
.0743935693\C,-0.5979881938,1.1567532736,0.041399076\C,0.5183664618,2.
1733536185,-0.1588726302\N,1.8221393759,1.5290110584,-0.0453994365\C,2
.9457157133,2.3094894675,0.0347638849\O,2.9092410257,3.5221504368,0.13
22635068\N,4.1308980638,1.5715892349,0.029708471\C,5.4356186189,2.0582
333087,0.0620162185\C,5.7519439037,3.4266046246,0.0374284985\C,6.47332
97834,1.1185424186,0.1248147935\C,7.7939255906,1.5308174969,0.14043570
59\C,8.0964148976,2.8846153733,0.0748085108\C,7.0786995758,3.843215559
1,0.0340899126\H,-2.7711822265,1.0741265791,0.0721825569\H,-2.11314200
46,2.2628061725,-1.0609042435\H,-2.098867125,2.594374661,0.6774641467\
H,-0.5069220117,0.3576899585,-0.7076542375\H,-0.481067923,0.6877261511
,1.0255231131\H,0.4720571883,2.9534405162,0.6057165612\H,0.4175323368,
2.6705390481,-1.1337652116\H,1.9044140171,0.605826923,-0.4529969127\H,
4.0433024454,0.5673805647,0.1154476273\H,4.9562756426,4.1574343408,0.0
0404785465\H,6.2447774601,0.0564592484,0.1585816452\C,7.331696866,5.342
5798193,0.0568299258\F,6.2160761973,6.0014106888,0.415656203\F,7.68969
67997,5.8224866796,-1.1377286734\F,8.2740748502,5.671815069,0.95089076
84\N,9.5222919386,3.2310767065,0.0117549002\O,10.3009411288,2.47755959
01,0.571921867\O,9.8349201249,4.2181475989,-0.6238281177\H,8.604741189
6,0.8134308036,0.1933765923\\Version=ES64L-G09RevE.01\State=1-A\HF=-11
15.3915663\RMSD=2.107e-09\RMSF=2.631e-06\Dipole=-2.9671422,-2.9888594,
-0.2429525\Quadrupole=-6.3576759,7.3458022,-0.9881263,3.2836212,1.7880
44,2.1060722\PG=C01 [X(C11H12F3N3O3)]\\@

13_anion.M062X_6-31pGd_opt

1\1\GINC-R3715\FOpt\RM062X\Gen\C11H11F3N3O3(1-)\ROOT\05-Nov-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268
4354560\\3TMF4Nitro_a1.M062X_6-31pGd_opt\\-1,1\C,-1.3581310006,2.20540
81771,-0.7458211021\C,0.0613748678,1.6778421972,-0.5481016245\C,0.4957
968866,1.7456802352,0.9190271108\N,1.8474166395,1.2987795197,1.1567395
427\C,2.9224160159,2.0936207262,0.7577023166\O,2.7167195396,3.28533043
47,0.4838416936\N,4.0838718565,1.3761751616,0.7516294331\C,5.260008906
,1.9409889777,0.4458049673\C,5.5150125359,3.3115744175,0.0871365766\C,
6.4047791501,1.0868363826,0.4628984188\C,7.6652219371,1.5504556019,0.1
841670566\C,7.8924491552,2.900817413,-0.1284926255\C,6.7846634402,3.78
3500305,-0.1856946706\H,-1.6687553969,2.1510121001,-1.7945405548\H,-1.
4278432069,3.2526790353,-0.4301889722\H,-2.0805113738,1.630609461,-0.1
524247392\H,0.7734997752,2.2670765489,-1.1362365324\H,0.1313731838,0.6
385824956,-0.8971867848\H,-0.1829284666,1.1442670489,1.5391205866\H,0.
429427814,2.7830156342,1.2635278883\H,2.0426131458,0.3069451522,1.1358
460353\H,4.667380009,3.9769089567,0.0204101016\H,6.2421824982,0.044277
2026,0.7188989898\C,6.8821240697,5.2398616424,-0.6030429437\F,5.660002
8898,5.7757756591,-0.810191975\F,7.5425987933,5.4028764364,-1.76494664
1\F,7.4619282122,6.0264806111,0.3195946127\N,9.2553532754,3.3011869866
,-0.3307146512\O,10.1080216898,2.4217919052,-0.4797228752\O,9.53262646
09,4.4956486353,-0.3291867085\H,8.5212766973,0.8865449392,0.2156680703
\\Version=ES64L-G09RevE.01\State=1-A\HF=-1114.8714964\RMSD=8.671e-09\R
MSF=1.512e-06\Dipole=-2.0757671,-0.8498793,-0.1704433\Quadrupole=-24.8
592574,9.8745548,14.9847026,-5.101336,5.9663187,2.0737726\PG=C01 [X(C1
1H11F3N3O3)]\\@

13_anion.M062X_6-31pGd_opt_water

1\1\GINC-R3720\FOpt\RM062X\Gen\C11H11F3N3O3(1-)\ROOT\30-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2684354560\\3TMF4Nitro_a1.M062X_6-31pGd_opt_water\
\-1,1\C,-1.8861077475,1.9057841803,-0.0561628562\C,-0.508347472,1.3429
660982,-0.3904025832\C,0.5987088259,2.1966485739,0.2104247844\N,1.9041
740684,1.6381930266,-0.1056513847\C,3.0563561695,2.1989764817,0.353830
3957\O,3.0194124338,3.3289596644,0.9021675073\N,4.1590805126,1.3994476

616,0.2063791684\C,5.3870283533,1.9312910138,0.1792617575\C,5.69779823
75,3.3093075073,-0.0924284663\C,6.5054375226,1.0601708597,0.3418245549
\C,7.7929162143,1.5299123206,0.3183777161\C,8.0671772149,2.894873449,0
.1153554999\C,6.9870455239,3.787025279,-0.1225288352\H,-2.679149541,1.
2923496168,-0.4942596353\H,-1.9963733401,2.9252479771,-0.4423529945\H,
-2.0440163835,1.9373548415,1.0276059267\H,-0.3764131661,1.2942494238,-
1.478199277\H,-0.4208312712,0.3177133803,-0.0087745485\H,0.4695415173,
2.2633852733,1.2998654521\H,0.5382678787,3.2168291778,-0.1846093666\H,
1.9504203875,0.6683308307,-0.3947340403\H,4.8818607299,3.9816100027,-0
.3156267348\H,6.3170411426,0.0050572954,0.5141506774\C,7.1552945521,5.
243970998,-0.5095219876\F,6.001232762,5.765133216,-0.972574421\F,8.049
7922955,5.4158371278,-1.4996452444\F,7.5172697259,6.0342343897,0.51635
29238\N,9.4196890211,3.3075328688,0.2075900365\O,10.3130892289,2.45009
03435,0.1904007501\O,9.6824578638,4.5074457269,0.3217944245\H,8.622116
7754,0.8526213938,0.4876108005\\Version=ES64L-G09RevE.01\State=1-A\HF=
-1114.944651\RMSD=2.302e-09\RMSF=7.686e-06\Dipole=-3.6005609,-1.752201
,-1.0370036\Quadrupole=-20.2487377,8.6914595,11.5572782,-2.8889577,3.7
547633,-0.7691535\PG=C01 [X(C11H11F3N3O3)]\\@

1_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3717\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\27-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) S
CRF=(SMD,Solvent=h2o) maxdisk=2684354560\\3TFM4Chloro_EtO.M062X_6-31pG
d_opt_water\\-1,1\C,-1.8844404543,2.1747068131,-0.158925398\C,-0.48535
22647,1.6160429001,0.0798005718\C,0.5824531103,2.6429793427,-0.2684176
851\N,1.9092564812,2.0901298074,-0.0391614833\C,3.0134457734,2.8284086
41,-0.2642906714\O,2.9614643096,3.9976455783,-0.6913417422\N,4.1973870
601,2.1751134772,0.010147846\C,5.4906133422,2.6697570897,-0.1404898574
\C,5.8034547926,4.0227995844,-0.3299290447\C,6.5420535202,1.7420443207
,-0.0629741339\C,7.8634583196,2.1461663163,-0.1771260574\C,8.166112179
7,3.4892254918,-0.3766669564\C,7.1331261052,4.4237874986,-0.4513751427
\H,-2.6513988653,1.4364322672,0.0935480342\H,-2.0198990529,2.456104496
6,-1.2091840975\H,-2.0598889832,3.3660484691,0.4537319198\H,-0.3317632
116,0.7143129594,-0.5258530774\H,-0.3733861056,1.3197496895,1.13015567
5\H,0.4449542914,3.5456372537,0.3404290873\H,0.4846398069,2.9426364004
,-1.3190901038\H,1.9863253901,1.1516445649,0.3740596811\H,5.0161949739
,4.7602427281,-0.3782500937\H,6.3154854984,0.6903407215,0.0892871283\H
,8.6623338761,1.4150665452,-0.1156995916\Cl,9.8421724673,3.9562400983,
-0.5260669576\C,7.4308617446,5.8843307266,-0.6598573328\F,6.3177292036
,6.633432134,-0.6999625676\F,8.0857045485,6.111861697,-1.8162581626\F,
8.2003411187,6.3944622633,0.3224554694\H,4.1312765351,1.1677351524,0.2
29953857\O,1.971406319,-0.5696652895,1.1158770811\O,4.1232109026,-0.63
39777092,0.5145228584\C,3.0499544099,-1.1927867368,0.8813249705\C,3.02
44185101,-2.707707951,1.0606213264\C,4.3418675392,-3.4155953709,0.7792
63036\H,2.2302065208,-3.0914421231,0.4088984206\H,2.6901137967,-2.9019
300004,2.0868371045\H,4.6684225708,-3.2496654502,-0.2519778369\H,4.235
4102869,-4.4944647628,0.930577113\H,5.1338836526,-3.0578096346,1.44443
68137\\Version=ES64L-G09RevE.01\State=1-A\HF=-1638.411338\RMSD=4.988e-
09\RMSF=2.811e-06\Dipole=1.2524818,0.0109244,-0.2620435\Quadrupole=-1.
2681178,-10.3946419,11.6627597,-17.3327898,5.8214479,8.942544\PG=C01 [
X(C14H17Cl1F3N2O3)]\\@

29.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3714\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\27-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) SCRF=
(SMD,Solvent=n-Pentadecane) maxdisk=2147483648\\3TFM4Chloro.M062X_6-31
pGd_opt_Pentadecane\\0,1\C,-1.9258572339,2.0831568688,-0.0525783215\C,
-0.5337648158,1.4892504194,0.1416775058\C,0.5551386138,2.4779377813,-0
.2540810077\N,1.8722747255,1.883688445,-0.0664386205\C,2.9914182555,2.
665903514,-0.1372738732\O,2.9456893384,3.8845939318,-0.2235326626\N,4.
1776531577,1.9466203961,-0.0737078406\C,5.4823371999,2.4472891459,-0.1
158105471\C,5.7926943534,3.7896180794,-0.3677068628\C,6.5289674049,1.5
393632746,0.0911265842\C,7.8520404924,1.9522147399,0.047038312\C,8.158
2216145,3.2851859969,-0.2039841211\C,7.1238650441,4.1996119944,-0.4102
754047\H,-2.7027709982,1.3687108527,0.2351879999\H,-2.0951520954,2.359
1062421,-1.099192753\H,-2.0565497299,2.9841219205,0.5566966342\H,-0.43
62299409,0.5764643457,-0.4622371016\H,-0.3884599109,1.19881455,1.18918
10345\H,0.5026703862,3.3749906734,0.3689942632\H,0.4203576494,2.797719
7581,-1.2969952457\H,1.958137244,0.893965308,-0.2650403254\H,4.1034710
619,0.9546896808,0.116916521\H,4.9995598443,4.507061879,-0.5240784214\
H,6.3064617854,0.4936946915,0.2895386404\H,8.6531544513,1.2387239844,0
.2092218499\Cl,9.8330736959,3.7615304596,-0.2507581505\C,7.4231135514,
5.6528582012,-0.685032139\F,6.3047894366,6.3740370678,-0.8546065702\F,

8.1600127896,5.813586489,-1.799102627\F,8.1053826287,6.2267093086,0.32
20832503\\Version=ES64L-G09RevE.01\State=1-A\HF=-1370.5493271\RMSD=9.3
96e-09\RMSF=1.495e-06\Dipole=-1.8148754,-3.2513507,0.2501586\Quadrupol
e=1.8775832,3.984965,-5.8625482,3.1863918,1.4652031,-0.5900867\PG=C01
[X(C11H12Cl1F3N2O1)]\\@

1_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3790\SP\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\28-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671
088640\\3TFM4Chloro_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-1.9350471484,2.2
180103752,-0.1305899469\C,0,-0.5267463045,1.6325114566,-0.204318874\C,
0,0.5409143418,2.7061072276,-0.0204448896\N,0,1.8535955703,2.103443856
7,-0.0425519102\C,0,2.9604201904,2.8729704502,-0.1788478344\O,0,2.9246
413093,4.0911499807,-0.3719013675\N,0,4.1351539459,2.1390500798,-0.088
9275035\C,0,5.4264431378,2.6124030987,-0.1892682154\C,0,5.7739863527,3
.9562732232,-0.4172035704\C,0,6.461761235,1.6660985425,-0.0520074491\C
,0,7.7902817015,2.0491121585,-0.140295105\C,0,8.1280351024,3.380111748
,-0.3666863109\C,0,7.1149365649,4.3301361761,-0.5034130508\H,0,-2.6974
399595,1.4451714128,-0.2737647043\H,0,-2.0846327559,2.9844767849,-0.90
05660336\H,0,-2.1145067424,2.6883633217,0.843407443\H,0,-0.3681448857,
1.1399912832,-1.1713353482\H,0,-0.3926202656,0.8563529761,0.5585852217
\H,0,0.370750312,3.2430627655,0.9272795483\H,0,0.4792978,3.4556571089,
-0.8185480229\H,0,1.9371537681,1.1057409244,0.2256767957\H,0,4.9902615
644,4.693407817,-0.523659052\H,0,6.1945179882,0.6268886367,0.126482641
1\H,0,8.5799525766,1.3119960874,-0.0332470618\Cl,0,9.823821932,3.80511
681,-0.4704670077\C,0,7.4476957309,5.7776867488,-0.7465780376\F,0,6.35
17941009,6.5473283673,-0.8438002967\F,0,8.1434089801,5.960389457,-1.88
86867407\F,0,8.1970469314,6.3056336101,0.2439579979\H,0,4.0547176561,1
.1152344938,0.0850242947\O,0,1.9574329375,-0.6148767426,0.7009336492\O
,0,4.183767369,-0.5925567902,0.4062706288\C,0,3.0911518052,-1.15739702
25,0.6850781007\C,0,3.1330638089,-2.6527171218,1.0411307738\C,0,4.5263
617659,-3.2689559345,1.0171860787\H,0,2.4619650162,-3.1674510275,0.342
3414726\H,0,2.6708581682,-2.7599073253,2.0302603216\H,0,4.9773533324,-
3.164363788,0.0261462711\H,0,4.4943024122,-4.3342900849,1.2770106522\H
,0,5.1868026539,-2.7573211419,1.7233664421\\Version=ES64L-G09RevE.01\S
tate=1-A\HF=-267.7285057\RMSD=3.997e-09\Dipole=0.7114536,0.2849117,-0.
1323476\Quadrupole=-7.900656,-11.3059268,19.2065828,-16.8875241,4.2637
662,6.4054948\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

1_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3761\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\27-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) S
CRF=(SMD,Solvent=n-Pentadecane) maxdisk=2684354560\\3TFM4Chloro_EtO.M0
62X_6-31pGd_opt_Pentadecane\\-1,1\C,-1.9406332924,2.2410976224,-0.1174
961003\C,-0.5388689799,1.6406662499,-0.0625681477\C,0.5356435567,2.721
551927,-0.0710273607\N,1.8497253656,2.1173109035,-0.0072333658\C,2.959
9007033,2.8747854904,-0.1597473086\O,2.9248032561,4.0881842356,-0.3896
922449\N,4.1349755055,2.1487217099,-0.0372020131\C,5.4283503482,2.6221
329897,-0.1465852843\C,5.7739912719,3.9577600078,-0.4160904008\C,6.465
5028836,1.6844464994,0.0250952436\C,7.7941301952,2.0663416508,-0.06740
56978\C,8.1290618512,3.3904958513,-0.3340348004\C,7.1141670033,4.33220
4128,-0.5077548422\H,-2.7076791418,1.4597233019,-0.1138297079\H,-2.078
6505212,2.841236631,-1.0247432705\H,-2.1251073949,2.8937644053,0.74398
39558\H,-0.3784525666,0.9715268855,-0.9166737629\H,-0.4245825835,1.024
6006383,0.8372371241\H,0.3850979665,3.4065226732,0.7770295156\H,0.4572
868717,3.3290556426,-0.9817250541\H,1.924702809,1.1133390105,0.2347849
168\H,4.9917593255,4.6910730594,-0.5516596598\H,6.2036897083,0.6496796
109,0.2326338781\H,8.5826685979,1.3326460563,0.0675792964\Cl,9.8227227
184,3.8201192403,-0.4406691281\C,7.4433362081,5.771727602,-0.798118191
1\F,6.3450372437,6.5314967459,-0.9376408784\F,8.1530685677,5.917250935
4,-1.9364216184\F,8.1761339646,6.3395099025,0.1823129089\H,4.058157250
6,1.1294816929,0.160721708\O,1.9730574154,-0.6354863791,0.6416424355\O
,4.2093670109,-0.5805401989,0.4854129982\C,3.1100580858,-1.1734517748,
0.6628769225\C,3.1411898933,-2.6857802551,0.9256437189\C,4.5335670237,
-3.3006087877,0.9700521399\H,2.531350654,-3.1575172022,0.1449340009\H,
2.6056408589,-2.8594761756,1.8670959939\H,5.0597866917,-3.145299988,0.
0234595032\H,4.4809616914,-4.3791126058,1.619581241\H,5.1395919827,-2
.8411399323,1.7568944533\\Version=ES64L-G09RevE.01\State=1-A\HF=-1638.
3803077\RMSD=4.516e-09\RMSF=4.115e-06\Dipole=0.7183327,0.207717,-0.127
1292\Quadrupole=-5.5421119,-11.8829516,17.4250634,-17.0216086,4.194242
7,6.4760968\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

29.M062X_6-31pGd_opt

1\1\GINC-R3718\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\27-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) maxdi
sk=2147483648\\3TFM4Chloro.M062X_6-31pGd_opt\\0,1\C,-1.9238118665,2.13
02060249,-0.0240079758\C,-0.5429143905,1.4923382681,0.1105817285\C,0.5
655679541,2.4874657783,-0.2071689609\N,1.872892206,1.8558202101,-0.071
8067082\C,2.9968520996,2.6475966299,-0.109349224\O,2.9498935416,3.8648
380839,-0.1160847102\N,4.1813751465,1.9201664846,-0.106434271\C,5.4874
750784,2.4263847924,-0.1351449561\C,5.7900361879,3.7720181627,-0.37456
6838\C,6.5364316884,1.5211782723,0.0630119031\C,7.8576652566,1.9411742
67,0.0220745769\C,8.1582485447,3.2777412516,-0.2168317359\C,7.11888143
52,4.189165086,-0.4140953478\H,-2.7147920025,1.4116712985,0.2076565257
\H,-2.0906467037,2.4972341989,-1.0422625423\H,-2.0301418537,2.97921784
72,0.6593440632\H,-0.4700464089,0.630914136,-0.5681065784\H,-0.3978293
366,1.1102735155,1.1279793269\H,0.5371674955,3.3309517059,0.4877451983
\H,0.435628158,2.8992092059,-1.2182088599\H,1.9491634331,0.9130890974,
-0.4341078472\H,4.1077510669,0.9330023215,0.1008931075\H,4.9935104698,
4.4878714164,-0.5198244001\H,6.3194677656,0.4721620893,0.250682255\H,8
.6643388522,1.2326654297,0.1770699552\Cl,9.8281376784,3.7588369322,-0.
2597943325\C,7.411075842,5.6480748895,-0.6756822117\F,6.2864576725,6.3
609571409,-0.8354179655\F,8.1431281052,5.8180777815,-1.7895677907\F,8.
0911368843,6.2109870818,0.3366546157\\Version=ES64L-G09RevE.01\State=1
-A\HF=-1370.5329301\RMSD=3.506e-09\RMSF=1.227e-06\Dipole=-1.5885245,-2
.7672284,0.09641\Quadrupole=2.5521173,2.8576786,-5.4097959,2.539066,1.
8461054,-0.1723318\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

1_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3782\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\27-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) m
axdisk=2684354560\\3TFM4Chloro_EtO.M062X_6-31pGd_opt\\-1,1\C,-1.935047
1484,2.2180103752,-0.1305899469\C,-0.5267463045,1.6325154166,-0.204318
874\C,0.5409143418,2.7061072276,-0.0204448896\N,1.8535955703,2.1034438
567,-0.0425519102\C,2.9604201904,2.8729704502,-0.1788478344\O,2.924641
3093,4.0911499807,-0.3719013675\N,4.1351539459,2.1390500798,-0.0889275
035\C,5.4264431378,2.6124030987,-0.1892682154\C,5.7739863527,3.9562732
232,-0.4172035704\C,6.461761235,1.6660985425,-0.0520074491\C,7.7902817
015,2.0491121585,-0.140295105\C,8.1280351024,3.380111748,-0.3666863109
\C,7.1149365649,4.3301361761,-0.5034130508\H,-2.6974399595,1.445171412
8,-0.2737647043\H,-2.0846327559,2.9844767849,-0.9005660336\H,-2.114506
7424,2.6883633217,0.843407443\H,-0.3681448857,1.1399912832,-1.17133534
82\H,-0.3926202656,0.8563529761,0.5585852217\H,0.370750312,3.243062765
5,0.9272795483\H,0.4792978,3.4556571089,-0.8185480229\H,1.9371537681,1
.1057409244,0.2256767957\H,4.9902615644,4.693407817,-0.523659052\H,6.1
945179882,0.6268886367,0.1264826411\H,8.5799525766,1.3119960874,-0.033
2470618\Cl,9.823821932,3.80511681,-0.4704670077\C,7.4476957309,5.77768
67488,-0.7465780376\F,6.3517941009,6.5473283673,-0.8438002967\F,8.1434
089801,5.960389457,-1.8886867407\F,8.1970469314,6.3056336101,0.2439579
979\H,4.0547176561,1.1152344938,0.0850242947\O,1.9574329375,-0.6148767
426,0.7009336492\O,4.183767369,-0.5925567902,0.4062706288\C,3.09115180
52,-1.1573970225,0.6850781007\C,3.1330638089,-2.6527171218,1.041130773
8\C,4.5263617659,-3.2689559345,1.0171860787\H,2.4619650162,-3.16745102
75,0.3423414726\H,2.6708581682,-2.7599073253,2.0302603216\H,4.97735333
24,-3.164363788,0.0261462711\H,4.4943024122,-4.3342900849,1.2770106522
\H,5.1868026539,-2.7573211419,1.7233664421\\Version=ES64L-G09RevE.01\S
tate=1-A\HF=-1638.3401141\RMSD=8.284e-09\RMSF=1.027e-06\Dipole=0.71023
19,0.3137589,-0.1395016\Quadrupole=-7.8235341,-11.5002611,19.3237952,-
16.9855432,4.2898447,6.4785243\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

29.M062X_6-31pGd_opt_water

1\1\GINC-R3741\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\27-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) SCRF=
(SMD,Solvent=h2o) maxdisk=2147483648\\3TFM4Chloro.M062X_6-31pGd_opt_wa
ter\\0,1\C,-1.9242305017,2.0591355712,-0.1305165714\C,-0.5324883817,1.
4949760555,0.1359820335\C,0.5459946396,2.5119576818,-0.2055934555\N,1.
867250505,1.9528576485,0.0528612208\C,2.9871122186,2.6713508328,-0.174
6062174\O,2.9503977216,3.8575858235,-0.5369271189\N,4.1665046975,1.985
1881227,0.0351253059\C,5.4730232011,2.4601588653,-0.1028456508\C,5.800
826279,3.8100603532,-0.2761091453\C,6.5072797756,1.5156366436,-0.03720
65254\C,7.8345175143,1.9019455587,-0.1461813046\C,8.1556526882,3.24319
27918,-0.3267667575\C,7.1362597153,4.1932777432,-0.3907706592\H,-2.698
0224932,1.326787448,0.1178737322\H,-2.0417522701,2.329728065,-1.185593
4516\H,-2.1040509548,2.9572990842,0.4704814881\H,-0.3753888052,0.58786
20479,-0.4606729402\H,-0.4384430857,1.2097006808,1.1908046277\H,0.4149

98265,3.4169651479,0.3979811533\H,0.4682293655,2.8045281316,-1.2600243
298\H,1.936940364,0.9674589784,0.2834534437\H,4.0881512136,0.997888441
1,0.259251221\H,5.0241729836,4.5589739765,-0.3184286614\H,6.2672074753
,0.4647996648,0.100738294\H,8.6229741991,1.1583061295,-0.0941844108\Cl
,9.8370630088,3.6893851195,-0.4652875873\C,7.4533683416,5.6529690339,-
0.5788273484\F,6.3487249905,6.4144530967,-0.6166907427\F,8.1186091916,
5.8861950739,-1.727513336\F,8.2212181382,6.1405961886,0.415423694\\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-1370.5529019\RMSD=4.075e-09\RMSF=2
.875e-06\Dipole=-2.0557969,-4.3024863,0.9144214\Quadrupole=0.9241778,6
.0361921,-6.9603699,5.2681364,-2.0183325,-2.0343225\PG=C01 [X(C11H12Cl
1F3N2O1)]\\@

2.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3757\FOpt\RM062X\Gen\C10H13F5N2O1S1\ROOT\25-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=n-Pentadecane) maxdisk=2147483648\\4SF5.M062X_6-31pGd_opt_Pentade
cane\\0,1\C,-2.092236994,1.8823633087,-0.0462364898\C,-0.7308641846,1.
1946260171,-0.0003441166\C,0.4039743467,2.207494909,0.0818595655\N,1.6
908386328,1.5258972876,0.1264470411\C,2.8467557688,2.2282152676,-0.069
9404079\O,2.8640622696,3.405649315,-0.3966564048\N,3.9939458189,1.4626
59561,0.1073492796\C,5.3227317463,1.8750174924,0.0148923396\C,5.715242
9139,3.2047236129,-0.2011862267\C,6.3078780809,0.8840409052,0.16413613
98\C,7.6548730431,1.2015709568,0.1040540074\C,8.0218494071,2.526646120
8,-0.1076301922\C,7.0673456254,3.5240950617,-0.2598637758\H,-2.9019514
638,1.1493285659,-0.1080046271\H,-2.169603756,2.5414517417,-0.91779807
64\H,-2.2584486798,2.4905860173,0.8496921942\H,-0.5896831248,0.5733881
095,-0.8929591209\H,-0.6873695436,0.5239904172,0.8688561351\H,0.277406
2222,2.8534233322,0.9621376378\H,0.4029216559,2.8559769457,-0.79850794
59\H,1.7308309632,0.6615852448,0.6534797597\H,3.8614509914,0.468857504
2,0.2515211192\H,4.969771482,3.9770664758,-0.3249038304\H,6.0130597691
,-0.1489876809,0.3305922149\H,8.4013936927,0.4237370906,0.2213667773\S
,9.7712480251,2.9542071513,-0.1847913801\H,7.3619175206,4.554784348,-0
.425700381\F,10.1168913485,1.7036041822,-1.1504484743\F,11.3375794961
,3.3340350715,-0.2525535635\F,9.5689321193,3.8990308809,-1.4796334817\
F,9.5836981693,4.240667298,0.774934575\F,10.1323486378,2.0455174883,1.
1038493661\\Version=ES64L-G09RevE.01\State=1-A\HF=-1470.5462802\RMSD=4
.062e-09\RMSF=7.645e-06\Dipole=-2.9372259,-2.1436125,0.6870021\Quadrup
ole=-0.7003529,5.2237386,-4.5233857,7.8870997,-3.853601,-2.4580699\PG=
C01 [X(C10H13F5N2O1S1)]\\@

2.M062X_6-31pGd_opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13F5N2O1S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=21474
83648\\4SF5.M062X_6-31pGd_opt\\0,1\C,-2.0948335042,1.9046393492,0.0044
342604\C,-0.7387005762,1.2091435064,0.0979128525\C,0.408084306,2.20365
44755,-0.0249872519\N,1.6878407,1.5158695525,0.0682705488\C,2.85177333
54,2.220609996,-0.034915754\O,2.8683270034,3.4287793658,-0.2037620392\
N,3.9992797709,1.4395905567,0.071456147\C,5.3292742418,1.8632288845,0.
0073631391\C,5.7138230818,3.1993799716,-0.1763848696\C,6.3187306185,0.
8755412601,0.1376630783\C,7.6646618585,1.201190052,0.0876681324\C,8.02
66286555,2.5310910273,-0.0950741354\C,7.0652418884,3.5245267145,-0.226
435952\H,-2.9135377655,1.1853756323,0.0927245266\H,-2.2037356321,2.422
8325913,-0.953942271\H,-2.2104659744,2.6459935776,0.8018584347\H,-0.65
27215837,0.4558511302,-0.6962839698\H,-0.6593480367,0.679465311,1.0565
080968\H,0.3465416167,2.9602827842,0.7662296943\H,0.3549141013,2.73501
8087,-0.9824559294\H,1.688479682,0.5155120816,0.2084528423\H,3.8730138
82,0.4459185867,0.2096761318\H,4.9621638561,3.9689113161,-0.2783096187
\H,6.0301970677,-0.1631051756,0.2802254097\H,8.41731823,0.4275780245,0
.1898297642\S,9.775366344,2.9694067766,-0.1619778373\H,7.358385244,4.5
588334301,-0.3686207991\F,10.1215643051,1.7341942428,-1.145352719\F,11
.3351324769,3.35722828,-0.2211755462\F,9.5624590014,3.9305039196,-1.44
15318488\F,9.5718424038,4.237262061,0.8165344846\F,10.1310894012,2.040
9426307,1.1124129979\\Version=ES64L-G09RevE.01\State=1-A\HF=-1470.5306
35\RMSD=4.697e-09\RMSF=3.326e-05\Dipole=-2.7126732,-1.98461,0.28297\Qu
adrupole=1.0205306,4.541292,-5.5618225,8.046695,-1.1271033,-1.450379\P
G=C01 [X(C10H13F5N2O1S1)]\\@

2.M062X_6-31pGd_opt_water

1\1\GINC-R3714\FOpt\RM062X\Gen\C10H13F5N2O1S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2147483648\\4SF5.M062X_6-31pGd_opt_water\\0,1\C,-2.0
874983117,1.8805065948,0.0189597345\C,-0.7268055172,1.1994554923,0.123
9606135\C,0.4020532443,2.1994084289,-0.0744248406\N,1.6939631322,1.533

8635482,0.0419683464\C,2.8454377421,2.2197985863,-0.1117044544\O,2.865
6735446,3.4215918137,-0.415035459\N,3.9911653428,1.4702449884,0.081135
3734\C,5.3181546514,1.8884149835,0.0080895559\C,5.7197028526,3.2267677
464,-0.1254226112\C,6.298606783,0.8840322528,0.0974702407\C,7.64687980
78,1.1957330538,0.050443926\C,8.0189649091,2.5306158907,-0.0872380303\
C,7.073177096,3.5440382396,-0.1734955657\H,-2.8985787841,1.1598611384,
0.1588681164\H,-2.21654674,2.3474651913,-0.9636798573\H,-2.1942821804,
2.6611738624,0.7801590987\H,-0.64396145,0.4066648505,-0.6293296882\H,-
0.6203347073,0.7249212149,1.1073636379\H,0.3313821637,3.0008536204,0.6
71352024\H,0.3257821824,2.6630733979,-1.0641110643\H,1.713432322,0.574
6490841,0.3711392352\H,3.8611701975,0.4774613767,0.2516164683\H,4.9887
376242,4.0191928392,-0.1873247487\H,5.9950265495,-0.1534685656,0.20523
86517\H,8.3845311347,0.403440359,0.1195510582\S,9.7671329868,2.9501620
068,-0.15193494\H,7.3673391676,4.5834012593,-0.2745409286\F,10.1065168
611,1.7627577044,-1.1979075374\F,11.3421278343,3.3263337872,-0.2101401
321\F,9.5706537518,3.9785036301,-1.3856027126\F,9.6062986077,4.1798385
542,0.8874065125\F,10.1428872017,1.9644930696,1.0751799774\\Version=ES
64L-G09RevE.01\State=1-A\HF=-1470.5502283\RMSD=6.128e-09\RMSF=7.732e-0
6\Dipole=-3.3558652,-3.1069071,0.7806074\Quadrupole=-1.3209659,7.06165
37,-5.7406879,12.5173808,-4.1283499,-1.5860141\PG=C01 [X(C10H13F5N2O1S
1)]\\@

2_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3777\FOpt\RM062X\Gen\C13H18F5N2O3S1(1-)\ROOT\19-Feb-2019\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=n-Pentadecane) maxdisk=3221225472\\4SF5_EtO.M062X_6-31pGd_opt
_Pentadecane\\-1,1\C,-2.1603464566,2.3378583421,-0.089024084\C,-0.8157
249329,1.6317428169,0.0597884595\C,0.3476219408,2.5846439935,-0.186983
6024\N,1.6063950709,1.8857308841,-0.0314410794\C,2.7740622416,2.552998
235,-0.1621659133\O,2.8382374089,3.7602505125,-0.4134979036\N,3.888158
6504,1.7414894652,0.0180011472\C,5.2126783146,2.1107408782,-0.05293533
62\C,5.673331125,3.4124808561,-0.3373140277\C,6.1637264482,1.090738594
2,0.1794109124\C,7.5201489947,1.3545921304,0.1299555883\C,7.948550088,
2.6512550793,-0.1543575982\C,7.0366791312,3.6748785116,-0.3866072334\H
,-2.9921481474,1.6478218276,0.0863676324\H,-2.2786344699,2.7548056749,
-1.09618552\H,-2.2543988493,3.1637311348,0.6260506472\H,-0.7486448907,
0.7915600145,-0.6415853652\H,-0.7211725131,1.2022805717,1.0643160737\H
,0.3015054036,3.428106261,0.5156056578\H,0.2758345721,3.0144017147,-1.
1964476942\H,1.5918793358,0.8675272765,0.1609945672\H,3.7219796665,0.7
370389923,0.241819801\H,4.9585713729,4.2032701949,-0.5159283777\H,5.80
66324327,0.0880045417,0.3993697584\H,8.2328712552,0.5570909001,0.31133
2992\S,9.7077742423,3.0014439969,-0.2211504852\H,7.3761113472,4.681594
3928,-0.6070869536\F,10.0379678837,1.6759421516,-1.092938712\F,11.2999
337121,3.3156529041,-0.2810581764\F,9.5865463026,3.8682348324,-1.58526
14996\F,9.5722197935,4.3661558104,0.6424661981\F,10.0235322162,2.17396
96588,1.1358951999\O,1.4694069752,-0.8845749382,0.4960809892\O,3.70626
00974,-0.9550926067,0.6329791055\C,2.5605514634,-1.4801936622,0.690253
7341\C,2.4700763515,-2.9741264979,1.0313016366\C,3.8105175599,-3.67659
45807,1.2004357235\H,1.8754928348,-3.4500270239,0.241980312\H,1.869763
9197,-3.0560587338,1.9462862439\H,4.4059358902,-3.6090283844,0.2848404
366\H,3.670081848,-4.7371239333,1.441630296\H,4.3951943691,-3.21584278
97,2.0020964493\\Version=ES64L-G09RevE.01\State=1-A\HF=-1738.3778944\R
MSD=7.134e-09\RMSF=2.984e-06\Dipole=1.1122167,0.470444,-0.0660437\Quad
rupole=-24.5349361,4.0905982,20.4443379,-14.7604008,2.5360805,3.382577
4\PG=C01 [X(C13H18F5N2O3S1)]\\@

2_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3739\FOpt\RM062X\Gen\C13H18F5N2O3S1(1-)\ROOT\24-Feb-2019\0\\
# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) ma
xdisk=3221225472\\4SF5_EtO.M062X_6-31pGd_opt\\-1,1\C,-2.151296941,2.30
95142078,-0.0573528405\C,-0.7953929468,1.6567221286,0.2006703446\C,0.3
548580319,2.5558104354,-0.2394818505\N,1.6154617928,1.8883593001,-0.00
82548755\C,2.7801577031,2.5582794943,-0.1637114767\O,2.8427061826,3.75
57736752,-0.4530208579\N,3.8939805714,1.7505709156,0.0458980546\C,5.21
63114766,2.1155412829,-0.0330097143\C,5.6776874046,3.4113670574,-0.345
971881\C,6.1668280549,1.099411583,0.2228299353\C,7.5230331365,1.363270
9617,0.1698934078\C,7.9540384962,2.6530361608,-0.1420416404\C,7.041232
2648,3.670460576,-0.3987548187\H,-2.9736439462,1.662974661,0.266124033
8\H,-2.2902962685,2.5190623382,-1.1246063386\H,-2.2403602744,3.2608684
611,0.4807972837\H,-0.7242485288,0.6965027472,-0.3235662692\H,-0.67799
37055,1.427327562,1.2666055465\H,0.337655226,3.5033699794,0.3146366946
\H,0.2432156776,2.8161821886,-1.3040349293\H,1.6058141109,0.864801649,
0.1612600896\H,3.7232780591,0.7495609896,0.2838346355\H,4.9595232093,4

.1951658581,-0.5428399418\H,5.8058112455,0.1019396644,0.46201987\H,8.2
377583626,0.5721673915,0.3692801622\S,9.7121773705,3.0029328835,-0.212
948922\H,7.3857402984,4.6703018059,-0.6408005681\F,10.0479403791,1.651
594056,-1.0429119704\F,11.3043194464,3.3181035625,-0.2764601328\F,9.59
42611482,3.8282461469,-1.6035595817\F,9.5712205368,4.3936388096,0.6083
691274\F,10.0243717548,2.2164879847,1.1698250178\O,1.4441052715,-0.881
3832337,0.4356849929\O,3.6775535182,-0.9412515342,0.6604293601\C,2.533
2988932,-1.4713638705,0.6503898572\C,2.4453177266,-2.9810399659,0.9264
480064\C,3.7888947658,-3.6586710454,1.1654597002\H,1.9206677914,-3.432
7630668,0.0755002613\H,1.7793020392,-3.1105179863,1.7886231692\H,4.443
6190886,-3.5346824125,0.29796601\H,3.6639257859,-4.7311977792,1.358881
4572\H,4.3023257903,-3.2071056234,2.0191915912\\Version=ES64L-G09RevE.
01\State=1-A\HF=-1738.3394464\RMSD=7.802e-09\RMSF=1.515e-06\Dipole=1.1
547189,0.4921597,-0.0581641\Quadrupole=-26.3736143,4.2078613,22.165753
,-14.8219137,2.2866939,3.8471914\PG=C01 [X(C13H18F5N2O3S1)]\\@

2_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3757\SP\RM062X\Gen\C13H18F5N2O3S1(1-)\ROOT\25-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=6710
88640\\4SF5_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-2.151296941,2.3095142078
,-0.0573528405\C,0,-0.7953929468,1.6567221286,0.2006703446\C,0,0.35485
80319,2.5558104354,-0.2394818505\N,0,1.6154617928,1.8883593001,-0.0082
548755\C,0,2.7801577031,2.5582794943,-0.1637114767\O,0,2.8427061826,3.
7557736752,-0.4530208579\N,0,3.8939805714,1.7505709156,0.0458980546\C,
0,5.2163114766,2.1155412829,-0.0330097143\C,0,5.6776874046,3.411367057
4,-0.345971881\C,0,6.1668280549,1.099411583,0.2228299353\C,0,7.5230331
365,1.3632709617,0.1698934078\C,0,7.9540384962,2.6530361608,-0.1420416
404\C,0,7.0412322648,3.670460576,-0.3987548187\H,0,-2.9736439462,1.662
974661,0.2661240338\H,0,-2.2902962685,2.5190623382,-1.1246063386\H,0,-
2.2403602744,3.2608684611,0.4807972837\H,0,-0.7242485288,0.6965027472,
-0.3235662692\H,0,-0.6779937055,1.427327562,1.2666055465\H,0,0.3376552
26,3.5033699794,0.3146366946\H,0,0.2432156776,2.8161821886,-1.30403492
93\H,0,1.6058141109,0.864801649,0.1612600896\H,0,3.7232780591,0.749560
9896,0.2838346355\H,0,4.9595232093,4.1951658581,-0.5428399418\H,0,5.80
58112455,0.1019396644,0.46201987\H,0,8.2377583626,0.5721673915,0.36928
01622\S,0,9.7121773705,3.0029328835,-0.212948922\H,0,7.3857402984,4.67
03018059,-0.6408005681\F,0,10.0479403791,1.651594056,-1.0429119704\F,0
,11.3043194464,3.3181035625,-0.2764601328\F,0,9.5942611482,3.828246146
9,-1.6035595817\F,0,9.5712205368,4.3936388096,0.6083691274\F,0,10.0243
717548,2.2164879847,1.1698250178\O,0,1.4441052715,-0.8813832337,0.4356
849929\O,0,3.6775535182,-0.9412515342,0.6604293601\C,0,2.5332988932,-1
.4713638705,0.6503898572\C,0,2.4453177266,-2.9810399659,0.9264480064\C
,0,3.7888947658,-3.6586710454,1.1654597002\H,0,1.9206677914,-3.4327630
668,0.0755002613\H,0,1.7793020392,-3.1105179863,1.7886231692\H,0,4.443
6190886,-3.5346824125,0.29796601\H,0,3.6639257859,-4.7311977792,1.3588
814572\H,0,4.3023257903,-3.2071056234,2.0191915912\\Version=ES64L-G09R
evE.01\State=1-A\HF=-267.7284824\RMSD=4.017e-09\Dipole=1.1526371,0.463
6717,-0.0531301\Quadrupole=-26.4117661,4.3625971,22.049169,-14.6538166
,2.2545629,3.7915317\PG=C01 [X(C13H18F5N2O3S1)]\\@

2_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R4227\FOpt\RM062X\Gen\C13H18F5N2O3S1(1-)\ROOT\01-Mar-2019\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=(CalcFC,MaxStep=1) IO
P(2/17=4) SCRF=(SMD,Solvent=h2o) maxdisk=3221225472\\4SF5_EtO.M062X_6-
31pGd_opt_water\\-1,1\C,-2.1381338244,2.3236995085,-0.1520202739\C,-0.
799218178,1.611481992,0.011650082\C,0.3617149145,2.5702167624,-0.21030
17273\N,1.6315453223,1.8755863898,-0.0527003912\C,2.7963674252,2.53755
07366,-0.1852644659\O,2.849768116,3.7523478117,-0.4518108161\N,3.91840
21746,1.7503993719,-0.0061384464\C,5.2506577073,2.1345969146,-0.074482
4801\C,5.6991120066,3.4610638604,-0.2002690843\C,6.2038152494,1.099882
6377,0.0082209262\C,7.5607176122,1.369338635,-0.0362036387\C,7.9761180
351,2.6927905561,-0.1670233809\C,7.0617177913,3.7354691482,-0.24770339
93\H,-2.9727101604,1.6346425676,0.0083237466\H,-2.23725854,2.744811246
1,-1.1586903437\H,-2.2355922601,3.1444052088,0.5673719042\H,-0.7253069
68,0.781184436,-0.7015338871\H,-0.7241937473,1.1785003684,1.0167991854
\H,0.3029490002,3.3997018477,0.5054692413\H,0.300541768,3.0048593684,-
1.2158113281\H,1.6176877459,0.8755424123,0.1905413021\H,3.7542894629,0
.7422275425,0.1450305515\H,4.994374935,4.2773102305,-0.2567855797\H,5.
8667093368,0.072384569,0.107713574\H,8.2727383898,0.5533648484,0.02843
3171\S,9.7347538254,3.0585248721,-0.2291364213\H,7.3894907783,4.765356
2821,-0.3434851091\F,10.0466691253,1.8444203924,-1.2534754538\F,11.321
6096496,3.3868166117,-0.2848708669\F,9.5770724057,4.0723532277,-1.4812
927118\F,9.6075119913,4.3107758206,0.7885954782\F,10.0766950147,2.0828

788667,1.0168385746\O,1.3793554726,-0.9140870554,0.6738004822\O,3.5952
538544,-1.0605608813,0.4200796381\C,2.472446261,-1.553234792,0.7279550
455\C,2.3991337635,-3.0049023913,1.1924646435\C,3.7339814035,-3.732476
0292,1.2611590878\H,1.709854321,-3.5211604728,0.5132792357\H,1.9074735
062,-3.0014004294,2.1726541671\H,4.2172735211,-3.7675818465,0.27990099
4\H,3.5901612365,-4.7620336873,1.6039357405\H,4.419610555,-3.237677458
7,1.956073034\\Version=ES64L-G09RevE.01\State=1-A\HF=-1738.4087576\RMS
D=8.422e-09\RMSF=3.020e-06\Dipole=1.7134045,0.4518131,0.077097\Quadrup
ole=-23.4089258,5.5455162,17.8634096,-15.4628755,2.9231961,3.1060093\P
G=C01 [X(C13H18F5N2O3S1)]\\@

4_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3726\SP\RM062X\Gen\C14H21N2O5S1(1-)\ROOT\21-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671088
640\\4SulfOxyMethyl_C2_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-2.1138528668,
2.4434768491,-0.4531644221\C,0,-0.802685361,1.7655864782,-0.062487788\
C,0,0.4040058079,2.6265251475,-0.4203202077\N,0,1.6231580602,1.9352301
831,-0.0681226456\C,0,2.8099562601,2.5835622122,-0.1088076913\O,0,2.92
17043009,3.7808354687,-0.3827156849\N,0,3.8838902269,1.7527433325,0.19
93833586\C,0,5.216181756,2.0861075318,0.2337520138\C,0,5.7287989598,3.
3793641123,-0.0107428266\C,0,6.1179403267,1.0385695424,0.5446519648\C,
0,7.4798248692,1.2689212297,0.5918133178\C,0,7.9718634871,2.5534125824
,0.3354958792\C,0,7.0987279539,3.5994486594,0.0371819732\H,0,-2.977651
0508,1.8254326377,-0.1870839435\H,0,-2.1546732342,2.6281344664,-1.5332
222699\H,0,-2.2242596995,3.4105429737,0.0520580868\H,0,-0.7107125147,0
.7911004291,-0.556244375\H,0,-0.7842639142,1.56114586,1.0147958629\H,0
,0.3657172143,3.5857654142,0.1114922576\H,0,0.3889570387,2.8661136515,
-1.4957658914\H,0,1.5786679465,0.9087794191,0.0768556029\H,0,3.6711029
238,0.7516094153,0.3994669135\H,0,5.0426189351,4.1848994758,-0.2323297
734\H,0,5.7101143273,0.0505465959,0.745148549\H,0,8.1689685742,0.46727
59703,0.8431840941\S,0,9.7091872677,2.8260132285,0.2827528983\O,0,10.3
840507684,1.8209656198,1.1117854336\O,0,9.9834652192,4.2527412407,0.48
91150243\H,0,7.4985233665,4.5943806571,-0.1400722058\C,0,10.1601922694
,2.4648752997,-1.4168670317\H,0,9.9006283481,1.4274395682,-1.633375751
2\H,0,11.2390200166,2.620175043,-1.4913672847\H,0,9.621765014,3.150408
6286,-2.0730373746\O,0,1.3457504508,-0.8391331479,0.2878242112\O,0,3.5
46600369,-0.9481694174,0.7197278058\C,0,2.3986098687,-1.454439899,0.59
36834618\C,0,2.2563245208,-2.9658912666,0.8356234396\C,0,3.5588742992,
-3.6746560307,1.1856018158\H,0,1.8028435575,-3.3943909257,-0.066716052
\H,0,1.5118757206,-3.0936683412,1.6313607666\H,0,4.2926511508,-3.55259
84477,0.3835115666\H,0,3.395857037,-4.7468828076,1.3502845544\H,0,4.00
08404284,-3.2454086402,2.0893123672\\Version=ES64L-G09RevE.01\State=1-
A\HF=-267.7284863\RMSD=4.016e-09\Dipole=0.2424068,-0.1686383,-1.351430
7\Quadrupole=-24.8848572,0.2837493,24.6011079,-16.4363066,-15.7002718,
0.4063578\PG=C01 [X(C14H21N2O5S1)]\\@

4_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R4188\FOpt\RM062X\Gen\C14H21N2O5S1(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2684354560\\4SulfOxyMethyl_C2_EtO.M062X_6-31pGd_op
t_water\\-1,1\C,-2.0802836593,2.4217905092,-0.5600885176\C,-0.78034241
05,1.7079355187,-0.2035011678\C,0.418002092,2.628518306,-0.3841128046\
N,1.6499019888,1.9288920626,-0.0489419839\C,2.8398307805,2.5528000336,
-0.1363345099\O,2.9512248814,3.7348231475,-0.5094436671\N,3.918099112,1
.7612821572,0.2155676901\C,5.2628812879,2.1035899902,0.2204077103\C,5.
7591752989,3.4079453469,0.0416171655\C,6.1730190039,1.0487957557,0.443
3411738\C,7.5361664886,1.2806506378,0.4797414576\C,8.0095446068,2.5818
610478,0.2950740208\C,7.1298190415,3.6383566593,0.0735004149\H,-2.9416
329058,1.7601917453,-0.4281800373\H,-2.0693760325,2.7572431364,-1.6031
414164\H,-2.230888476,3.3018894335,0.0749948172\H,-0.6535508195,0.8199
647947,-0.8351015914\H,-0.816113252,1.3596253197,0.8361321854\H,0.3077
655984,3.5147744926,0.2536669328\H,0.4665013533,2.9800975862,-1.422014
6236\H,1.585663414,0.9709384719,0.3220910606\H,3.7129297285,0.76524925
21,0.3964279864\H,5.0828304741,4.2347778319,-0.1172384719\H,5.79237292
66,0.0422252494,0.5901610987\H,8.2235957937,0.4584215749,0.6555007774\
S,9.7495416033,2.8771491662,0.2856111205\O,10.4000255867,1.8693482534,
1.1463630489\O,9.9857882913,4.2996359507,0.6006695769\H,7.5065786514,4
.6475330744,-0.0647829536\C,10.2762954866,2.587910104,-1.3860416635\H,
10.0404077467,1.5537790152,-1.6454164513\H,11.3555068392,2.7612219564,
-1.4143149054\H,9.750923847,3.2882294173,-2.0384521966\O,1.2769936083,
-0.7494979245,0.9767605476\O,3.4620027896,-1.034154694,0.605725128\C,2
.3085495213,-1.4781453674,0.8714555677\C,2.1202220565,-2.9774323951,1.

0824843342\C,3.3851275659,-3.8137225955,0.9509684728\H,1.3599416996,-3
.3067544306,0.3639944079\H,1.6707285012,-3.1056156365,2.0745487344\H,3
.8254021883,-3.7124054884,-0.0457648894\H,3.161073621,-4.8724717206,1.
115411482\H,4.1389141481,-3.510356746,1.6840749383\\Version=ES64L-G09R
evE.01\State=1-A\HF=-1429.6968354\RMSD=9.371e-09\RMSF=3.091e-06\Dipole
=0.793754,-0.4363049,-2.3607874\Quadrupole=-19.6460447,0.2286701,19.41
73746,-17.092765,-19.793628,-0.6143231\PG=C01 [X(C14H21N2O5S1)]\\@

4.M062X_6-31pGd_opt

1\1\GINC-R3717\FOpt\RM062X\Gen\C11H16N2O3S1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483
648\\4SulfOxyMethyl.M062X_6-31pGd_opt\\0,1\C,-2.004263388,1.8464310338
,-0.0619611429\C,-0.6364865026,1.173271879,-0.1508238027\C,0.491430347
4,2.1644063527,0.1050600288\N,1.7859964779,1.5005241731,0.010388262\C,
2.9256908545,2.2693583333,0.0027417071\O,2.9039951239,3.4856778398,-0.
0561231676\N,4.0946538437,1.5149515788,0.0320442189\C,5.4106605759,1.9
866672237,0.0576462473\C,5.7447564566,3.3304413867,0.2884984485\C,6.43
08061142,1.0385648995,-0.1264199383\C,7.7642466362,1.4151355017,-0.087
9587748\C,8.0827586951,2.7526253088,0.1344028277\C,7.0838751806,3.7024
376149,0.3284910275\H,-2.8095746333,1.1299437332,-0.2454841161\H,-2.09
32757984,2.6490466794,-0.8015645517\H,-2.1638570882,2.2849385298,0.928
8121993\H,-0.4976929599,0.7231664482,-1.1409418453\H,-0.582099623,0.35
65017316,0.5825208025\H,0.3699568775,2.6405506529,1.0884724605\H,0.478
7227364,2.9636249124,-0.6409158263\H,1.8432166431,0.5770077191,0.42231
31816\H,3.9962960489,0.5214934954,-0.1316070473\H,4.9642025641,4.06354
60007,0.4350274309\H,6.172380869,-0.0049657857,-0.2909688177\H,8.55678
81999,0.6823373587,-0.2081265147\S,9.7881599085,3.2506208111,0.1597084
041\O,10.5984677656,2.063190585,0.4320968977\O,9.9005993094,4.44923006
66,0.0897965512\H,7.3567033401,4.7339662248,0.5334050209\C,10.12212679
74,3.7447920648,-1.5287554839\H,9.9618936343,2.8881474885,-2.18503237\
H,11.1683710732,4.0584682241,-1.5517379059\H,9.4649239201,4.5758499335
,-1.7890544113\\Version=ES64L-G09RevE.01\State=1-A\HF=-1161.800096\RMS
D=5.841e-09\RMSF=8.042e-06\Dipole=-2.4401217,-1.6292881,-1.2398018\Qua
drupole=-4.2302542,4.6076668,-0.3774126,8.1990254,-15.3396003,-3.35054
94\PG=C01 [X(C11H16N2O3S1)]\\@

4.M062X_6-31pGd_opt_water

1\1\GINC-R3717\FOpt\RM062X\Gen\C11H16N2O3S1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2147483648\\4SulfOxyMethyl.M062X_6-31pGd_opt_water\\0,
1\C,-2.0090827246,1.7753965897,-0.0139678909\C,-0.6236195031,1.1420022
119,-0.0895583396\C,0.4666267849,2.186714157,0.0937141935\N,1.78251760
34,1.5658040467,0.0016176282\C,2.9072983041,2.2969312163,0.1484766621\
O,2.8814689615,3.5008316619,0.4418059523\N,4.0802721639,1.5890422342,-
0.0398578996\C,5.3923282378,2.0503270955,0.0337058381\C,5.7488514022,3
.3943456619,0.2363785129\C,6.4038718122,1.0831301448,-0.1208199396\C,7
.7401571886,1.4397419359,-0.0719761342\C,8.076997449,2.7780715458,0.13
75191508\C,7.0919023697,3.7506937914,0.2856618498\H,-2.7920095479,1.02
19890751,-0.1411197895\H,-2.1372893254,2.5310406663,-0.79678599\H,-2.1
641089363,2.2632786038,0.9546467258\H,-0.4908158232,0.6475374156,-1.05
98686592\H,-0.5194599433,0.3715641926,0.683951544\H,0.3666524498,2.668
769452,1.0723012931\H,0.3722790853,2.9686245235,-0.6701474329\H,1.8391
028178,0.6078194885,-0.3270360986\H,3.9835291075,0.5961913928,-0.23089
01851\H,4.9897709106,4.1531251738,0.354583452\H,6.1293323926,0.0433912
137,-0.2762423854\H,8.5104150361,0.6830502948,-0.1868484746\S,9.779273
2296,3.2518373349,0.1620831634\O,10.5813882382,2.0813011539,0.56720220
75\O,9.9103605622,4.4828812764,0.9651383233\H,7.3634255177,4.789965106
2,0.4462051552\C,10.189900076,3.6469324356,-1.5201109789\H,10.03197629
56,2.7562618857,-2.1316508822\H,11.2419794252,3.9444204197,-1.52857537
96\H,9.5491383824,4.468936602,-1.8455651922\\Version=ES64L-G09RevE.01\
State=1-A\HF=-1161.8383679\RMSD=4.572e-09\RMSF=7.413e-06\Dipole=-3.218
0021,-2.8364289,-2.9900456\Quadrupole=-6.9046103,6.610839,0.2937713,12
.486628,-16.9460975,-3.1831732\PG=C01 [X(C11H16N2O3S1)]\\@

4.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3714\FOpt\RM062X\Gen\C11H16N2O3S1\ROOT\22-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=n-Pentadecane) maxdisk=2147483648\\4SulfOxyMethyl.M062X_6-31pGd_opt
_Pentadecane\\0,1\C,-2.0094015236,1.8061928988,-0.064431641\C,-0.62708
81574,1.1712437993,-0.1852478087\C,0.4758064504,2.1658152331,0.1538330
504\N,1.7836947257,1.5344376014,0.0370685661\C,2.9158322605,2.30211498
93,0.0237807635\O,2.8932831982,3.5232559359,-0.0131569296\N,4.08721272
48,1.5534946109,0.0210343662\C,5.402352006,2.0178516025,0.0515540155\C

,5.7478906558,3.3639046415,0.2546616266\C,6.417983416,1.0580505502,-0.
1063397219\C,7.7532159799,1.4256116998,-0.0666913664\C,8.0821837791,2.
765328672,0.1317351435\C,7.0892013566,3.7271296133,0.2960940256\H,-2.7
961171149,1.0880962995,-0.3139424654\H,-2.108957056,2.6612820793,-0.74
19233248\H,-2.1927264978,2.1633236152,0.9549365617\H,-0.4686486654,0.7
978580755,-1.2041029323\H,-0.560386932,0.305951614,0.4885247734\H,0.32
92032849,2.5692105532,1.1658224915\H,0.4542864425,3.0120321631,-0.5381
541291\H,1.8550502722,0.5769142714,0.3608189278\H,3.9873528949,0.55316
53788,-0.102773457\H,4.9743159811,4.1077408556,0.3820771294\H,6.151767
3663,0.0139263256,-0.2524475498\H,8.537016736,0.6810790289,-0.17140013
03\S,9.7898164963,3.2509371787,0.1558784754\O,10.592994628,2.068050274
9,0.4806456033\O,9.9100529739,4.4685933238,0.9623601928\H,7.3633885899
,4.7629792622,0.4755193402\C,10.1501743618,3.6938133719,-1.5367108364\
H,9.9896984706,8.2814031574,-2.1730962077\H,11.1999743358,3.9983650105
,-1.5603300511\H,9.5040065597,4.5227963125,-1.8316265014\\Version=ES64
L-G09RevE.01\State=1-A\HF=-1161.8212177\RMSD=2.656e-09\RMSF=3.811e-06\
Dipole=-2.6793962,-1.9653809,-1.4565624\Quadrupole=-4.919226,5.1859827
,-0.2667567,9.2908242,-17.0240649,-3.6837728\PG=C01 [X(C11H16N2O3S1)]\
\@

4_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R4380\FOpt\RM062X\Gen\C14H21N2O5S1(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=n-Pentadecane) maxdisk=2684354560\\4SulfOxyMethyl_C2_EtO.M062X_
6-31pGd_opt_Pentadecane\\-1,1\C,-2.1191212041,2.4466744476,-0.51055337
08\C,-0.8030573827,1.7136868036,-0.267172392\C,0.3853789335,2.66701755
77,-0.3080067171\N,1.6145254991,1.9387516588,-0.0725293262\C,2.8045911
396,2.5772427415,-0.1216427582\O,2.9164868966,3.7798893272,-0.37764394
81\N,3.881845101,1.73852052,0.1407134577\C,5.2172304986,2.0726045407,0
.1777479694\C,5.7296721432,3.3700944435,-0.0355732234\C,6.1194957095,1
.0185163033,0.4572491284\C,7.4816258834,1.247531045,0.5123891392\C,7.9
725419298,2.538249833,0.2920266786\C,7.0998567927,3.5907650531,0.02019
06628\H,-2.9691393768,1.7573366262,-0.4771459443\H,-2.1236258066,2.936
138781,-1.4917533059\H,-2.2866997384,3.2206175266,0.247827114\H,-0.659
1310145,0.9296406109,-1.0202225696\H,-0.8245728289,1.2051851112,0.7039
879996\H,0.2617730116,3.4573477573,0.4466546542\H,0.433668058,3.170793
0686,-1.2829882528\H,1.5554529419,0.9347802803,0.1783090486\H,3.672985
8183,0.7333473871,0.3189388017\H,5.0472939863,4.1834923986,-0.23850785
81\H,5.7153204304,0.0246953427,0.6324950875\H,8.1676964877,0.436592537
8,0.7408918438\S,9.7134294583,2.8188765302,0.2817470528\O,10.366001155
1,1.7964833152,1.110192942\O,9.9708449041,4.2401810398,0.5484774426\H,
7.4948526026,4.5915132704,-0.1328041097\C,10.2107019855,2.5102002323,-
1.4091933571\H,9.9658017178,1.4777567566,-1.6659770079\H,11.2909881068
,2.6727817188,-1.4535980149\H,9.6880605006,3.2104210577,-2.0636753549\
O,1.3308920533,-0.7873575858,0.5889512048\O,3.5649729376,-0.9768971888
,0.6180064994\C,2.3971097602,-1.4441264285,0.7127618226\C,2.2434168279
,-2.9448452963,0.9971932928\C,3.5514637634,-3.6960925,1.2056904189\H,1
.6789272051,-3.3717423668,0.1584343841\H,1.5919786981,-3.0421988609,1.
874203718\H,4.1930257811,-3.616883037,0.3231010485\H,3.3665320304,-4.7
587619294,1.4036542242\H,4.1100666029,-3.281959431,2.0505610753\\Versi
on=ES64L-G09RevE.01\State=1-A\HF=-1429.6517097\RMSD=3.622e-09\RMSF=3.5
87e-06\Dipole=0.3884804,-0.1737006,-1.6441906\Quadrupole=-21.9838274,-
0.6868538,22.6706812,-15.9288085,-16.4634746,-0.0800464\PG=C01 [X(C14H
21N2O5S1)]\\@

4_propanoate.M062X_6-31pGd_opt

1\1\GINC-R4176\FOpt\RM062X\Gen\C14H21N2O5S1(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268
4354560\\4SulfOxyMethyl_C2_EtO.M062X_6-31pGd_opt\\-1,1\C,-2.1138528668
,2.4434768491,-0.4531644221\C,-0.802685361,1.7655864782,-0.062487788\C
,0.4040058079,2.6265251475,-0.4203202077\N,1.6231580602,1.9352301831,-
0.0681226456\C,2.8094562601,2.5835622122,-0.1088076913\O,2.9217043009,
3.7808354687,-0.3827156849\N,3.8838902269,1.7527433325,0.1993833586\C,
5.216181756,2.0861075318,0.2337520138\C,5.7287989598,3.3793641123,-0.0
107428266\C,6.1179403267,1.0385695424,0.5446519648\C,7.4798248692,1.26
89212297,0.5918133178\C,7.9718634871,2.5534125824,0.3354958792\C,7.098
7279539,3.5994486594,0.0371819732\H,-2.9776510508,1.8254326377,-0.1870
839435\H,-2.1546732342,2.6281344664,-1.5332222699\H,-2.2242596995,3.41
05429737,0.0520580868\H,-0.7107125147,0.7911004291,-0.556244375\H,-0.7
842639142,1.56114586,1.0147958629\H,0.3657172143,3.5857654142,0.111492
2576\H,0.3889570387,2.8661136515,-1.4957658914\H,1.5786679465,0.908779
4191,0.0768556029\H,3.6711029238,0.7516094153,0.3994669135\H,5.0426189
351,4.1848994758,-0.2323297734\H,5.7101143273,0.0505465959,0.745148549

1\C,-1.9529072718,1.7850364894,-0.1521107346\C,-0.5769891008,1.1520883
555,0.0282790047\C,0.5263306866,2.1856109742,-0.1382417603\N,1.8334815
591,1.5667482074,0.0483967279\C,2.9664454673,2.28590839,-0.0834257173\
O,2.9590766261,3.4809694504,-0.4127416873\N,4.1305222423,1.5811895592,
0.1662286649\C,5.4430704985,2.0419692235,0.1081359436\C,5.79112872,3.3
922448447,-0.0453046487\C,6.4620975666,1.0836785871,0.2332606953\C,7.7
926479081,1.4621629972,0.2001303677\C,8.1536994645,2.8020135709,0.0405
90888\C,7.1329253097,3.7466889145,-0.0774179383\H,-2.7454252713,1.0401
039575,-0.0349776869\H,-2.0517352336,2.2292738271,-1.1486814305\H,-2.1
203154201,2.5754031,0.5878289497\H,-0.4334360101,0.3493176397,-0.70504
34972\H,-0.5005343947,0.6989463089,1.0244572492\H,0.3960697995,2.99710
65193,0.5882456943\H,0.4799084335,2.6288391368,-1.1390784577\H,1.87198
66718,0.6108011411,0.3849701229\H,4.0315992983,0.5877023744,0.35434155
78\H,5.0330190906,4.1564182313,-0.1340041578\H,6.2011588727,0.03665157
14,0.356401045\H,8.56392445,0.7057711744,0.2968667246\Cl,7.50526169,5.
4424274723,-0.2680941106\C,9.6008841939,3.1902630547,0.0021311099\F,9.
938313689,4.0421519515,0.9927850963\F,9.9459878663,3.7988437939,-1.151
8564575\F,10.4093925979,2.1240291817,0.1259484427\\Version=ES64L-G09Re
vE.01\State=1-A\HF=-1370.5545512\RMSD=7.957e-09\RMSF=2.551e-06\Dipole=
-2.6963403,-3.8839872,0.8325572\Quadrupole=-0.6090646,6.140591,-5.5315
265,7.4986795,-2.8790258,-1.7701773\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

8_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R4273\SP\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\21-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671
088640\\3Chloro4TFM_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-1.989832681,1.96
06498839,-0.0564907278\C,0,-0.590289146,1.351388508,-0.0214347335\C,0,
0.4902445132,2.4267913415,-0.0027834451\N,0,1.7962943343,1.8095238128,
0.0369814133\C,0,2.9107608736,2.574531478,-0.0040956732\O,0,2.88565187
52,3.8046597668,-0.0886940666\N,0,4.0801857607,1.8232504152,0.05711534
04\C,0,5.3720860894,2.2884633263,0.0363643092\C,0,5.7314470864,3.64873
17467,-0.0540583671\C,0,6.398324837,1.3206169389,0.1113023608\C,0,7.72
5337109,1.7036721772,0.0957384305\C,0,8.0973945868,3.0510159569,0.0060
11418\C,0,7.0725261397,3.9986480353,-0.067209148\H,0,-2.7625046688,1.1
850337441,-0.0725351081\H,0,-2.1247199762,2.5872913702,-0.9461660936\H
,0,-2.1667542569,2.5919777062,0.8223967085\H,0,-0.4332406542,0.7018274
098,-0.8907437132\H,0,-0.4735466011,0.707945985,0.8585569345\H,0,0.353
9532119,3.0868152671,0.8670828433\H,0,0.4080354325,3.0671970783,-0.892
2373692\H,0,1.8549546737,0.7791600508,0.1303684886\H,0,3.98434931,0.78
51624845,0.1273522798\H,0,0.4.9622986246,4.4064283156,-0.1125912534\H,0,
6.1178595688,0.2726798622,0.1811329499\H,0,8.5000786885,0.9465204157,0
.1539562912\Cl,0,7.4530166084,5.7053972204,-0.1814398905\C,0,9.5427361
84,3.4331676518,-0.0088204351\F,0,9.9089549339,4.0890275034,-1.1312066
675\F,0,10.3473175645,2.3509835418,0.0693572132\F,0,9.8932321363,4.232
7396064,1.0217285242\O,0,1.8115805738,-0.9971868191,0.2886451692\O,0,4
.055997177,-0.9293360528,0.2502002687\C,0,2.9475692911,-1.5310771349,0
.3142376443\C,0,3.0238679183,-3.0615253306,0.433393891\C,0,1.668557869
4,-3.7525016718,0.5167903866\H,0,3.63712131,-3.2856534575,1.3149398674
\H,0,3.5991500392,-3.4226285226,-0.4281502128\H,0,1.1051389506,-3.3929
272394,1.3827211768\H,0,1.7814920046,-4.8405433252,0.5990281609\H,0,1.
0668227074,-3.5289390473,-0.3688651662\\Version=ES64L-G09RevE.01\State
=1-A\HF=-267.7284768\RMSD=3.841e-09\Dipole=0.4336193,0.1460925,-0.0227
397\Quadrupole=-14.7936018,-6.6211777,21.4147795,-18.355143,1.1914903,
1.969942\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

8_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R4140\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=h2o) maxdisk=2684354560\\3Chloro4TFM_EtO.M062X_6-31pGd_opt_w
ater\\-1,1\C,-1.9388764401,1.93787865,-0.1551202771\C,-0.5493086506,1.
3257552323,-0.0105197593\C,0.536020264,2.3801200217,-0.1742261312\N,1.
8522244831,1.771040747,-0.0474853494\C,2.969660838,2.5152395917,-0.145
6332116\O,2.9464745734,3.7372030603,-0.3777147953\N,4.1406289395,1.794
8922265,0.0143724458\C,5.4360263601,2.2909599938,0.0172263478\C,5.7526
293093,3.6498518212,0.179886704\C,6.4829294583,1.3611320191,-0.1113948
072\C,7.8025460082,1.7773966875,-0.0913863679\C,8.1291035794,3.1281122
399,0.0545380602\C,7.0829794092,4.0427857954,0.1928816852\H,-2.7174698
467,1.1785173214,-0.0359779549\H,-2.0638121237,2.3971438758,-1.1420427
152\H,-2.1057865252,2.7132436344,0.6008589578\H,-0.4046238157,0.538504
7926,-0.7608223547\H,-0.4483427147,0.8528572661,0.9741794152\H,0.41217
46647,3.1652726447,0.5827331533\H,0.4487592156,2.8591276932,-1.1567475
272\H,1.9125054374,0.7949622307,0.2695184602\H,4.0492529354,0.76513374
27,-0.002082945\H,4.9746996939,4.3895413864,0.3033481136\H,6.251070369

8,0.3069805874,-0.2288158457\H,8.5938388108,1.0428844683,-0.1960194679
\Cl,7.4107660529,5.7468781029,0.401496427\C,9.5634284567,3.5587246579,
0.0638990396\F,9.8519789054,4.4347004468,-0.9222093082\F,10.4013092282
,2.5198463172,-0.0949760896\F,9.9206885365,4.1625607661,1.2175732183\O
,1.9092852956,-0.9757194733,0.8789555784\O,3.8756508977,-1.0434271836,
-0.1804866083\C,2.8596206606,-1.6039886977,0.3348919728\C,2.8172253821
,-3.1277232042,0.2799426235\C,1.5483922559,-3.759728812,0.8336511077\H
,3.6992602467,-3.4886362819,0.823210485\H,2.9709970374,-3.4153889277,-
0.7667485107\H,1.4073402071,-3.5071686521,1.8890460386\H,1.5974670843,
-4.8500541791,0.750828734\H,0.6647355195,-3.4184306295,0.2852914582\\V
ersion=ES64L-G09RevE.01\State=1-A\HF=-1638.4133092\RMSD=6.419e-09\RMSF
=2.688e-06\Dipole=0.8650381,-0.0233224,-0.0273266\Quadrupole=-7.161178
2,-6.3968642,13.5580423,-17.8069272,2.4995487,4.0418626\PG=C01 [X(C14H
17Cl1F3N2O3)]\\@

8_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3736\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
2684354560\\3Chloro4TFM_EtO.M062X_6-31pGd_opt\\-1,1\C,-1.989832681,1.9
606498839,-0.0564907278\C,-0.590289146,1.351388508,-0.0214347335\C,0.4
902445132,2.4267913415,-0.0027834451\N,1.7962943343,1.8095238128,0.036
9814133\C,2.9107608736,2.574531478,-0.0040956732\O,2.8856518752,3.8046
597668,-0.0886940666\N,4.0801857607,1.8232504152,0.0571153404\C,5.3720
860894,2.2884633263,0.0363643092\C,5.7314470864,3.6487317467,-0.054058
3671\C,6.398324837,1.3206169389,0.1113023608\C,7.725337109,1.703672177
2,0.0957384305\C,8.0973945868,3.0510159569,0.006011418\C,7.0725261397,
3.9986480353,-0.067209148\H,-2.7625046688,1.1850337441,-0.0725351081\H
,-2.1247199762,2.5872913702,-0.9461660936\H,-2.1667542569,2.5919777062
,0.8223967085\H,-0.4332406542,0.7018274098,-0.8907437132\H,-0.47354660
11,0.707945985,0.8585569345\H,0.3539532119,3.0868152671,0.8670828433\H
,0.4080354325,3.0671970783,-0.8922373692\H,1.8549546737,0.7791600508,0
.1303684886\H,3.98434931,0.7851624845,0.1273522798\H,4.9622986246,4.40
64283156,-0.1125912534\H,6.1178595688,0.2726798622,0.1811329499\H,8.50
00786885,0.9465204157,0.1539562912\Cl,7.4530166084,5.7053972204,-0.181
4398905\C,9.542736184,3.4331676518,-0.0088204351\F,9.9089549339,4.0890
275034,-1.1312066675\F,10.3473175645,2.3509835418,0.0693572132\F,9.893
2321363,4.2327396064,1.0217285242\O,1.8115805738,-0.9971868191,0.28864
51692\O,4.055997177,-0.9293360528,0.2502002687\C,2.9475692911,-1.53107
71349,0.3142376443\C,3.0238679183,-3.0615253306,0.433393891\C,1.668557
8694,-3.7525016718,0.5167903866\H,3.63712131,-3.2856534575,1.314939867
4\H,3.5991500392,-3.4226285226,-0.4281502128\H,1.1051389506,-3.3929272
394,1.3827211768\H,1.7814920046,-4.8405433252,0.5990281609\H,1.0668227
074,-3.5289390473,-0.3688651662\\Version=ES64L-G09RevE.01\State=1-A\HF
=-1638.3433304\RMSD=8.139e-09\RMSF=4.521e-06\Dipole=0.4298962,0.174182
2,-0.024709\Quadrupole=-14.7198236,-6.8123981,21.5322217,-18.4739804,1
.1978318,1.9907527\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

8_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3830\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=n-Pentadecane) maxdisk=2684354560\\3Chloro4TFM_EtO.M062X_6-3
1pGd_opt_Pentadecane\\-1,1\C,-2.0031928783,2.0070481199,-0.0478391275\
C,-0.6129673726,1.3821414344,0.0240659696\C,0.4809113579,2.4410149652,
-0.046624816\N,1.7854106112,1.8157592616,0.023294\C,2.9050713138,2.571
3046173,-0.0209967105\O,2.8864939657,3.8014674212,-0.1226880069\N,4.07
17876139,1.8202977397,0.0593031369\C,5.3674380222,2.2828585582,0.04104
05831\C,5.731132439,3.6400892314,-0.0650425819\C,6.3906811006,1.314814
6696,0.136525121\C,7.7195921739,1.692340813,0.1257204146\C,8.094056425
4,3.0372148186,0.0205862476\C,7.0733325808,3.9868285044,-0.0731063016\
H,-2.7851108565,1.2423351312,0.003373884\H,-2.1392895697,2.5621513824,
-0.9835517865\H,-2.1654458501,2.7070010916,0.7803942078\H,-0.474537250
9,0.6670164514,-0.7956829181\H,-0.5005394825,0.8105365471,0.9531345782
\H,0.3649652895,3.1596772619,0.7767229187\H,0.3904664452,3.0160122988,
-0.9787987099\H,1.8398402462,0.7858756091,0.1117578331\H,3.9759982838,
0.7835413104,0.1434646952\H,4.9670126739,4.4010591266,-0.1393980236\H,
6.1115230342,0.2678835297,0.2186346607\H,8.4898090205,0.9318371003,0.2
000370411\Cl,7.4583670719,5.6904244988,-0.2073382804\C,9.5403614468,3.
417310716,0.0113817105\F,9.9145646889,4.0571567908,-1.117742604\F,10.3
426968695,2.3377253636,0.1118434659\F,9.882025995,4.2330427336,1.03219
86114\O,1.826311613,-1.0079501776,0.2625959964\O,4.0670156736,-0.92939
21706,0.2852255693\C,2.961227803,-1.5416563516,0.3183506308\C,3.046239
2523,-3.0691197991,0.4373729856\C,1.7002993356,-3.7794503517,0.4769516
588\H,3.6324839401,-3.2895551619,1.3381905642\H,3.6519444478,-3.424119

6911,-0.405743377\H,1.1021669468,-3.4359185417,1.3262496449\H,1.830465
5157,-4.8649071831,0.5630754635\H,1.1228400628,-3.5727176694,-0.429058
3488\\Version=ES64L-G09RevE.01\State=1-A\HF=-1638.3832654\RMSD=4.590e-
09\RMSF=1.895e-05\Dipole=0.3933523,0.0961965,-0.0055991\Quadrupole=-12
.7059057,-6.8413914,19.5472971,-18.1088359,1.0158494,1.9310515\PG=C01
[X(C14H17Cl1F3N2O3)]\\@

12_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3737\FOpt\RM062X\Gen\C14H16Cl2F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=h2o) maxdisk=3221225472\\22Cl_4CF3_EtO.M062X_6-31pGd_opt_wat
er\\-1,1\C,-4.3174191736,4.0741337076,-0.8496333166\C,-4.4246978671,2.
7332336379,-0.4912660432\C,-3.2637131726,1.9930073076,-0.3280683983\C,
-1.9869625583,2.5441561132,-0.5306747744\C,-1.934028432,3.8929940966,-
0.9155827571\C,-3.0794384502,4.6660756914,-1.0637027769\N,-0.826722899
9,1.7806255383,-0.384996936\C,0.0817473883,2.0682438564,0.6236714393\N
,1.1803811286,1.2967719122,0.6196777098\O,-0.1232041118,2.9652626342,1
.4615223455\C,2.207479818,1.4402028434,1.6414358863\C,3.3146860279,0.4
199692845,1.4191087835\C,4.4032268232,0.5470391244,2.4798892283\H,-0.8
050276975,0.8225468668,-0.775048871\H,1.3325337488,0.6356928727,-0.153
9374853\H,1.7604769619,1.2995925103,2.6331303912\H,2.6231258636,2.4553
782119,1.6123590271\H,3.7446820755,0.5657875382,0.4202936963\H,2.88516
85116,-0.5893671234,1.4390890769\H,4.8554393351,1.5448692194,2.4592635
818\H,5.1987032684,-0.1863224545,2.3173547057\H,3.9934865757,0.3836716
17,3.4828745084\H,-5.3949008657,2.2745963978,-0.3246027887\H,-2.997496
0006,5.7064087349,-1.3583508042\C,-5.5815845573,4.865618132,-1.0185589
706\F,-5.3505134729,6.1618945349,-1.2746369577\F,-6.3380444148,4.39512
40541,-2.0315841023\F,-6.3575307349,4.8133479343,0.0820787842\Cl,-0.39
80135384,4.624442995,-1.2721101555\Cl,-3.3959387325,0.3317619595,0.167
5384887\O,1.6601530932,-0.5487271631,-1.5469538214\O,-0.5511002718,-0.
8591938478,-1.4388186135\C,0.6087613145,-1.2130926524,-1.795796238\C,0
.7870700195,-2.5157261934,-2.5702726871\C,-0.4972491362,-3.2737252207,
-2.8738566482\H,1.4766235338,-3.1386779933,-1.9876703871\H,1.318678195
7,-2.2654207024,-3.496160263\H,-1.0187378646,-3.5546802924,-1.95360081
06\H,-0.2770760733,-4.1900528514,-3.430644058\H,-1.1816036572,-2.66842
28317,-3.4764998883\\Version=ES64L-G09RevE.01\State=1-A\HF=-2097.97629
45\RMSD=3.288e-09\RMSF=5.520e-06\Dipole=-1.9875927,1.2304853,-0.128265
9\Quadrupole=-3.4952542,-2.103402,5.5986562,9.4274229,3.6975205,-8.777
7519\PG=C01 [X(C14H16Cl2F3N2O3)]\\@

12_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3734\FOpt\RM062X\Gen\C14H16Cl2F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
3221225472\\22Cl_4CF3_EtO.M062X_6-31pGd_opt\\-1,1\C,-4.3479994194,3.95
82982951,-0.8744042446\C,-4.4110096018,2.5928867123,-0.6188091548\C,-3
.2328424583,1.881524542,-0.4382440646\C,-1.9601551605,2.4861090012,-0.
5142580415\C,-1.9483449792,3.8652973538,-0.82217638\C,-3.1161843117,4.
5980701516,-0.9769334629\N,-0.8063158274,1.7529886695,-0.3454571922\C,
0.1537927619,2.1243518582,0.605788848\N,1.2556772731,1.3471121718,0.57
49605607\O,-0.0245133774,3.0506512331,1.3955059385\C,2.3202830003,1.54
99791872,1.530428932\C,3.2316926786,0.3275928915,1.5666158528\C,4.4001
766989,0.5256289272,2.529494038\H,-0.7494010976,0.7817269844,-0.737989
8147\H,1.3801279579,0.6223956895,-0.1581233855\H,1.8832220174,1.737298
4534,2.5194130148\H,2.9076515216,2.4464139248,1.2742074381\H,3.5972692
283,0.1187517317,0.5544387147\H,2.6383036667,-0.5471146036,1.858648187
5\H,5.0161179134,1.3818314728,2.229455645\H,5.0475009709,-0.3571187163
,2.559766215\H,4.0438834223,0.7161572863,3.5491173875\H,-5.3636912947,
2.0801542543,-0.5448171709\H,-3.0564326213,5.6551024233,-1.2131634178\
C,-5.6056277477,4.7579970156,-0.9991667992\F,-5.4870444411,5.765259803
4,-1.8881540904\F,-6.6554644964,4.0099250506,-1.3910111759\F,-5.970980
5883,5.3351141746,0.1679226256\Cl,-0.445220412,4.6739202976,-1.1314707
127\Cl,-3.3387042702,0.1866379271,-0.0834563029\O,1.7227315396,-0.7071
907687,-1.2689639623\O,-0.5162198417,-0.7485486019,-1.465416019\C,0.64
03245223,-1.1986603704,-1.68061957\C,0.7559531828,-2.4801227594,-2.524
1580703\C,-0.5758062367,-3.0293487676,-3.0206492399\H,1.2840956639,-3.
2210919899,-1.9108315563\H,1.4277517036,-2.2542127471,-3.3615670067\H,
-1.2371622348,-3.254758069,-2.1791260802\H,-0.4341337172,-3.9428991663
,-3.6117142586\H,-1.0918815882,-2.2890709239,-3.6388222245\\Version=ES
64L-G09RevE.01\HF=-2097.8962914\RMSD=5.520e-09\RMSF=4.812e-0
6\Dipole=-1.4206293,0.9821265,-0.0094694\Quadrupole=-7.1148797,-4.0344
292,11.1493089,15.4974705,-1.1462459,-8.566641\PG=C01 [X(C14H16Cl2F3N2
O3)]\\@

12_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3710\SP\RM062X\Gen\C14H16Cl2F3N2O3(1-)\ROOT\21-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671
088640\\22Cl_4CF3_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-4.3479994194,3.958
2982951,-0.8744042446\C,0,-4.4110096018,2.5928867123,-0.6188091548\C,0
,-3.2328424583,1.881524542,-0.4382440646\C,0,-1.9601551605,2.486109001
2,-0.5142580415\C,0,-1.9483449792,3.8652973538,-0.82217638\C,0,-3.1161
843117,4.5980701516,-0.9769334629\N,0,-0.8063158274,1.7529886695,-0.34
54571922\C,0,0.1537927619,2.1243518582,0.605788848\N,0,1.2556772731,1.
3471121718,0.5749605607\O,0,-0.0245133774,3.0506512331,1.3955059385\C,
0,2.3202830003,1.5499791872,1.530428932\C,0,3.2316926786,0.3275928915,
1.5666158528\C,0,4.4001766989,0.5256289272,2.529494038\H,0,-0.74940109
76,0.7817269844,-0.7379898147\H,0,1.3801279579,0.6223956895,-0.1581233
855\H,0,1.8832220174,1.7372984534,2.5194130148\H,0,2.9076515216,2.4464
139248,1.2742074381\H,0,3.5972692283,0.1187517317,0.5544387147\H,0,2.6
383036667,-0.5471146036,1.8586481875\H,0,5.0161179134,1.3818314728,2.2
29455645\H,0,5.0475009709,-0.3571187163,2.559766215\H,0,4.0438834223,0
.7161572863,3.5491173875\H,0,-5.3636912947,2.0801542543,-0.5448171709\
H,0,-3.0564326213,5.6551024233,-1.2131634178\C,0,-5.6056277477,4.75799
70156,-0.9991667992\F,0,-5.4870444411,5.7652598034,-1.8881540904\F,0,-
6.6554644964,4.0099250506,-1.3910111759\F,0,-5.9709805883,5.3351141746
,0.1679226256\Cl,0,-0.445220412,4.6739202976,-1.1314707127\Cl,0,-3.338
7042702,0.1866379271,-0.0834563029\O,0,1.7227315396,-0.7071907687,-1.2
689639623\O,0,-0.5162198417,-0.7485486019,-1.465416019\C,0,0.640324522
3,-1.1986603704,-1.68061957\C,0,0.7559531828,-2.4801227594,-2.52415807
03\C,0,-0.5758062367,-3.0293487676,-3.0206492399\H,0,1.2840956639,-3.2
210919899,-1.9108315563\H,0,1.4277517036,-2.2542127471,-3.3615670067\H
,0,-1.2371622348,-3.254758069,-2.1791260802\H,0,-0.4341337172,-3.94289
91663,-3.6117142586\H,0,-1.0918815882,-2.2890709239,-3.6388222245\\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-267.7286106\RMSD=3.874e-09\Dipole=
-1.4149125,0.9562979,-0.0312322\Quadrupole=-7.1835154,-3.8854404,11.06
89559,15.3543435,-1.2036027,-8.4276522\PG=C01 [X(C14H16Cl2F3N2O3)]\\@

12.M062X.opt

1\1\GINC-R3771\FOpt\RM062X\Gen\C11H11Cl2F3N2O1\ROOT\10-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
maxdisk=2147483648\\aryl_urea_dichloro_CF3.M062X.opt\\0,1\C,-4.102067
2406,3.4964938621,-0.1116510989\C,-4.1881832392,2.2963878828,-0.311816
3197\C,-3.0214728883,1.6101242639,-0.0167946945\C,-1.758593676,2.07675
32369,-0.4168090302\C,-1.7179970922,3.270187356,-1.1522819433\C,-2.874
8969743,3.9887428376,-1.434613624\N,-0.5905621491,1.3613440121,-0.1313
400836\C,0.3933033967,1.9465020578,0.6982775681\N,1.4703050599,1.12572
41131,0.8895594068\O,0.269313819,3.046670427,1.1941120142\C,2.61447741
46,1.6145287809,1.6481988808\C,3.5462406832,0.4663436862,2.0139277475\
C,4.7540987215,0.956805829,2.8090990578\H,-0.7290152035,0.3678163463,0
.0176337884\H,1.6573645191,0.4407269505,0.1672776833\H,2.2250858209,2.
0977315983,2.5485942375\H,3.1556051717,2.2834187692,1.0787607796\H,3.8
888858962,-0.0346376214,1.0978882135\H,2.9854068152,-0.2767741485,2.59
29696407\H,5.3349701728,1.6855533429,2.2337871682\H,5.4185310846,0.128
2451091,3.0692375277\H,4.4390391803,1.4400048224,3.7399644223\H,-5.146
7428617,1.9060830266,0.0147191213\H,-2.8082205867,4.9133650486,-1.9964
027429\C,-5.3757632216,4.2363626169,-1.3131299621\F,-5.1553088474,5.38
0496628,-1.9757357508\F,-6.2114593595,3.493525124,-2.0626989992\F,-6.0
456221302,4.5448042931,-0.1883530227\Cl,-0.2131578039,3.8497484863,-1.
7795847456\Cl,-3.1284844814,0.1205412621,0.8785847598\\Version=ES64L-G
09RevE.01\State=1-A\HF=-1830.1007854\RMSD=9.502e-09\RMSF=5.760e-06\Dip
ole=1.2868621,-1.5537144,-0.0445701\Quadrupole=3.4211721,0.4361818,-3.
857354,-3.8762883,-0.1015435,-2.3401996\PG=C01 [X(C11H11Cl2F3N2O1)]\\@

12_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3734\FOpt\RM062X\Gen\C14H16Cl2F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=n-Pentadecane) maxdisk=3221225472\\22Cl_4CF3_EtO.M062X_6-31p
Gd_opt_Pentadecane\\-1,1\C,-4.3393904945,3.9613965301,-0.8804118321\C,
-4.4195789596,2.6089834342,-0.5682719063\C,-3.2465518372,1.8925222006,
-0.3728647173\C,-1.9702985548,2.4770511949,-0.4939112353\C,-1.94363944
86,3.8428130616,-0.8471462349\C,-3.1031460243,4.5851389305,-1.01892909
67\N,-0.8182742523,1.7338884961,-0.3156613659\C,0.1321506619,2.0935486
854,0.6430547009\N,1.2264885245,1.3042425756,0.6301417660\O,-0.0432052
635,3.0279450914,1.4264930421\C,2.3089658197,1.530499273,1.5637034911\
C,3.239635734,0.323250186,1.5925212092\C,4.4174533545,0.5425440028,2.5
376844792\H,-0.7641036211,0.7705378032,-0.7238720982\H,1.3651767897,0.
61718265,-0.1343013299\H,1.8889813077,1.7150374961,2.5597863932\H,2.87

73577109,2.4329448011,1.2889952654\H,3.5990051874,0.121328357,0.576380
6138\H,2.6652892434,-0.5598273692,1.8977956027\H,5.0165913022,1.406997
1693,2.2278136424\H,5.0784797011,-0.3302187679,2.5590124385\H,4.073481
6724,0.7269853833,3.5625246011\H,-5.3788856726,2.1142146599,-0.4607673
37\H,-3.0351355418,5.633583797,-1.2898003852\C,-5.5901948422,4.7711337
556,-1.0273743387\F,-5.4646128761,5.7426748804,-1.952488559\F,-6.64912
36328,4.0212475217,-1.3852742256\F,-5.9395927524,5.3930997629,0.120596
4458\Cl,-0.428168206,4.6228622884,-1.1752223195\Cl,-3.3647565567,0.215
9927245,0.0642920032\O,1.6802470182,-0.6260495381,-1.3597992507\O,-0.5
574750989,-0.756465402,-1.4901936276\C,0.6076256996,-1.1659327151,-1.7
395675622\C,0.7538937027,-2.4463384165,-2.5757856183\C,-0.5604653822,-
3.0560946283,-3.0434014406\H,1.3219918325,-3.1614140655,-1.9673168243\
H,1.3990322553,-2.202682969,-3.4289974922\H,-1.1976162696,-3.308523422
8,-2.1907227702\H,-0.3868201071,-3.9676003487,-3.6283290035\H,-1.11939
21237,-2.3494590695,-3.6641251243\\Version=ES64L-G09RevE.01\State=1-A\
HF=-2097.9384453\RMSD=3.385e-09\RMSF=2.492e-06\Dipole=-1.5464573,1.049
7759,-0.0035856\Quadrupole=-5.5270054,-3.8679307,9.3949361,13.7184474,
0.3227698,-8.7382958\PG=C01 [X(C14H16Cl2F3N2O3)]\\@

12.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3834\FOpt\RM062X\Gen\C11H11Cl2F3N2O1\ROOT\21-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,So
lvent=n-Pentadecane) maxdisk=2147483648\\aryl_urea_dichloro_CF3.M062X_
6-31pGd_opt_Pentadecane\\0,1\C,-4.112171219,3.4937888923,-0.9966298854
\C,-4.1778437335,2.3001383287,-0.2838755277\C,-3.0000347417,1.62633521
6,-0.0036678696\C,-1.7473839429,2.0981601903,-0.4306587613\C,-1.731511
0122,3.2843843001,-1.1793192937\C,-2.8976369397,3.9919962189,-1.449135
0078\N,-0.5688449473,1.3976226966,-0.1530802073\C,0.4192123961,1.97803
82907,0.6675171373\N,1.4810715473,1.151931703,0.8834917466\O,0.3081439
468,3.0960761161,1.1356135842\C,2.6379539797,1.6261272619,1.6318194262
\C,3.5215695965,0.4568930241,2.0464758381\C,4.7451554211,0.9297979096,
2.8260853703\H,-0.6762137408,0.3938366946,-0.0541244289\H,1.6376096808
,0.4041640191,0.2174628417\H,2.2661263208,2.1571670479,2.5124511775\H,
3.2131528752,2.3478197523,1.0349757505\H,3.8455274677,-0.0922122178,1.
1518002831\H,2.9301869155,-0.2389360996,2.6536187089\H,5.3589426181,1.
6091572757,2.224360233\H,5.3738916095,0.0850933426,3.1228693014\H,4.44
88475269,1.4631378937,3.7359581451\H,-5.1275981585,1.9076855576,0.0660
359468\H,-2.8485508927,4.9121481283,-2.0207091018\C,-5.3964201213,4.21
16426741,-1.3013828604\F,-5.1911359077,5.4232251945,-1.837507965\F,-6.
1585195521,3.5192055366,-2.1714424428\F,-6.1458019876,4.3831762396,-0.
1972181727\Cl,-0.242009239,3.8680969921,-1.844154033\Cl,-3.0806357663,
0.1479218207,0.9137500663\\Version=ES64L-G09RevE.01\State=1-A\HF=-1830
.1158119\RMSD=5.588e-09\RMSF=5.037e-06\Dipole=1.3428152,-1.8118322,-0.
0487861\Quadrupole=3.3053743,0.9282065,-4.2335808,-5.0230627,-0.169843
7,-2.4199572\PG=C01 [X(C11H11Cl2F3N2O1)]\\@

12.M062X.SMD.h2o.opt

1\1\GINC-R3771\FOpt\RM062X\Gen\C11H11Cl2F3N2O1\ROOT\10-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_dichloro_CF3.M06
2X.SMD.h2o.opt\\0,1\C,-4.0977807217,3.4993409941,-1.0160881138\C,-4.15
95492663,2.3656665111,-0.2108722127\C,-2.9829805823,1.6907337813,0.075
6006447\C,-1.7435113545,2.1005592118,-0.4400087194\C,-1.734432149,3.23
32346194,-1.2652560628\C,-2.8945732609,3.9446343332,-1.548266367\N,-0.
5644725679,1.3941720136,-0.1650983682\C,0.4167200142,1.9607875547,0.64
43347632\N,1.4732647057,1.1684256105,0.8947308805\O,0.3134447017,3.113
9717649,1.0832477004\C,2.5577073217,1.601727645,1.7685065068\C,3.59749
35867,0.5001945138,1.9047166607\C,4.7367546623,0.930840559,2.822772771
5\H,-0.6299085217,0.3800625698,-0.1592141732\H,1.5154037845,0.24175291
05,0.4843261296\H,2.1483285151,1.8595857708,2.7522934984\H,3.018068246
6,2.5062893756,1.3546505615\H,3.9897085364,0.2495863934,0.9114814543\H
,3.1171094215,-0.4027624239,2.3010502347\H,5.2370323657,1.8243951559,2
.4335342299\H,5.485537761,0.1387110655,2.9155517655\H,4.3641497966,1.1
626955903,3.8265720078\H,-5.1032224923,2.0211629792,0.2012769021\H,-2.
8523900011,4.8205804385,-2.1862469485\C,-5.3790756334,4.2191189101,-1.
3254927657\F,-5.1778286458,5.3810072222,-1.9642695438\F,-6.1924787879,
3.4786198575,-2.1060546489\F,-6.080388849,4.497071604,-0.2098503194\Cl
,-0.2476304955,3.7491584066,-1.9979248076\Cl,-3.0454200905,0.302295061
9,1.1213763392\\Version=ES64L-G09RevE.01\State=1-A\HF=-1830.1175567\RM
SD=5.930e-09\RMSF=1.000e-05\Dipole=1.2433274,-2.7440607,-0.1444095\Qua
drupole=2.7160312,2.5957037,-5.3117349,-8.554226,0.7462797,-4.2646706\
PG=C01 [X(C11H11Cl2F3N2O1)]\\@

9.M062X_6-31pGd_opt

1\1\GINC-R3716\FOpt\RM062X\Gen\C11H13F3N2O3S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26843
54560\\4SulfOxyCf3.M062X_6-31pGd_opt\\0,1\C,-2.0010428586,1.8457922452
,-0.0802217512\C,-0.6280795585,1.1881093543,-0.199730912\C,0.490966029
7,2.1715336782,0.1173105902\N,1.7911286441,1.5222062396,-0.0032823291\
C,2.9251796531,2.2937181757,0.0193232059\O,2.9015059241,3.5108533237,0
.0178274491\N,4.1005460897,1.5424107228,0.0071138117\C,5.4113364331,2.
012427542,0.0606729887\C,5.7425655791,3.3610018192,0.2773447257\C,6.43
42840347,1.0581770941,-0.0921500446\C,7.7652610177,1.4299920546,-0.031
0973253\C,8.0771422241,2.772448547,0.184766214\C,7.0789643815,3.732583
1006,0.339631109\H,-2.7997741089,1.1353626376,-0.3098762045\H,-2.09188
46795,2.6891412553,-0.7726990896\H,-2.1693865933,2.2248341767,0.933325
1295\H,-0.4814448853,0.7954775369,-1.2128901096\H,-0.5713299435,0.3320
24479,0.4870890679\H,0.3608399052,2.5921329934,1.1244367314\H,0.478366
2693,3.0098810218,-0.5843934688\H,1.8513475808,0.5717171322,0.34065927
27\H,4.0043590024,0.5523619711,-0.1778058341\H,4.9602517835,4.09741663
48,0.392322073\H,6.1767146157,0.0142069758,-0.2528271913\H,8.558538358
1,0.6963002065,-0.1368037693\S,9.766966969,3.2587831967,0.2541742781\O
,10.5974129768,2.1023086784,0.5509458271\O,9.8898497575,4.5227285377,0
.9612589667\H,7.3514008765,4.7684492823,0.5190100027\C,10.1373533318,3
.6665644804,-1.5237031214\F,11.4021855692,4.0489420082,-1.6277020261\F
,9.9370507346,2.5949543986,-2.2878909408\F,9.343684886,4.6485984999,-1
.9425773257\\Version=ES64L-G09RevE.01\State=1-A\HF=-1459.435642\RMSD=3
.887e-09\RMSF=2.086e-06\Dipole=-3.1182809,-2.0747144,-0.3116659\Quadru
pole=-1.3693055,5.0674997,-3.6981942,8.4847527,-7.1167572,-1.851644\PG
=C01 [X(C11H13F3N2O3S1)]\\@

9_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3722\FOpt\RM062X\Gen\C14H18F3N2O5S1(1-)\ROOT\19-Feb-2019\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=3
221225472\\4SulfOxyCF3_EtO.M062X_6-31pGd_opt\\-1,1\C,-2.1691580428,2.1
810960156,-0.1733823084\C,-0.7914550342,1.5709307017,0.0726737597\C,0.
3177351597,2.6023057132,-0.1007763432\N,1.603202987,1.9855124683,0.139
2993175\C,2.7344597808,2.7119458042,0.0223691841\O,2.7503030106,3.9055
161652,-0.2836947561\N,3.8826325882,1.9603016066,0.2858758079\C,5.1809
54749,2.3860311271,0.2540915383\C,5.5881145535,3.7075954017,-0.0510191
634\C,6.1697122831,1.4119612476,0.5552500623\C,7.5083345313,1.73970275
9,0.5477635434\C,7.8917700171,3.054541915,0.2430514924\C,6.9340363135,
4.0297015868,-0.0558990899\H,-2.9625652908,1.4369763493,-0.0491628708\
H,-2.2452085223,2.585992456,-1.1895595934\H,-2.3672817133,3.0024184558
,0.5255344764\H,-0.6138677842,0.7343160635,-0.6132674411\H,-0.73362407
5,1.1471316215,1.08212527\H,0.1686571268,3.4436246485,0.5916047111\H,0
.2896100899,3.0272652259,-1.1144808307\H,1.6290588476,0.9803077213,0.3
996908577\H,3.749015392,0.9527819221,0.5337145682\H,4.8366087955,4.451
9331389,-0.2736872316\H,5.8416226446,0.4034861134,0.7952503923\H,8.264
7291397,0.9973421781,0.7847610882\S,9.5789265659,3.4653461181,0.184526
0689\O,10.3761053467,2.5088912051,0.9434858863\O,9.7720467454,4.904519
7223,0.3190031739\H,7.2540835604,5.0429323484,-0.2813910516\C,10.05192
22831,3.124607404,-1.5834719103\F,11.3436841738,3.4028399037,-1.757713
2883\F,9.8466232456,1.8438920615,-1.8876045613\F,9.3372177349,3.880624
0178,-2.4161584001\O,1.5224945097,-0.7257276998,0.8313244276\O,3.76352
50121,-0.7052025868,0.958976192\C,2.6370430533,-1.2681035167,1.0397457
567\C,2.6097556227,-2.7542550284,1.4277429683\C,3.9819776283,-3.367210
2728,1.6779425349\H,2.080420201,-3.2845724696,0.6264329052\H,1.9700579
114,-2.8419645679,2.3145846953\H,4.6103818334,-3.284606624,0.786509770
5\H,3.8993262402,-4.4262885453,1.9509056027\H,4.500040785,-2.838869775
7,2.4834827885\\Version=ES64L-G09RevE.01\State=1-A\HF=-1727.2488192\RM
SD=9.587e-09\RMSF=4.975e-06\Dipole=0.4793203,0.1375795,-0.8549522\Quad
rupole=-28.3003504,3.6628616,24.6374888,-18.3517442,-0.1978947,4.18509
17\PG=C01 [X(C14H18F3N2O5S1)]\\@

9_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3762\FOpt\RM062X\Gen\C14H18F3N2O5S1(1-)\ROOT\19-Feb-2019\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=n-Pentadecane) maxdisk=3221225472\\4SulfOxyCF3_EtO.M062X_6-31
pGd_opt_Pentadecane\\-1,1\C,-2.1762893785,2.2119658266,-0.1879332421\C
,-0.8087695217,1.5953349628,0.0911902431\C,0.3135606929,2.6035539924,-
0.1228098848\N,1.5967662486,1.9842793208,0.1400472748\C,2.7314226193,2
.7043957697,0.0241657691\O,2.7503623057,3.8955794491,-0.2956788503\N,3
.8782410308,1.9596172301,0.3019356984\C,5.1789573871,2.3875326411,0.26
7869456\C,5.5848820174,3.7095211659,-0.0315224708\C,6.1689952974,1.414
1974777,0.5609841744\C,7.5082071586,1.7408328191,0.5485120295\C,7.8887

866795,3.0567308057,0.2478747292\C,6.9307303903,4.0335695462,-0.041203
3965\H,-2.9788099941,1.4841668615,-0.030008053\H,-2.2462654684,2.56747
88123,-1.2227767927\H,-2.3665418321,3.0673730613,0.471096903\H,-0.642
4377626,0.7283846818,-0.5592614259\H,-0.7634741459,1.2205366011,1.1206
6205\H,0.175554668,3.4709497673,0.5374409414\H,0.28707927,2.9866662808
,-1.1526149298\H,1.6199005075,0.9834349151,0.4121371306\H,3.7480284733
,0.9530120889,0.5516263971\H,4.8360964021,4.4577326612,-0.2484121105\H
,5.8462553057,0.4038355674,0.7979887346\H,8.2621429286,0.9930337668,0.
7762959478\S,9.5776731545,3.4670638096,0.1768619013\O,10.380113047,2.5
148136349,0.936484397\O,9.7725400824,4.9067637291,0.307657616\H,7.2444
949481,5.0492545228,-0.2642653833\C,10.0382696759,3.1207561773,-1.5922
8067\F,11.3244648679,3.4133305208,-1.7755375111\F,9.8444612124,1.83642
82772,-1.8841308163\F,9.3074169846,3.8638593793,-2.4209053794\O,1.5413
921681,-0.7334091871,0.8668400638\O,3.7801513966,-0.7113053259,0.97594
88462\C,2.6572916137,-1.28208788,1.0565569896\C,2.6342177213,-2.774713
2485,1.4097288759\C,4.0006777407,-3.388379693,1.6827757715\H,2.1337697
729,-3.2902240919,0.5802517705\H,1.9710262176,-2.8909079083,2.27556889
61\H,4.6545908943,-3.2889709989,0.8114094189\H,3.9109400922,-4.4535153
428,1.9274051082\H,4.4961871302,-2.8849024474,2.5184737825\\Version=ES
64L-G09RevE.01\State=1-A\HF=-1727.2878759\RMSD=6.371e-09\RMSF=3.993e-0
6\Dipole=0.483354,0.1148352,-0.9361986\Quadrupole=-26.7181429,3.596054
8,23.1220881,-18.4768833,-0.3529703,3.9343858\PG=C01 [X(C14H18F3N2O5S1
)]\\@

9_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3748\SP\RM062X\Gen\C14H18F3N2O5S1(1-)\ROOT\21-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=6710
88640\\4SulfOxyCF3_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-2.1691518038,2.18
11031174,-0.1737462307\C,0,-0.7914325814,1.570967769,0.0723154464\C,0,
0.3176937215,2.6025303916,-0.1004481368\N,0,1.6031642402,1.9857265324,
0.1395667749\C,0,2.7344558547,2.7121655484,0.0227499145\O,0,2.75035950
45,3.9057755048,-0.2831510539\N,0,3.8825448409,1.960467313,0.286337017
7\C,0,5.1808865899,2.3860737943,0.2543056783\C,0,5.5880636399,3.707594
3063,-0.0509636564\C,0,6.1696105963,1.4119854763,0.5555713965\C,0,7.50
82433857,1.7396537581,0.547927945\C,0,7.8916919494,3.0544470563,0.2430
009639\C,0,6.934002035,4.029629163,-0.0559429495\H,0,-2.962498214,1.43
68353866,-0.0500388319\H,0,-2.2450251885,2.5864572151,-1.1897544013\H,
0,-2.3675153792,3.0020794468,0.5255081125\H,0,-0.6136143249,0.73469037
55,-0.6139739561\H,0,-0.7337567973,1.146688583,1.0815705911\H,0,0.1684
049552,3.4435220213,0.5922896477\H,0,0.2897560249,3.0279384495,-1.1139
641222\H,0,1.6289763806,0.980466249,0.4000106729\H,0,3.7488965096,0.95
29675207,0.5342245644\H,0,4.8365890126,4.4519651527,-0.2736262123\H,0,
5.8414927849,0.4035543246,0.7956826402\H,0,8.2646194442,0.9972714055,0
.7849131261\S,0,9.5787905211,3.4652187858,0.1842324503\O,0,10.37605514
74,2.5089280362,0.9433115115\O,0,9.7717732963,4.904446373,0.3184680311
\H,0,7.2541364374,5.0428225181,-0.2815557748\C,0,10.0515643956,3.12413
69591,-1.5837269553\F,0,11.3432462511,3.402493685,-1.7582007302\F,0,9.
8464110915,1.8433350087,-1.8875738541\F,0,9.3366723504,3.8798641911,-2
.416497161\O,0,1.5227077451,-0.7256611959,0.8314776774\O,0,3.763713311
2,-0.7049662198,0.9594712324\C,0,2.6372635354,-1.2679690845,1.04005655
86\C,0,2.610093782,-2.7543268697,1.4272777662\C,0,3.9822856531,-3.3670
737938,1.6782002923\H,0,2.0815083357,-3.2844038379,0.6253078595\H,0,1.
9697432366,-2.8426497278,2.3135822765\H,0,4.6113446628,-3.2838445084,0
.787291116\H,0,3.8996889837,-4.4263133404,1.9505554275\H,0,4.499604082
6,-2.8390228401,2.4844073353\\Version=ES64L-G09RevE.01\State=1-A\HF=-2
67.7284139\RMSD=4.108e-09\Dipole=0.4785322,0.1091848,-0.8485355\Quadru
pole=-28.3467033,3.8168661,24.5298371,-18.1786782,-0.2372481,4.1018176
\PG=C01 [X(C14H18F3N2O5S1)]\\@

9_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3711\FOpt\RM062X\Gen\C14H18F3N2O5S1(1-)\ROOT\19-Feb-2019\0\\
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD
,Solvent=h2o) maxdisk=3221225472\\4SulfOxyCF3_EtO.M062X_6-31pGd_opt_wa
ter\\-1,1\C,-2.1536142262,2.1967989739,-0.219191744\C,-0.7915750904,1.
5842693725,0.0911322835\C,0.3239841986,2.5980562047,-0.1178786092\N,1.
6177519853,1.9998787961,0.1806302128\C,2.7491334743,2.7128973702,0.042
9592822\O,2.7564314342,3.8993642514,-0.3281157483\N,3.9016701645,2.004
7964498,0.3515220982\C,5.2103843388,2.4393976498,0.2921658274\C,5.6084
648572,3.7483592219,-0.0511538135\C,6.1993045984,1.4788032074,0.607932
1589\C,7.5401219923,1.8017935889,0.5775178278\C,7.9108496752,3.1079109
603,0.2335411771\C,6.9548301879,4.0758307704,-0.0829947163\H,-2.955941
5239,1.4681789084,-0.069677922\H,-2.2003115821,2.5413312395,-1.2582781
071\H,-2.3535591318,3.0566161661,0.4299040379\H,-0.6154014494,0.713635

5245,-0.5525344302\H,-0.767587446,1.2269330978,1.1279888131\H,0.163077
7078,3.4701749712,0.5279908204\H,0.3150915372,2.9561484017,-1.15482272
26\H,1.6451369894,1.0162999906,0.4842302039\H,3.7736526533,1.014966001
9,0.6233401502\H,4.8715685805,4.5009081803,-0.2877931715\H,5.892860450
5,0.4729826524,0.8787714038\H,8.2899178011,1.0550320763,0.8205993498\S
,9.6001794602,3.5158023533,0.1355374296\O,10.4100799111,2.5939245372,0
.9307409919\O,9.7994575741,4.9604955464,0.2404211414\H,7.2571107697,5.
0846659192,-0.3481352023\C,10.053096286,3.1194004461,-1.6243157989\F,1
1.3345753788,3.4112765697,-1.8136950348\F,9.8552800639,1.8282726837,-1
.8623449203\F,9.3097679712,3.8388813664,-2.4568636862\O,1.4661417188,-
0.7712044435,0.9900031691\O,3.6995171248,-0.7411747236,1.0677826053\C,
2.5880801979,-1.339293,1.1444930161\C,2.5684689084,-2.8353113853,1.443
4076582\C,3.9361106029,-3.4815408907,1.6104992503\H,2.0082172176,-3.31
50179187,0.6319150889\H,1.9619721163,-2.970536261,2.3471324494\H,4.539
0143416,-3.3730845791,0.703614967\H,3.8297970596,-4.5506639588,1.81981
19658\H,4.4899511204,-3.0286862895,2.4386602473\\Version=ES64L-G09RevE
.01\State=1-A\HF=-1727.3222222\RMSD=3.503e-09\RMSF=4.698e-06\Dipole=0.
8748859,-0.051099,-1.2768538\Quadrupole=-26.9268021,4.8869258,22.03987
63,-20.2257718,-1.067181,3.1441385\PG=C01 [X(C14H18F3N2O5S1)]\\@

9.M062X_6-31pGd_opt_water

1\1\GINC-R3752\FOpt\RM062X\Gen\C11H13F3N2O3S1\ROOT\30-Oct-2018\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2684354560\\4SulfOxyCf3.M062X_6-31pGd_opt_water\\0,1
\C,-1.9975838106,1.7789303913,-0.0127286701\C,-0.610608386,1.151263683
4,-0.1041962688\C,0.4774723441,2.2028797606,0.0493724132\N,1.794425303
5,1.5849970306,-0.0507827099\C,2.9174085035,2.3162594073,0.0822768171\
O,2.8966739987,3.5343150794,0.3030423412\N,4.0931013522,1.5907393613,-
0.0484500269\C,5.4000302381,2.0427878792,0.0443302077\C,5.7584955071,3
.3777580913,0.3123992442\C,6.4105507279,1.076276379,-0.1451335991\C,7.
7449987777,1.4223041057,-0.0729218922\C,8.0792526846,2.7536305764,0.19
91308953\C,7.0980120613,3.7285375752,0.3869854927\H,-2.7785333445,1.02
03876371,-0.1196879738\H,-2.1422075045,2.5257564623,-0.8010975163\H,-2
.1395495067,2.2758914276,0.9532268312\H,-0.4905262078,0.6457302795,-1.
0702467072\H,-0.4900597744,0.3909721104,0.6771576258\H,0.3856701649,2.
7029034106,1.0203619322\H,0.3751603128,2.9694357671,-0.7278733862\H,1.
8499577573,0.5882236005,-0.2299295885\H,3.9920858528,0.5988920371,-0.2
445908711\H,5.0003113687,4.1312766154,0.4630955418\H,6.1327381882,0.04
59962874,-0.3476741677\H,8.5150201005,0.6710577701,-0.2188647192\S,9.7
600087543,3.216919327,0.2469202327\O,10.61391652,2.056993648,0.4945756
988\O,9.9418658674,4.4522209012,1.0066560192\H,7.3737280542,4.75774554
59,0.5964266491\C,10.1360187529,3.700341513,-1.5095086221\F,11.4070188
959,4.0757898479,-1.585240613\F,9.9318213922,2.6672029367,-2.317682829
4\F,9.3555844536,4.7090235543,-1.8777877806\\Version=ES64L-G09RevE.01\
State=1-A\HF=-1459.4630757\RMSD=5.273e-09\RMSF=4.772e-06\Dipole=-4.230
0964,-3.3556381,-1.2227587\Quadrupole=-4.6992877,8.7517511,-4.0524634,
14.6666191,-5.4570017,-1.2607973\PG=C01 [X(C11H13F3N2O3S1)]\\@

9.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3711\FOpt\RM062X\Gen\C11H13F3N2O3S1\ROOT\24-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=n-Pentadecane) maxdisk=2684354560\\4SulfOxyCF3.M062X_6-31pGd_opt_
Pentadecane\\0,1\C,-2.0061981748,1.796604628,-0.0304454332\C,-0.621718
0477,1.1763680691,-0.1945128989\C,0.478710936,2.1679032394,0.160307919
7\N,1.7892730321,1.5525444029,-0.0069315611\C,2.9163425288,2.320311501
3,0.0311901901\O,2.892375808,3.5389751365,0.1070602946\N,4.0938970283,
1.5785599614,-0.0565330395\C,5.4029738631,2.0383584849,0.0195387483\C,
5.7462165999,3.3812374714,0.2591372748\C,6.4211591441,1.077878913,-0.1
420554497\C,7.753555706,1.4375390886,-0.0665208313\C,8.0758973595,2.77
74729829,0.1747150546\C,7.0841567285,3.7416739645,0.3367023112\H,-2.791
5752223,1.0795316646,-0.2866553164\H,-2.1241923534,2.6699353457,-0.681
0467087\H,-2.1735285246,2.1225655364,1.0019762915\H,-0.4784882067,0.83
88122006,-1.2281631813\H,-0.5372553218,0.2899043157,0.4490753899\H,0.3
519316236,2.5283644603,1.1905405295\H,0.4340002521,3.0410553754,-0.496
7371391\H,1.8617910204,0.5625602264,0.1963535919\H,3.9960309947,0.5894
987318,-0.2535248039\H,4.9714015248,4.1239394697,0.3829240437\H,6.1557
964433,0.0389378788,-0.3201574319\H,8.5373311926,0.6950842098,-0.18190
79664\S,9.7651307182,3.2458517221,0.2568993833\O,10.5947820375,2.08499
46425,0.5472652741\O,9.9045114042,4.5027341008,0.9770787836\H,7.358246
433,4.774320031,0.5317007288\C,10.1605313093,3.6711204742,-1.511079876
1\F,11.4310896301,4.0445041947,-1.592286758\F,9.9648339614,2.611536376
,-2.292294238\F,9.3832395718,4.6655043539,-1.930053176\\Version=ES64L-
G09RevE.01\State=1-A\HF=-1459.4532732\RMSD=8.416e-09\RMSF=4.108e-06\Di

pole=-3.5098275,-2.431978,-0.4821404\Quadrupole=-2.206564,6.1733495,-3
.9667855,10.161983,-6.9527574,-1.6965976\PG=C01 [X(C11H13F3N2O3S1)]\\@

11_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R4192\FOpt\RM062X\Gen\C13H17Cl1F5N2O3S1(1-)\ROOT\19-Feb-2019\
0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(
SMD,Solvent=n-Pentadecane) maxdisk=3221225472\\3SF5Chloro_EtO.M062X_6-
31pGd_opt_Pentadecane\\-1,1\C,-2.0007278213,2.0547400527,-0.0184641843
\C,-0.5777411189,1.5036284129,-0.0175089311\C,0.4565901796,2.622678804
3,0.0004912093\N,1.7930461627,2.0645628337,0.0101892724\C,2.8705285267
,2.8778463664,-0.0169609129\O,2.791059776,4.1089514373,-0.068731981\N,
4.0752469763,2.1854206656,0.0162461772\C,5.3436963091,2.7201062622,-0.
0105694472\C,5.6282614384,4.0991899362,-0.0583440081\C,6.4148447057,1.
8014603941,0.0128704209\C,7.7175920867,2.2631913963,-0.0147698725\C,8.
037161178,3.6173415316,-0.065073255\C,6.9579158235,4.4907791174,-0.083
468746\H,-2.7390863941,1.2464590788,-0.0341565874\H,-2.1788251392,2.68
7777703,-0.8958213466\H,-2.189551707,2.662856566,0.874083281\H,-0.4134
337698,0.8770133984,-0.902405182\H,-0.4222197274,0.8546758658,0.852584
6375\H,0.3067504319,3.2608651909,0.8831722762\H,0.3305987078,3.2696317
471,-0.8782722475\H,1.9067591368,1.0370448138,0.0806751976\H,4.0392695
215,1.1428324834,0.0608155499\H,4.8152888708,4.8113638169,-0.075341947
1\H,6.1966222243,0.7371647402,0.0530018097\H,9.0654976958,3.9550267973
,-0.0867524461\S,7.3170026791,6.2697500869,-0.142071083\F,6.1789835197
,6.5598228491,-1.2470798732\F,8.4130562246,6.0927838361,-1.3220063788\
F,6.2669135599,6.6144502147,1.0328433678\Cl,9.0281356447,1.1029022099,
0.0157832015\F,7.6506502418,7.8535649445,-0.194006081\F,8.5014017263,6
.1513437952,0.956897042\O,2.0393990758,-0.7382241659,0.2252522435\O,4.
2729861932,-0.5594283899,0.1595758285\C,3.2009501684,-1.2196259076,0.2
52073488\C,3.3072339438,-2.7426956144,0.4019849841\C,4.728323248,-3.27
09255814,0.543095601\H,2.8130573098,-3.1832098412,-0.4734886044\H,2.69
32336061,-3.0266403464,1.2651120251\H,5.3333793297,-2.9975046314,-0.32
60137402\H,4.7344316523,-4.3632341883,0.6400354509\H,5.2183278025,-2.8
45168682,1.4242137914\\Version=ES64L-G09RevE.01\State=1-A\HF=-2197.945
1674\RMSD=7.563e-09\RMSF=4.809e-06\Dipole=1.0569629,0.8675614,-0.04259
7\Quadrupole=-0.9175919,-19.3140254,20.2316172,-14.1065776,0.7660678,1
.9961472\PG=C01 [X(C13H17Cl1F5N2O3S1)]\\@

11_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3711\SP\RM062X\Gen\C13H17Cl1F5N2O3S1(1-)\ROOT\27-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=6
71088640\\3SF5Chloro_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-1.6761737953,3.
0057081687,0.4889021821\C,0,-0.2421517185,2.5179465304,0.6838177214\C,
0,0.3975428859,2.0977390265,-0.641201788\N,0,1.7597502553,1.639750027,
-0.4982758092\C,0,2.7676576721,2.5357376075,-0.3825018747\O,0,2.604709
9744,3.7582540765,-0.4289795585\N,0,4.0072648525,1.9295408245,-0.21500
29589\C,0,5.2218592942,2.5547757621,-0.0591671272\C,0,5.4068287071,3.9
526632811,-0.0592890766\C,0,6.344467644,1.714855843,0.1105594448\C,0,7
.5990728357,2.2718411579,0.2731037807\C,0,7.8202562795,3.6462578638,0.
2794626753\C,0,6.6933118863,4.4402177143,0.1101819807\H,0,-2.134631804
4,3.3014851187,1.4383981651\H,0,-2.3022191544,2.221788609,0.0451018796
\H,0,-1.7047769933,3.873293755,-0.1807808727\H,0,-0.2183213818,1.66421
48751,1.3719756751\H,0,0.3737044453,3.3105073907,1.1234524744\H,0,0.37
97143786,2.9459243794,-1.3365646282\H,0,-0.1763285415,1.2782925396,-1.
0895836004\H,0,1.9401857105,0.6228191928,-0.4068594987\H,0,4.042473872
7,0.8847235573,-0.1884632855\H,0,4.5525451301,4.6024286513,-0.18973996
52\H,0,6.2010662226,0.6367914527,0.1116889923\H,0,8.8120698433,4.05905
13519,0.4092315785\S,0,6.9276468643,6.2405816729,0.1135448784\F,0,5.98
16704419,6.4616596264,-1.1730743133\F,0,8.2230827665,6.1560985224,-0.8
575452338\F,0,5.6691147665,6.497235513,1.0877856058\Cl,0,8.9778460252,
1.2121915149,0.4825340593\F,0,7.152623841,7.8449146658,0.1195530037\F,
0,7.9106945268,6.1915656365,1.4019279953\O,0,2.1649952286,-1.131101751
,-0.2614213499\O,0,4.3769913133,-0.7881653018,-0.0899131208\C,0,3.3513
986549,-1.5231502017,-0.1334190673\C,0,3.5600712161,-3.0413599158,-0.0
021865284\C,0,5.0122477793,-3.4682974714,0.1528219366\H,0,3.1220915705,
-3.4910144266,-0.9216835495\H,0,2.9419092592,-3.3893708082,0.81848525
55\H,0,5.6200114674,-3.1243128035,-0.6889416607\H,0,5.0988387029,-4.559
4207457,0.2248371801\H,0,5.4397570747,-3.0241824829,1.0564198582\\Vers
ion=ES64L-G09RevE.01\State=1-A\HF=-267.7284252\RMSD=4.146e-09\Dipole=1
.039879,1.3007982,0.3152966\Quadrupole=-1.0392127,-20.9478892,21.98710
19,-13.6962321,-2.2619466,-0.8964817\PG=C01 [X(C13H17Cl1F5N2O3S1)]\\@

11_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3717\FOpt\RM062X\Gen\C13H17Cl1F5N2O3S1(1-)\ROOT\26-Feb-2019\
0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4)
 SCRF=(SMD,Solvent=h2o) maxdisk=3221225472\\3SF5Chloro_EtO.M062X_6-31p
Gd_opt_water\\-1,1\C,-1.9278368656,2.0482007752,-0.0458299236\C,-0.507
5645326,1.4923500445,-0.0662143061\C,0.5201638479,2.606553662,0.069033
8125\N,1.8671895047,2.0540413328,0.057421992\C,2.9428769152,2.85747380
24,0.1391772537\O,2.8561745871,4.0938797178,0.2514742255\N,4.152536914
2,2.1860494863,0.1035434824\C,5.4155093464,2.7602327219,0.1673077388\C
,5.679256327,4.0939775154,-0.1808135343\C,6.478900585,1.9305799052,0.5
589164598\C,7.767592485,2.4362408947,0.6056641394\C,8.0655823833,3.757
1357763,0.2852173871\C,6.9890044299,4.5431192815,-0.101910274\H,-2.665
6840173,1.2464994717,-0.1452070942\H,-2.0839124607,2.7539212407,-0.869
3587195\H,-2.1280834386,2.5765195011,0.8929543151\H,-0.3303619902,0.94
88190788,-1.0025832075\H,-0.3726545781,0.7741271733,0.7520398448\H,0.3
567598755,3.155823012,1.0041737542\H,0.4048763406,3.3236664251,-0.7536
350156\H,1.9879783226,1.0484188492,-0.1258943603\H,4.1159516929,1.1582
717879,0.2119943111\H,4.8780137622,4.7404144141,-0.5084299154\H,6.2847
172073,0.8964452732,0.8271817355\H,9.0803172183,4.1337696993,0.3377078
131\S,7.3170445274,6.2712724046,-0.544560256\F,6.0433970227,6.81611956
37,0.2854994613\F,6.4096049495,6.1921337413,-1.8783298132\F,8.25653659
26,6.5094934748,0.7483834013\Cl,9.0686280314,1.3823952332,1.0969601019
\F,7.6126576095,7.8110648272,-0.9379481371\F,8.6225701466,5.8871123559
,-1.4154410256\O,2.0972091571,-0.7712290165,-0.5031966261\O,4.10569868
63,-0.6363452973,0.4678458234\C,3.1394908073,-1.2974245443,-0.01018863
85\C,3.2072955727,-2.8212459341,-0.004334506\C,4.4795155849,-3.4096666
268,0.5886128216\H,3.0737332523,-3.1499484724,-1.0419979739\H,2.323919
1571,-3.1774146889,0.539270497\H,4.6052473169,-3.1097104087,1.63352506
53\H,5.3640426904,-3.0794500268,0.0351881679\H,4.4469730783,-4.5032074
269,0.5526597222\\Version=ES64L-G09RevE.01\State=1-A\HF=-2197.9736801\
RMSD=5.115e-09\RMSF=1.406e-06\Dipole=1.7587518,0.8708144,0.0625184\Qua
drupole=3.8287609,-18.7698435,14.9410827,-14.1150107,-0.9558991,0.4574
511\PG=C01 [X(C13H17Cl1F5N2O3S1)]\\@

11_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3713\FOpt\RM062X\Gen\C13H17Cl1F5N2O3S1(1-)\ROOT\26-Feb-2019\
0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4)
 maxdisk=3221225472\\3SF5Chloro_EtO.M062X_6-31pGd_opt\\-1,1\C,-1.67617
37953,3.0057081687,0.4889021821\C,-0.2421517185,2.5179465304,0.6838177
214\C,0.3975428859,2.0977390265,-0.641201788\N,1.7597502553,1.63975002
7,-0.4982758092\C,2.7676576721,2.5357376075,-0.3825018747\O,2.60470997
44,3.7582540765,-0.4289795585\N,4.0072648525,1.9295408245,-0.215002958
9\C,5.2218592942,2.5547757621,-0.0591671272\C,5.4068287071,3.952663281
1,-0.0592890766\C,6.344467644,1.714855843,0.1105594448\C,7.5990728357,
2.2718411579,0.2731037807\C,7.8202562795,3.6462578638,0.2794626753\C,6
.6933118863,4.4402177143,0.1101819807\H,-2.1346318044,3.3014851187,1.4
383981651\H,-2.3022191544,2.221788609,0.0451018796\H,-1.7047769933,3.8
73293755,-0.1807808727\H,-0.2183213818,1.6642148751,1.3719756751\H,0.3
737044453,3.3105073907,1.1234524744\H,0.3797143786,2.9459243794,-1.336
5646282\H,-0.1763285415,1.2782925396,-1.0895836004\H,1.9401857105,0.62
28191928,-0.4068594987\H,4.0424738727,0.8847235573,-0.1884632855\H,4.5
525451301,4.6024286513,-0.1897399652\H,6.2010662226,0.6367914527,0.111
6889923\H,8.8120698433,4.0590513519,0.4092315785\S,6.9276468643,6.2405
816729,0.1135448784\F,5.9816704419,6.4616596264,-1.1730743133\F,8.2230
827665,6.1560985224,-0.8575452338\F,5.6691147665,6.497235513,1.0877856
058\Cl,8.9778460252,1.2121915149,0.4825340593\F,7.152623841,7.84491466
58,0.1195530037\F,7.9106945268,6.1915656365,1.4019279953\O,2.164995228
6,-1.131101751,-0.2614213499\O,4.3769913133,-0.7881653018,-0.089913120
8\C,3.3513986549,-1.5231502017,-0.1334190673\C,3.5600712161,-3.0413599
158,-0.021865284\C,5.0122477793,-3.4682974714,0.1528219366\H,3.1220915
705,-3.4910144266,-0.9216835495\H,2.9419092592,-3.3893708082,0.8148525
555\H,5.6200114674,-3.1243128035,-0.6889416607\H,5.0988387029,-4.55942
07457,0.2248371801\H,5.4397570747,-3.0241824829,1.0564198582\\Version=
ES64L-G09RevE.01\State=1-A\HF=-2197.9082652\RMSD=8.001e-09\RMSF=3.999e
-06\Dipole=1.0371109,1.3287006,0.3130705\Quadrupole=-0.9374839,-21.206
9143,22.1443981,-13.7648135,-2.2631529,-0.8915638\PG=C01 [X(C13H17Cl1F
5N2O3S1)]\\@

11.M062X_6-31pGd_opt

1\1\GINC-R3751\FOpt\RM062X\Gen\C10H12Cl1F5N2O1S1\ROOT\31-Oct-2018\0\\#
 M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26
84354560\\3SF55Chloro.M062X_6-31pGd_opt\\0,1\C,-1.8313614645,1.5664542
783,0.1428751125\C,-0.4028537498,1.0268055488,0.1286769734\C,0.6143487

873,2.1473274355,-0.042876205\N,1.9706831447,1.6107368696,-0.045657926
8\C,3.027619147,2.4831739217,0.0300145314\O,2.8914250719,3.6775959876,
0.2228544977\N,4.2668560775,1.8598484081,-0.1029688818\C,5.5241371208,
2.469933185,-0.0615582737\C,5.7055606952,3.8594474363,-0.0974141921\C,
6.6423085702,1.6277691458,-0.0070858381\C,7.919325697,2.1681053241,0.0
101822777\C,8.1346329797,3.5409016127,-0.0232017179\C,7.0046058648,4.3
453330402,-0.0768418135\H,-2.5572109911,0.758217505,0.2667817414\H,-2.
0648815813,2.2879160649,-0.7913844228\H,-1.9728520603,2.2746254262,0.9
659860407\H,-0.293371117,0.3014179341,-0.689652227\H,-0.1896963532,0.4
912770949,1.0613734188\H,0.5469220844,2.8590979363,0.7842412601\H,0.41
8112631,2.7084079686,-0.9674188508\H,2.1066143735,0.7409941318,-0.5463
3904\H,4.2755319665,0.8496892866,-0.052122342\H,4.8518674269,4.5211144
854,-0.12990053\H,6.5203752268,0.5487038092,0.0214740744\H,9.136705718
1,3.950934494,-0.0070436455\S,7.2408031133,6.1477680661,-0.1248846485\
F,6.1664904541,6.3244667561,-1.3123427275\F,8.4242111064,6.0251248554,
-1.2167205251\F,6.0819229495,6.3991032202,0.9630859962\Cl,9.2867865143
,1.0953068718,0.078791491\F,7.456737613,7.7380021819,-0.1694435944\F,8
.3393129835,6.0980797175,1.056871987\\Version=ES64L-G09RevE.01\State=1
-A\HF=-1930.0962802\RMSD=9.203e-09\RMSF=4.360e-06\Dipole=-1.5333625,-2
.7430307,-0.3073349\Quadrupole=5.4712852,0.3739384,-5.8452236,8.104772
8,2.1052901,1.5223336\PG=C01 [X(C10H12Cl1F5N2O1S1)]\\@

11.M062X_6-31pGd_opt_water
1\1\GINC-R4423\FOpt\RM062X\Gen\C10H12Cl1F5N2O1S1\ROOT\30-Oct-2018\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,
Solvent=h2o) maxdisk=2684354560\\3SF55Chloro.M062X_6-31pGd_opt_water\\
0,1\C,-1.8209571608,1.5055211498,-0.0992953652\C,-0.3995589595,1.04436
21793,0.2063773557\C,0.606014931,2.1496847962,-0.0771310243\N,1.961462
4612,1.6884196919,0.2024038999\C,3.0185763471,2.5088997088,0.028973772
9\O,2.8916091967,3.7087202509,-0.2537421753\N,4.2521337789,1.907346418
,0.2071879382\C,5.5050587443,2.4973184623,0.0498424836\C,5.7153209616,
3.8822862059,0.0851691998\C,6.5997773549,1.6360907774,-0.1142414887\C,
7.8749639778,2.1607759862,-0.2454140831\C,8.1236743225,3.5297626936,-0
.2310856434\C,7.0144913939,4.3462112952,-0.0636217646\H,-2.5439992052,
0.7113806652,0.108786736\H,-1.9229848253,1.7873223216,-1.1530509514\H,
-2.0898674162,2.3753204489,0.5101639044\H,-0.1522667826,0.1655054662,-
0.4020959357\H,-0.3194097412,0.7437909335,1.2579469961\H,0.3924781311,
3.0225872754,0.5486916906\H,0.5318213906,2.4682432945,-1.1245702312\H,
2.1135650714,0.6923821486,0.3235944207\H,4.2590372376,0.8970042592,0.3
117395539\H,4.8857809958,4.5585884683,0.2312829502\H,6.4434189923,0.56
15502583,-0.1394139578\H,9.1289516275,3.9188695642,-0.3432799326\S,7.2
777563561,6.1406040159,-0.0252276541\F,6.0194245873,6.4312004182,-0.99
38085171\F,8.2548704217,6.106204752,-1.310949719\F,6.3260634874,6.3371
782545,1.2642476428\Cl,9.2186475731,1.0681259335,-0.4463806734\F,7.514
4914119,7.7388211916,0.0086959447\F,8.5613233373,6.0136007148,0.946594
6275\\Version=ES64L-G09RevE.01\State=1-A\HF=-1930.1146211\RMSD=4.435e-
09\RMSF=5.702e-06\Dipole=-1.752688,-4.3353976,0.4212078\Quadrupole=4.2
952473,3.555779,-7.8510263,12.8889754,-2.1346836,-1.286257\PG=C01 [X(C
10H12Cl1F5N2O1S1)]\\@

11.M062X_6-31pGd_opt_Pentadecane
1\1\GINC-R3837\FOpt\RM062X\Gen\C10H12Cl1F5N2O1S1\ROOT\25-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,
Solvent=n-Pentadecane) maxdisk=2684354560\\3SF5Chloro.M062X_6-31pGd_op
t_Pentadecane\\0,1\C,-1.8271176415,1.4827347266,0.2250737577\C,-0.3855
654414,0.9928465089,0.1226568927\C,0.5927707093,2.1562685433,0.0267810
342\N,1.9613089639,1.6635620592,-0.0660621052\C,3.0103398772,2.5202882
677,0.0998044136\O,2.874409734,3.6873764646,0.4350774417\N,4.249958207
7,1.9273764957,-0.1223073878\C,5.5057834532,2.5255137023,-0.0239797166
\C,5.6940735211,3.9023740712,0.1647861543\C,6.6233429317,1.686521851,-
0.1410097268\C,7.900900131,2.2186869987,-0.0699409055\C,8.1251840699,3
.57802615,0.1179097783\C,6.9958495822,4.3771912349,0.2289079849\H,-2.5
245638047,0.6426921321,0.293191744\H,-2.1052268722,2.079322073,-0.6506
549494\H,-1.9666826568,2.107325922,1.1141032004\H,-0.2774345584,0.3497
318236,-0.7616606173\H,-0.1299829002,0.3829414357,0.9975468359\H,0.526
8991885,2.7864209257,0.9179784807\H,0.3515468687,2.7892126552,-0.83855
0604\H,2.1075751207,0.8061894923,-0.5856293703\H,4.25901353,0.92418030
88,-0.2606515243\H,4.8419990261,4.5597010312,0.2619194193\H,6.49251323
2,0.6179686411,-0.2870060591\H,9.1305473538,3.9775456475,0.1730789822\
S,7.2352306623,6.1626945073,0.4724836256\F,6.1341404996,6.5379703197,-
0.6434855021\F,8.3933297862,6.2311132792,-0.6517187468\F,6.1030478166,
6.2366124055,1.6157213461\Cl,9.2680044438,1.1492306624,-0.217861096\F,
7.4536680111,7.7431318058,0.6863104171\F,8.3619071544,5.928047858,1.60

55968024\\Version=ES64L-G09RevE.01\State=1-A\HF=-1930.1117592\RMSD=5.5
38e-09\RMSF=8.118e-06\Dipole=-1.7052442,-3.1634647,-0.7428637\Quadrupo
le=5.2924756,0.5750414,-5.867517,9.1590116,3.0288367,2.3655916\PG=C01
[X(C10H12Cl1F5N2O1S1)]\\@

10_propanoate.M062X_6-31pGd_opt
1\1\GINC-R3748\FOpt\RM062X\Gen\C15H17F6N2O3(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=322
1225472\\34TFM_EtO.M062X_6-31pGd_opt\\-1,1\C,-2.115626308,2.2467108197
,-0.1609901682\C,-0.7436330215,1.5776695724,-0.1295830364\C,0.38230404
52,2.6052292183,-0.1027365064\N,1.6601082849,1.9306952932,-0.065887376
6\C,2.806637287,2.6446484885,-0.103668245\O,2.8408385502,3.8746441065,
-0.1825970944\N,3.9415455951,1.839063313,-0.0460292419\C,5.2527542123,
2.2428020351,-0.0662482607\C,5.6797645228,3.5844988077,-0.1608160077\C
,6.2338751253,1.2344830476,0.0100724768\C,7.5781588724,1.5599288149,-0
.0014495194\C,8.0119139475,2.885867081,-0.0880511722\C,7.0345116116,3.
8926318579,-0.1755739257\H,-2.9206919767,1.5049481871,-0.1826638823\H,
-2.2231044295,2.8845986926,-1.046386838\H,-2.2660706751,2.878890741,0.
7221787954\H,-0.6138615214,0.928227405,-1.0034375384\H,-0.6551139245,0
.9235998987,0.7458311711\H,0.2743157221,3.2646094495,0.7715013695\H,0.
3297691154,3.2544043553,-0.987985396\H,1.674140393,0.897025393,0.02229
98882\H,3.7990823886,0.8072042907,0.0236031047\H,4.9351358259,4.365493
9954,-0.226505096\H,5.910060611,0.1988433226,0.0806685707\H,8.31404658
1,0.7656692001,0.0632688937\C,7.3960419363,5.3573770745,-0.2504751016\
C,9.4900790457,3.1434151854,-0.1228156627\F,9.8675380083,4.19143097,0.
6332191797\F,9.9605627264,3.3796437994,-1.3676385357\F,10.1892516474,2
.0804605854,0.3334581496\F,6.3715812499,6.1133585499,-0.679352456\F,8.
420088565,5.5934900997,-1.0930992724\F,7.7559725182,5.8576043348,0.949
4268139\O,1.5731967979,-0.8670617728,0.1731589743\O,3.8179566527,-0.91
39494671,0.1484023631\C,2.6815513917,-1.4588018057,0.2061050507\C,2.63
14824686,-2.990153343,0.3277187498\C,3.9966339135,-3.6653472632,0.3723
14899\H,2.0360948056,-3.359155989,-0.5166284924\H,2.0468318187,-3.2214
422842,1.2266727333\H,4.5697144439,-3.4374301211,-0.5310593247\H,3.898
1860378,-4.7543864825,0.4590838941\H,4.5809551377,-3.2990794569,1.2214
130733\\Version=ES64L-G09RevE.01\State=1-A\HF=-1515.728782\RMSD=4.754e
-09\RMSF=4.216e-06\Dipole=0.8450125,0.3313186,-0.040794\Quadrupole=-15
.1982587,-7.7842424,22.9825011,-18.5954096,1.3835206,2.0135448\PG=C01
[X(C15H17F6N2O3)]\\@

10_propanoate.M062X_6-31pGd_opt_Pentadecane
1\1\GINC-R3752\FOpt\RM062X\Gen\C15H17F6N2O3(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=n-Pentadecane) maxdisk=3221225472\\34TFM_EtO.M062X_6-31pGd_opt_
Pentadecane\\-1,1\C,-2.1222600899,2.2779405546,-0.1186410834\C,-0.7581
574984,1.5948656651,-0.0903071803\C,0.3778716268,2.6092795842,-0.13910
91653\N,1.6550927951,1.9267628281,-0.1101595282\C,2.8045186785,2.63461
91196,-0.1391172876\O,2.8406521288,3.867066422,-0.1970451368\N,3.93917
72565,1.8308256174,-0.0975532538\C,5.252444446,2.2372973679,-0.1032681
844\C,5.6775768079,3.5805804638,-0.1655261995\C,6.2348302204,1.2302074
865,-0.044765047\C,7.5793673637,1.5557434718,-0.039675948\C,8.00956632
96,2.8840980376,-0.0916666407\C,7.0318448342,3.8910368793,-0.163959904
2\H,-2.9339046845,1.5439160064,-0.0835029106\H,-2.2483191809,2.8722924
751,-1.0313705709\H,-2.2446364148,2.9527213692,0.7368746733\H,-0.66018
46446,0.9053722639,-0.9374027685\H,-0.6564869043,0.9857707562,0.815806
6228\H,0.3038179496,3.3018321853,0.7109493076\H,0.300623837,3.22097938
34,-1.0487169059\H,1.6660647405,0.8920133973,-0.0549518935\H,3.7987718
158,0.7982173898,-0.0404922023\H,4.93462126,4.3636840651,-0.2178474197
\H,5.9167299009,0.1918388136,0.0007763743\H,8.3142566862,0.7594221322,
0.0107526148\C,7.3904171298,5.3577696243,-0.204758801\C,9.4871260442,3
.1483588814,-0.1024331951\F,9.8482328005,4.1794137898,0.6851807493\F,9
.9708037203,3.4215345027,-1.3346017973\F,10.1859703103,2.0794335762,0.
3340222744\F,6.3691800394,6.1196636707,-0.6302872664\F,8.4234139219,5.
6137276657,-1.0301967921\F,7.7351486835,5.8355891767,1.0085877813\O,1.
5828934347,-0.8941229238,0.0639718051\O,3.8248545887,-0.9240262527,0.0
890713893\C,2.6930798398,-1.4798047235,0.1457531708\C,2.6497938102,-3.
0020272653,0.3353254395\C,4.0125227014,-3.6762900506,0.4164436936\H,2.
0581095635,-3.4133802676,-0.4917470254\H,2.0648534767,-3.1934952201,1.
2435898147\H,4.5884909859,-3.5068569405,-0.4983231472\H,3.907210532,-4
.7581974707,0.5611894595\H,4.598599157,-3.2732935082,1.2478620845\\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-1515.7662467\RMSD=5.598e-09\RMSF=3
.957e-06\Dipole=0.8573368,0.2429803,0.0339491\Quadrupole=-13.4226217,-

7.9792569,21.4018786,-19.1693258,0.6153463,1.2848488\\PG=C01 [X(C15H17F
6N2O3)]\\@

10_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3732\FOpt\RM062X\Gen\C15H17F6N2O3(1-)\ROOT\19-Feb-2019\0\\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent=h2o) maxdisk=3221225472\\34TFM_EtO.M062X_6-31pGd_opt_water\\-1,
1\C,-2.0631831615,2.2129757523,-0.2372989322\C,-0.699120058,1.54854777
09,-0.081439893\C,0.427384851,2.5441282561,-0.3178576492\N,1.718791578
4,1.8867323518,-0.176327777\C,2.8633972521,2.5815875117,-0.3117374186\
O,2.8878893041,3.7924920114,-0.5965486342\N,4.0056811611,1.8231168508,
-0.1255917094\C,5.3207064376,2.2605198773,-0.1302485281\C,5.7058877234
,3.6115795139,-0.093721777\C,6.3233414463,1.2790614327,-0.1399810789\C
,7.6616431476,1.6340954401,-0.1082805688\C,8.0521595638,2.9732691671,-
0.0692976295\C,7.0516323682,3.9580266632,-0.0718594644\H,-2.8718905081
,1.4964508541,-0.0652696987\H,-2.1856134024,2.624332508,-1.2454227047\
H,-2.182626673,3.3041735913,0.4782176256\H,-0.6019986268,0.716990086,-
0.7903983353\H,-0.601303783,1.1245223086,0.9256161731\H,0.3498004981,3
.3731887803,0.3971927909\H,0.3441261063,2.973607534,-1.3234218842\H,1.
7439582482,0.9225891892,0.1824122094\H,3.8751866553,0.7991897421,-0.06
24430105\H,4.9522046904,4.3845706088,-0.0780731909\H,6.0433669357,0.22
97720635,-0.1686225294\H,8.4139306315,0.8529348231,-0.114259046\C,7.36
83294219,5.4337339651,-0.0079722655\C,9.5239398142,3.278886178,-0.0541
357193\F,9.8464475768,4.2670647964,0.8028757081\F,9.9961784573,3.65187
74002,-1.2663705748\F,10.2502115254,2.2077786551,0.3129284415\F,6.3267
630388,6.1922806525,-0.3870996717\F,8.3967968118,5.7756595985,-0.80537
04597\F,7.6911829975,5.8329052324,1.2387178167\O,1.6968504498,-0.80186
78249,0.8823314713\O,3.7122737671,-1.0108334496,-0.0599154123\C,2.6709
250723,-1.4983268502,0.4665192693\C,2.5522785097,-3.0112638263,0.62418
96682\C,3.7284041584,-3.8163794448,0.0901793304\H,1.6204317171,-3.3102
146735,0.1295119301\H,2.4009541942,-3.2077241285,1.6925719447\H,3.8717
928209,-3.6453021583,-0.981240671\H,3.5573942757,-4.8868747156,0.24147
46107\H,4.6580730049,-3.5474790946,0.6011972441\\Version=ES64L-G09RevE
.01\State=1-A\HF=-1515.7958967\RMSD=9.974e-09\RMSF=2.153e-06\Dipole=1.
3219898,0.006714,-0.069757\Quadrupole=-8.8721171,-6.8185429,15.69066,-
19.6744475,3.3789945,4.1855952\PG=C01 [X(C15H17F6N2O3)]\\@

10_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R4186\SP\RM062X\Gen\C15H17F6N2O3(1-)\ROOT\21-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671088
640\\34TFM_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-2.115626308,2.2467108197,
-0.1609901682\C,0,-0.7436330215,1.5776695724,-0.1295830364\C,0,0.38230
40452,2.6052292183,-0.1027365064\N,0,1.6601082849,1.9306952932,-0.0658
873766\C,0,2.806637287,2.6446484885,-0.103668245\O,0,2.8408385502,3.87
46441065,-0.1825970944\N,0,3.9415455951,1.839063313,-0.0460292419\C,0,
5.2527542123,2.2428020351,-0.0662482607\C,0,5.6797645228,3.5844988077,
-0.1608160077\C,0,6.2338751253,1.2344830476,0.0100724768\C,0,7.5781588
724,1.5599288149,-0.0014495194\C,0,8.0119139475,2.885867081,-0.0880511
722\C,0,7.0345116116,3.8926318579,-0.1755739257\H,0,-2.9206919767,1.50
49481871,-0.1826638823\H,0,-2.2231044295,2.8845986926,-1.046376838\H,0
,-2.2660706751,2.878890741,0.7221787954\H,0,-0.6138615214,0.928227405,
-1.0034375384\H,0,-0.6551139245,0.9235998987,0.7458311711\H,0,0.274315
7221,3.2646094495,0.7715013695\H,0,0.3297691154,3.2544043553,-0.987985
396\H,0,1.674140393,0.897025393,0.0222998882\H,0,3.7990823886,0.807204
2907,0.0236031047\H,0,4.9351358259,4.3654939954,-0.226505096\H,0,5.910
060611,0.1988433226,0.0806685707\H,0,8.314046581,0.7656692001,0.063268
8937\C,0,7.3960419363,5.3573770745,-0.2504751016\C,0,9.4900790457,3.14
34151854,-0.1228156627\F,0,9.8675380083,4.19143097,0.6332191797\F,0,9.
9605627264,3.3796637994,-1.3676385357\F,0,10.1892516474,2.0804605854,0
.3334581496\F,0,6.3715812499,6.1133585499,-0.679352456\F,0,8.420088565
,5.5934900997,-1.0930992724\F,0,7.7559725182,5.8576043348,0.9494268139
\O,0,1.5731967979,-0.8670617728,0.1731589743\O,0,3.8179566527,-0.91394
94671,0.1484023631\C,0,2.6815513917,-1.4588018057,0.2061050507\C,0,2.6
314824686,-2.990153343,0.3277187498\C,0,3.9966339135,-3.6653472632,0.3
72314899\H,0,2.0360948056,-3.359155989,-0.5166284924\H,0,2.0468318187,
-3.2214422842,1.2266727333\H,0,4.5697144439,-3.4374301211,-0.531059324
7\H,0,3.8981860378,-4.7543864825,0.4590838941\H,0,4.5809551377,-3.2990
794569,1.2214130733\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.728465
2\RMSD=4.029e-09\Dipole=0.8442586,0.3021579,-0.0384135\Quadrupole=-15.
2661765,-7.5841433,22.8503198,-18.4516722,1.3745749,1.9879571\PG=C01 [
X(C15H17F6N2O3)]\\@

10.M062X_6-31pGd_opt

1\1\GINC-R3925\FOpt\RM062X\Gen\C12H12F6N2O1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354
560\\34TFM.M062X_6-31pGd_opt\\0,1\C,-1.9142136395,1.8711942098,-0.0275
844978\C,-0.5417488004,1.216731799,0.1131114462\C,0.5809773684,2.21545
97893,-0.1356781701\N,1.8804491043,1.5683066565,0.0039888146\C,3.00978
28851,2.3477908737,0.041503696\O,2.9775159911,3.5638645288,0.087170474
\N,4.1893512042,1.6052101934,0.0563023624\C,5.4969805011,2.0935978519,
0.0825155847\C,5.8212567678,3.4442076695,-0.1110518889\C,6.5300867167,
1.1733125295,0.2863752566\C,7.8522954474,1.5892683813,0.3019080976\C,8
.1867817461,2.9288560103,0.1161105135\C,7.1510078933,3.850738753,-0.09
83903419\H,-2.7155744354,1.1498014753,0.1538387042\H,-2.0534246679,2.2
82487243,-1.0329565964\H,-2.0313685835,2.6910431882,0.6887605946\H,-0.
4584587075,0.3841326756,-0.5994702719\H,-0.4243313885,0.7912777056,1.1
167790788\H,0.5419403555,3.0293300585,0.59322875\H,0.4795579367,2.6696
572443,-1.131483024\H,1.9588769189,0.6355686214,-0.382533685\H,4.09837
32928,0.6111740735,0.2206890705\H,5.0338426688,4.1675364793,-0.2666320
837\H,6.2991949496,0.1215039288,0.4363196711\H,8.6382140384,0.86134785
8,0.4683179924\C,7.4095718742,5.3323001891,-0.2904360365\C,9.651524078
9,3.2964436152,0.1252015534\F,9.8967178293,4.4236407267,0.8063022357\F
,10.1438679761,3.4582195932,-1.1148004293\F,10.3872557431,2.3260308127
,0.7015603525\F,6.3498709059,5.9499580785,-0.835089734\F,8.4525225566,
5.5612473923,-1.1011368576\F,7.6588154723,5.9476777947,0.8764893682\\V
ersion=ES64L-G09RevE.01\State=1-A\HF=-1247.9178435\RMSD=7.521e-09\RMSF
=4.946e-06\Dipole=-2.2138725,-2.8311815,-0.0711439\Quadrupole=1.094665
8,3.8342639,-4.9289297,5.3666069,2.0775385,0.1281928\PG=C01 [X(C12H12F
6N2O1)]\\@

10.M062X_6-31pGd_opt_water

1\1\GINC-R3724\FOpt\RM062X\Gen\C12H12F6N2O1\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2684354560\\34TFM.M062X_6-31pGd_opt_water\\0,1\C,-1.91
64674437,1.8389407388,-0.028454318\C,-0.5315246213,1.2079429317,0.0708
834571\C,0.559553151,2.2636376158,-0.0204958431\N,1.8743572729,1.63943
37213,0.064468453\C,3.0006999857,2.3785808433,0.0230195177\O,2.9806994
912,3.6156699054,-0.0539617999\N,4.1739849385,1.6461560428,0.079727023
1\C,5.4824181469,2.1197701026,0.0836385362\C,5.8337568497,3.4533587525
,-0.1770356434\C,6.5006470703,1.1925949115,0.3415585774\C,7.8282736645
,1.5876625998,0.3532928955\C,8.1867643983,2.9135530543,0.1102352973\C,
7.1693048376,3.8393506887,-0.1657997277\H,-2.6993126372,1.0779492332,0
.0408047274\H,-2.0397641319,2.3643610142,-0.9818238528\H,-2.0761748699
,2.5621607122,0.7788014659\H,-0.3943868466,0.4761575421,-0.7347908\H,-
0.4319176263,0.6675770258,1.0201041847\H,0.4518192078,2.9895637076,0.7
933282054\H,0.4755306871,2.8128360689,-0.9660361181\H,1.9296848836,0.6
270407672,0.0925526458\H,4.0796450368,0.6427678163,0.2084205123\H,5.06
57666153,4.1807338227,-0.3928782925\H,6.2459259521,0.1551104155,0.5383
997047\H,8.5954978787,0.8499616229,0.5610050992\C,7.4529799749,5.29921
53949,-0.4346264798\C,9.6501402263,3.2617742499,0.1246090455\F,9.90482
99676,4.4322557116,0.7393887998\F,10.1760764169,3.3555498026,-1.114996
0047\F,10.3756065196,2.3297324503,0.7674839835\F,6.4164731532,5.913569
6542,-1.027179149\F,8.5141141855,5.4770892135,-1.2418237021\F,7.702507
6646,5.9868418657,0.6974095993\\Version=ES64L-G09RevE.01\State=1-A\HF=
-1247.937026\RMSD=4.094e-09\RMSF=5.886e-06\Dipole=-2.7981014,-4.472614
5,0.4009785\Quadrupole=-0.3475347,6.8620942,-6.5145595,9.765534,0.2654
655,-1.7842593\PG=C01 [X(C12H12F6N2O1)]\\@

10.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3916\FOpt\RM062X\Gen\C12H12F6N2O1\ROOT\22-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=n-Pentadecane) maxdisk=2684354560\\34TFM.M062X_6-31pGd_opt_Pentadec
ane\\0,1\C,-2.0644881492,2.3504320902,-0.3736343798\C,-0.702718932,1.6
651726143,-0.3078551894\C,0.4208514033,2.6753945098,-0.1159946016\N,1.
7087034757,1.9966069873,-0.0499845609\C,2.8669417045,2.7114786492,-0.1
509803183\O,2.8942815382,3.9050277239,-0.4104001957\N,4.0124812513,1.9
430103132,0.0412014719\C,5.3382233789,2.3689408171,0.0107818155\C,5.71
98095318,3.7166374432,-0.0805022374\C,6.3360931197,1.3909215036,0.0974
454906\C,7.6756541253,1.7451343776,0.0854111419\C,8.0659777333,3.07945
10267,-0.0129770581\C,7.0664495257,4.0618392755,-0.0863217508\H,-2.866
6808282,1.6198331316,-0.5131392503\H,-2.1073662051,3.058874217,-1.2080
60384\H,-2.2727943312,2.9050899814,0.5478575446\H,-0.5190235151,1.0978
504887,-1.2282270148\H,-0.6936297053,0.9450956608,0.521999145\H,0.2509
4551,3.2687377721,0.7933059586\H,0.4563949479,3.3734750935,-0.95681412
36\H,1.7282962182,1.0943409301,0.4101791911\H,3.8841703543,0.941052654

5,0.1203404551\H,4.9619384949,4.4837389565,-0.1467269093\H,6.061736401
8,0.3418273526,0.1719674031\H,8.4302293749,0.9689103575,0.1480831018\C
,7.3881163841,5.5365257063,-0.2100043133\C,9.5424918314,3.3849470597,-
0.0001150943\F,9.8872014965,4.3254094728,-0.8931617671\F,10.2685633957
,2.2896165022,-0.2953945365\F,9.9717170981,3.8057971182,1.2045878185\F
,6.3326976723,6.3037969474,0.1043827342\F,7.7444454761,5.8699058848,-1
.4629540695\F,8.3903912221,5.9074073809,0.602594483\\Version=ES64L-G09
RevE.01\State=1-A\HF=-1247.9328083\RMSD=8.143e-09\RMSF=2.368e-06\Dipol
e=-2.6360796,-3.1758481,0.5356929\Quadrupole=1.2908284,4.0961858,-5.38
70142,6.1196178,-2.6549127,-1.6915967\PG=C01 [X(C12H12F6N2O1)]\\@

6.M062X.opt

1\1\GINC-R4416\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\12-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
 maxdisk=2147483648\\aryl_urea_Cl_CF3.M062X.opt\\0,1\C,-4.2219699984,3
.0921246846,-0.7877862884\C,-4.0860658285,1.7210908982,-0.594821155\C,
-2.9206125605,1.1692311931,-0.0883323545\C,-1.8376349534,1.9975987313,
0.2435210443\C,-1.9485226508,3.380033916,0.0595955416\C,-3.1375662396,
3.893914998,-0.4526744958\H,-5.1379710026,3.5111662118,-1.1866389109\N
,-0.6844809784,1.3686914757,0.7256437899\C,0.4525478734,1.9801669072,1
.2448969887\N,1.422212427,1.0856900858,1.6291910956\O,0.5725351375,3.1
850372104,1.3755688755\C,2.7152587543,1.5963802709,2.0691798224\C,3.54
47831769,0.4820712492,2.6937989154\C,4.9045272736,0.9933818727,3.16447
3032\H,-2.8538695307,0.0929563222,0.0451160945\H,-1.1262277945,4.03440
2607,0.3163437809\H,-0.7540370686,0.3660221024,0.8384310167\H,1.430764
4765,0.1757216212,1.1847624924\H,2.5224912071,2.3882236922,2.797877339
2\H,3.2569741948,2.0559763393,1.2302380227\H,3.6903518926,-0.323801297
7,1.960787145\H,2.9881053282,0.0520780117,3.5348303083\H,5.4797650977,
1.408345654,2.3300298723\H,5.4950635542,0.1894626435,3.6122965998\H,4.
7867363757,1.7821757665,3.91481177\Cl,-5.4108235508,0.6667124053,-1.00
11954293\C,-3.2363338903,5.3887637593,-0.6121811063\F,-3.2919853725,6.
0093421806,0.5799395755\F,-4.3306088736,5.7558521014,-1.2989301101\F,-
2.1715687763,5.8909663863,-1.2597732725\\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-1370.5372523\RMSD=3.304e-09\RMSF=3.794e-06\Dipole=1.2919467,
-2.3044984,0.3422649\Quadrupole=4.2697816,-0.6453867,-3.6243949,-6.920
8459,2.1221183,-1.89227\PG=C01 [X(C11H12Cl1F3N2O1)]\\@

6_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R4179\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=n-Pentadecane) maxdisk=2684354560\\6_C2_EtO.M062X_6-31pGd_
opt_Pentadecane\\-1,1\C,-4.1088128341,3.7521201998,-0.8065102751\C,-2.
9371813792,4.4713152852,-0.6099526629\C,-1.7499869511,3.8971433399,-0.
1785204038\C,-1.716819042,2.51290352,0.0819374588\C,-2.8932703911,1.75
98955667,-0.1078930009\C,-4.0526070838,2.3834147156,-0.5443431913\H,-5
.0170533679,4.2344181933,-1.1464563253\N,-6.0038678283,1.8266358714,0.
5209924956\C,0.6639548164,2.3410613079,0.7529494993\N,1.5380124938,1.4
138244049,1.2053389746\O,0.9708405802,3.5229334538,0.564945662\C,2.906
7613106,1.7830537133,1.5008955908\C,3.6775630796,0.5741110335,2.017843
756\C,5.1290199891,0.9268206247,2.3300485901\H,-0.8586437467,4.4931023
739,-0.0403411735\H,-2.8723117978,0.6906269826,0.0935442668\H,-0.75413
11917,0.8065881447,0.6883900413\H,1.234961953,0.4392754573,1.378053781
8\H,2.9254224136,2.5894947575,2.2474732118\H,3.3908374731,2.181124578,
0.5979913367\H,3.6341733933,-0.2272683152,1.2705997853\H,3.1794079914,
0.1862684602,2.914416914\H,5.6477377229,1.2929574827,1.4361379788\H,5.
6782741638,0.0555009832,2.7014438023\H,5.1896780351,1.7108393202,3.094
151055\Cl,-2.9606722146,6.19855636,-0.920691589\C,-5.2778837657,1.5354
618796,-0.7290732985\F,-5.0734242629,0.52371921,-1.5959977997\F,-6.329
0636102,2.2365292507,-1.1985221847\F,-5.6831333075,0.9639482319,0.4232
493331\O,-1.2555620837,-0.8223785794,0.9013785627\O,0.7820217575,-1.26
53321823,1.7253606756\C,-0.3933807376,-1.5863021402,1.4223375832\C,-0.
8499956574,-3.0258814546,1.692447175\C,0.1843599907,-3.9009600679,2.38
67218057\H,-1.1398277288,-3.456455613,0.7253695801\H,-1.774037465,-2.9
664954063,2.2798870116\H,1.0987266328,-3.9735700159,1.7905202851\H,-0.
2033052158,-4.9136812781,2.5501797976\H,0.464477866,-3.4795796493,3.35
70658941\\Version=ES64L-G09RevE.01\State=1-A\HF=-1638.3841989\RMSD=3.3
53e-09\RMSF=4.997e-06\Dipole=-0.4575775,0.3758011,-0.1540784\Quadrupol
e=-3.8130731,-9.589749,13.4028221,1.9372823,-6.4793621,6.7088\PG=C01 [
X(C14H17Cl1F3N2O3)]\\@

6.M062X.SMD.pentadecane.opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\24-Feb-2019\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,So

lvent=n-Pentadecane) maxdisk=2147483648\\CLCF3.M062X_6-31pGd_opt_Penta
decane\\0,1\C,-4.2248035516,3.0770211789,-0.8007878367\C,-4.0576664151
,1.7049394179,-0.6404627554\C,-2.8886108892,1.1629023126,-0.1339543407
\C,-1.8262093471,2.0052141626,0.2340536745\C,-1.9679519445,3.389538331
8,0.084949095\C,-3.1620267474,3.89094746,-0.4289811217\H,-5.1461816331
,3.48568644,-1.1984752186\N,-0.672182937,1.3879950111,0.7204264435\C,0
.4689597753,2.0023548255,1.223617213\N,1.4396173402,1.1192348047,1.604
489232\O,0.5865846468,3.2131524922,1.3401458673\C,2.7395575146,1.60719
46605,2.0461792858\C,3.525940995,0.4897551971,2.7195287185\C,4.8945706
399,0.9742068214,3.1891987961\H,-2.7979400874,0.0858198213,-0.02403369
67\H,-1.1641717497,4.0558520539,0.3687192633\H,-0.7158494842,0.3779468
527,0.7853946433\H,1.4063953175,0.1734720029,1.2429475001\H,2.56466942
49,2.4281125039,2.7468845943\H,3.3068639072,2.0175698404,1.1989237457\
H,3.6534099537,-0.3445497673,2.0160647029\H,2.9466776264,0.1083522506,
3.569009624\H,5.4949641379,1.338607679,2.3483714127\H,5.4526850236,0.1
68053612,3.6744243989\H,4.7946924763,1.7935248707,3.9094479103\Cl,-5.3
58200335,0.6330113385,-1.0901403813\C,-3.2736897521,5.3848359088,-0.57
472731\F,-3.1360984622,6.0134669912,0.6073520945\F,-4.4552421773,5.765
9920806,-1.0870115258\F,-2.3168732664,5.8795688446,-1.3825540287\\Vers
ion=ES64L-G09RevE.01\State=1-A\HF=-1370.5534268\RMSD=5.050e-09\RMSF=9.
538e-06\Dipole=1.4252726,-2.6780452,0.4142071\Quadrupole=4.0885826,-0.
2581712,-3.8304114,-8.056063,2.2292295,-2.2947411\PG=C01 [X(C11H12Cl1F
3N2O1)]\\@

6_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3829\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=
2684354560\\6_C2_EtO.M062X_6-31pGd_opt\\-1,1\C,-4.0705611683,3.70750
68963,-0.9362405015\C,-2.874743224,4.4011244627,-0.8517935115\C,-1.699
1683193,3.8425963406,-0.3628459648\C,-1.7124383455,2.5039878164,0.0694
457618\C,-2.9205458749,1.7713489247,-0.0071420257\C,-4.0612413986,2.37
80798524,-0.5006207207\H,-4.9703568883,4.1741258591,-1.3215777002\N,-0
.620146224,1.8341929139,0.5724037606\C,0.6655779731,2.3318720221,0.741
8181782\N,1.5148009843,1.4139667503,1.2625785077\O,1.000098775,3.48557
20857,0.4599460768\C,2.9149047475,1.7272625702,1.43302161\C,3.57640993
69,0.6840563425,2.3275485202\C,5.0705786774,0.9505256042,2.4950019659\
H,-0.7841650184,4.416403236,-0.3106292918\H,-2.9262232332,0.7363915155
,0.3263061042\H,-0.7937623794,0.8388270573,0.8407122543\H,1.2184829694
,0.4282906953,1.3813907953\H,3.0053933734,2.7280834549,1.8722740734\H,
3.4301235922,1.7651829609,0.4591792028\H,3.4087415914,-0.3133643689,1.
904096117\H,3.0760441402,0.6887567732,3.3034993887\H,5.5859334234,0.92
09152964,1.5276912099\H,5.5390936979,0.2050802195,3.14596099\H,5.24811
16869,1.9395644519,2.9342606498\Cl,-2.8404375396,6.0720488856,-1.39045
19917\C,-5.3500030159,1.6155233157,-0.5935949145\F,-5.7888858805,1.520
2370425,-1.8703794948\F,-6.3472685634,2.2269292497,0.0871508769\F,-5.2
656748087,0.3661173789,-0.1189252227\O,-1.2892453754,-0.7623658346,1.1
782054715\O,0.8449003571,-1.3047876415,1.6183734615\C,-0.373830276,-1.
5760887657,1.486565896\C,-0.8210639742,-3.0278515702,1.7177703702\C,0.
3104139812,-3.9830198294,2.0766609742\H,-1.3403380673,-3.3533165264,0.
8080028631\H,-1.5856223345,-3.0071780928,2.5042067608\H,1.0639886163,-
4.0032454087,1.283972798\H,-0.0641210063,-5.0025424227,2.2303865498\H,
0.8172743921,-3.6550695133,2.9888401513\\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-1638.3444857\RMSD=4.800e-09\RMSF=2.141e-06\Dipole=-0.4666532
,0.3149217,-0.1658227\Quadrupole=-6.4460586,-8.6313017,15.0773603,3.99
34165,-7.0828714,8.7792411\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

6_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3927\FOpt\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\19-Feb-2019\0\
\# M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SM
D,Solvent=h2o) maxdisk=2684354560\\6_C2_EtO.M062X_6-31pGd_opt_water\
\-1,1\C,-4.0842755973,3.7832207262,-0.9619489795\C,-2.8633513219,4.444
8710615,-0.9330503657\C,-1.6922359058,3.8655190324,-0.4610090082\C,-1.
7313178919,2.5457088856,0.0191322828\C,-2.952838282,1.8533624312,-0.00
30738723\C,-4.0956170116,2.4738993877,-0.4878926524\H,-4.9790068494,4.
2657073429,-1.3373806493\N,-0.6287727528,1.8513720861,0.5048286915\C,0
.6289989817,2.3511989796,0.7790920438\N,1.4960126611,1.4347952983,1.24
88920429\O,0.9408039215,3.5453768142,0.6124675481\C,2.8608568849,1.805
8417595,1.5929671645\C,3.6285400755,0.5907787043,2.0938904744\C,5.0617
064675,0.9595575566,2.4634404035\H,-0.7674744482,4.4238372357,-0.46843
89949\H,-2.9957780635,0.8302006872,0.361330562\H,-0.8016033903,0.86262
73732,0.7520002003\H,1.2096454971,0.4528831221,1.358002683\H,2.8487271
354,2.5847989942,2.3654729651\H,3.3630067002,2.2285767617,0.7137616337
\H,3.628171334,-0.1834662603,1.3166714937\H,3.1120318056,0.1703087525,

2.9656599921\H,5.5983331032,1.3627456087,1.5973941757\H,5.61241788,0.0
854627497,2.8236037975\H,5.0794003273,1.7183552319,3.2536909524\Cl,-2.
7909331089,6.0895961954,-1.5252217582\C,-5.3705067044,1.6801710114,-0.
4934810025\F,-5.2801475688,0.5863632708,-1.2787242383\F,-6.4229816036,
2.3874127546,-0.9343097627\F,-5.6908947923,1.2292728774,0.7368750458\O
,-1.2617631531,-0.8567623256,1.1580633551\O,0.8689192426,-1.3657432625
,1.6035746322\C,-0.3467103015,-1.6786165079,1.4737196618\C,-0.77378262
,-3.1257495969,1.7006797921\C,0.3359175977,-4.0631537898,2.1551141036\
H,-1.216867295,-3.4764872605,0.7604239877\H,-1.5923436119,-3.108288145
,2.429839575\H,1.1404574615,-4.1135950955,1.4151001928\H,-0.0547630547
,-5.0754661886,2.2991327028\H,0.7710482524,-3.7307442598,3.1027791282\
\Version=ES64L-G09RevE.01\State=1-A\HF=-1638.4148471\RMSD=5.603e-09\RM
SF=5.619e-06\Dipole=-0.9285989,0.5081038,-0.4418741\Quadrupole=-2.4113
856,-8.7086377,11.1200233,0.3135338,-3.2313644,5.1734912\PG=C01 [X(C14
H17Cl1F3N2O3)]\\@

6.M062X.SMD.h2o.opt
1\1\GINC-R4493\FOpt\RM062X\Gen\C11H12Cl1F3N2O1\ROOT\12-Jul-2018\0\\# M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman
SCRF=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_Cl_CF3.M062X.SMD
.h2o.opt\\0,1\C,-4.2320811711,3.0839767232,-0.7844623646\C,-4.07831401
28,1.7174108925,-0.5669855614\C,-2.908898396,1.174906289,-0.0640005041
\C,-1.8236724454,2.0149367873,0.2411808117\C,-1.9463457573,3.392129601
8,0.027279577\C,-3.1459110193,3.8924734279,-0.4768194566\H,-5.15727554
81,3.4901184544,-1.1765097098\N,-0.6710785918,1.394347711,0.7254464162
\C,0.452369458,1.9951716602,1.2603693081\N,1.413783624,1.1383877891,1.
6628358232\O,0.5706696418,3.3243843827,1.3741823224\C,2.6816203312,1.6
286887429,2.19065385\C,3.5699342316,0.4643256051,2.6010242534\C,4.9070
343393,0.9593185171,3.1428098439\H,-2.8258113422,0.1036013792,0.095503
0662\H,-1.1254105081,4.0614644742,0.2442169958\H,-0.702152769,0.379348
4436,0.748913823\H,1.3167037726,0.1445368523,1.4857012287\H,2.48410639
11,2.2741567615,3.053484901\H,3.1862948242,2.2386733194,1.4312063663\H
,3.7350476291,-0.1875714495,1.7341991586\H,3.0536691776,-0.1329220353,
3.3622998882\H,5.4455425173,1.5396905788,2.3855819243\H,5.5437201394,0
.1212186764,3.4410628537\H,4.7610286382,1.6008019777,4.0188634651\Cl,-
5.4098333129,0.6505022566,-0.9381760578\C,-3.2323487267,5.3774890399,-
0.6875112472\F,-3.061579394,6.0597168368,0.463859427\F,-4.4116237021,5
.7659137405,-1.1973381966\F,-2.2772980187,5.8225825634,-1.5298722058\\
Version=ES64L-G09RevE.01\State=1-A\HF=-1370.5562207\RMSD=3.023e-09\RMS
F=2.834e-06\Dipole=1.43011,-3.6477761,0.5085546\Quadrupole=3.3949249,1
.1399976,-4.5349225,-10.9746854,2.7850249,-4.2831915\PG=C01 [X(C11H12C
l1F3N2O1)]\\@

6_propanoate.M062X_6-31pGd_bsse
1\1\GINC-R3845\SP\RM062X\Gen\C14H17Cl1F3N2O3(1-)\ROOT\21-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671
088640\\6_C2_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-4.0705611683,3.707506
8963,-0.9362405015\C,0,-2.874743224,4.4011244627,-0.8517935115\C,0,-1.
6991683193,3.8425963406,-0.3628459648\C,0,-1.7124383455,2.5039878164,0
.0694457618\C,0,-2.9205458749,1.7713489247,-0.0071420257\C,0,-4.061241
3986,2.3780798524,-0.5006207207\H,0,-4.9703568883,4.1741258591,-1.3215
777002\N,0,-0.620146224,1.8341929139,0.5724037606\C,0,0.6655779731,2.3
318720221,0.7418181782\N,0,1.5148009843,1.4139667503,1.2625785077\O,0,
1.000098775,3.4855720857,0.4599460768\C,0,2.9149047475,1.7272625702,1.
43302161\C,0,3.5764099369,0.6840563425,2.3275485202\C,0,5.0705786774,0
.9505256042,2.4950019659\H,0,-0.7841650184,4.416403236,-0.3106292918\H
,0,-2.9262232332,0.7363915155,0.3263061042\H,0,-0.7937623794,0.8388270
573,0.8407122543\H,0,1.2184829694,0.4282906953,1.3813907953\H,0,3.0053
933734,2.7280834549,1.8722740734\H,0,3.4301235922,1.7651829609,0.45917
92028\H,0,3.4087415914,-0.3133643689,1.904096117\H,0,3.0760441402,0.68
87567732,3.3034993887\H,0,5.5859334234,0.9209152964,1.5276912099\H,0,5
.5390936979,0.2050802195,3.14596099\H,0,5.2481116869,1.9395644519,2.93
42606498\Cl,0,-2.8404375396,6.0720488856,-1.3904519917\C,0,-5.35000301
59,1.6155233157,-0.5935949145\F,0,-5.7888858805,1.5202370425,-1.870379
4948\F,0,-6.3472685634,2.2269292497,0.0871508769\F,0,-5.2656748087,0.3
661173789,-0.1189252227\O,0,-1.2892453754,-0.7623658346,1.1782054715\O
,0,0.8449003571,-1.3047876415,1.6183734615\C,0,-0.373830276,-1.5760887
657,1.486565896\C,0,-0.8210639742,-3.0278515702,1.7177703702\C,0,0.310
4139812,-3.9830198294,2.0766609742\H,0,-1.3403380673,-3.3533165264,0.8
080028631\H,0,-1.5856223345,-3.0071780928,2.5042067608\H,0,1.063988616
3,-4.0032454087,1.283972798\H,0,-0.0641210063,-5.0025424227,2.23038654
98\H,0,0.8172743921,-3.6550695133,2.9888401513\\Version=ES64L-G09RevE.
01\State=1-A\HF=-267.7284526\RMSD=3.860e-09\Dipole=-0.4766584,0.288232

1,-0.1618144\Quadrupole=-6.534893,-8.468315,15.003208,3.9636542,-7.071
3931,8.6961445\PG=C01 [X(C14H17Cl1F3N2O3)]\\@

Propanoate.M062X_6-31pGd_opt_water
1\1\GINC-R3734\FOpt\RM062X\Gen\C3H5O2(1-)\ROOT\20-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=h2o) maxdisk=671088640\\Prop.M062X_6-31pGd_opt_water\\-1,1\C,-5.36193
1422,-2.1851750805,-0.0010493259\C,-3.9901278265,-1.5269845556,-0.0062
098952\C,-2.8018701603,-2.4897299901,-0.0036948422\O,-3.0165693554,-3.
7345453186,0.0023159164\O,-1.6480639674,-1.9630117113,-0.0079128531\H,
-6.1512583288,-1.4264304065,-0.0032632774\H,-5.4980804609,-2.810996842
,0.8865442624\H,-5.5008675187,-2.8190580647,-0.8824691686\H,-3.8719243
684,-0.8719220321,0.8655163482\H,-3.8746810839,-0.8798954932,-0.884238
03\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.8436842\RMSD=2.039e-09
\RMSF=3.576e-05\Dipole=-2.8998729,1.5078719,-0.0023025\Quadrupole=-5.0
406627,-0.9670921,6.0077547,-0.722816,0.0207007,0.0329233\PG=CS [SG(C3
H1O2),X(H4)]\\@

Propanoate.M062X_6-31pGd_opt
1\1\GINC-R3722\FOpt\RM062X\Gen\C3H5O2(1-)\ROOT\20-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=671088640
\\Prop.M062X_6-31pGd_opt\\-1,1\C,-5.3604901217,-2.1792620695,-0.001078
5416\C,-3.9877001921,-1.5147220948,-0.0062695987\C,-2.7836464279,-2.50
9262949,-0.0036345436\O,-3.0683394909,-3.7307125802,0.0023800142\O,-1.
6543796102,-1.96203547,-0.0079073515\H,-6.1740803926,-1.4393181008,-0.
0031685936\H,-5.4705963512,-2.8209328535,0.8789185652\H,-5.473359375,-
2.8289245607,-0.8748398729\H,-3.8700120765,-0.8573002989,0.8659698109\
H,-3.8727704402,-0.8652785273,-0.8848307535\\Version=ES64L-G09RevE.01\
State=1-A\HF=-267.7291889\RMSD=5.199e-09\RMSF=8.412e-05\Dipole=-2.026
0163,0.9674059,-0.0012164\Quadrupole=-5.1945784,-0.8343147,6.028893,-0
.1834739,0.0185188,0.0315648\PG=CS [SG(C3H1O2),X(H4)]\\@

Propanoate.M062X_6-31pGd_opt_Pentadecane
1\1\GINC-R3737\FOpt\RM062X\Gen\C3H5O2(1-)\ROOT\20-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=n-Pentadecane) maxdisk=671088640\\Prop.M062X_6-31pGd_opt_Pentadecane\
\-1,1\C,-5.3600696907,-2.180285733,-0.0010745393\C,-3.9873658129,-1.51
94156931,-0.0062487373\C,-2.7854190224,-2.5053647538,-0.0036495146\O,-
3.0537622797,-3.7308157195,0.002357518\O,-1.652508465,-1.9617200656,-0
.0079117368\H,-6.1676977658,-1.4359271617,-0.0031941015\H,-5.479990106
2,-2.8178245846,0.8807936761\H,-5.4827590363,-2.825833375,-0.876713625
4\H,-3.8715227808,-0.8612944382,0.8654756016\H,-3.8742795225,-0.869267
9751,-0.8842954062\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.777229
8\RMSD=3.585e-09\RMSF=6.233e-05\Dipole=-2.2407592,1.0781309,-0.0013827
\Quadrupole=-5.0485579,-0.8880239,5.9365818,-0.3320726,0.0188204,0.031
623\PG=CS [SG(C3H1O2),X(H4)]\\@

3_propanoate.M062X_6-31pGd_bsse
1\1\GINC-R3713\SP\RM062X\Gen\C13H18N3O5(1-)\ROOT\22-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=67108864
0\\3Nitro_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,11.8422003791,-0.0093140006
,-7.406870633\C,0,10.866875673,-0.2318581274,-6.253193625\C,0,10.48961
59427,1.0798747015,-5.5720591867\N,0,9.5200365692,0.8350186116,-4.5296
969509\C,0,9.2943101649,1.7621778254,-3.5657444579\O,0,9.9438561715,2.
8043935511,-3.4554937513\N,0,8.2612192768,1.4017353285,-2.7120670116\C
,0,7.7880355122,2.1113103946,-1.6285846348\C,0,8.3061095686,3.34239839
82,-1.1871598669\C,0,6.7052929987,1.5390966883,-0.9242337145\C,0,6.157
3847307,2.1729664624,0.1819231382\C,0,6.6564138272,3.3935457161,0.6343
305718\C,0,7.7213752671,3.9360589324,-0.0743008182\H,0,12.1197804264,-
0.9548649909,-7.8843047081\H,0,12.7625793791,0.4739804664,-7.056614449
2\H,0,11.3071486469,-0.9021764164,-5.5050485334\H,0,9.9560552247,-0.72
72056827,-6.6105623226\H,0,10.0940713387,1.7866319967,-6.3205037311\H,
0,11.3714738271,1.5556864862,-5.1279192856\H,0,8.8748597608,0.03416122
78,-4.6465636567\H,0,9.1341421411,3.8087168447,-1.7022744142\H,0,6.313
6035437,0.5871695606,-1.2763731265\H,0,5.3250312091,1.7077709394,0.702
4495606\N,0,8.2663634102,5.2261437734,0.3867433337\H,0,6.2472087104,3.
9083488466,1.4938473978\O,0,9.2040663202,5.7105989572,-0.22163442\O,0,
7.7473769434,5.750323776,1.3639245924\H,0,11.4008771952,0.6362531285,-
8.1753604744\H,0,7.7653037491,5.0444412784,-2.9017459185\O,0,6.7768482
391,-0.91642851,-3.0355757571\O,0,7.827446644,-1.3935625599,-4.9625682
393\C,0,6.9752745343,-1.6158633805,-4.0681978032\C,0,6.0746158144,-2.8
526776643,-4.220596633\C,0,6.3410901161,-3.6716931353,-5.4774035516\H,
0,5.0360703091,-2.5002365146,-4.1914253422\H,0,6.2075942576,-3.4606871

87,-3.3171035449\H,0,6.1991567076,-3.0600853105,-6.3731270158\H,0,5.67
28574534,-4.539762253,-5.5356934326\H,0,7.3761520165,-4.0250581587,-5.
4947975836\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.7285017\RMSD=3.
820e-09\Dipole=-0.3526007,-0.9378964,-0.2803204\Quadrupole=16.0157337,
-18.4232951,2.4075614,-9.4981782,-1.1398482,-24.0434363\PG=C01 [X(C13H
18N3O5)]\\@

3_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R4093\FOpt\RM062X\Gen\C13H18N3O5(1-)\ROOT\20-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=n-Pentadecane) maxdisk=2684354560\\3Nitro_EtO.M062X_6-31pGd_opt_P
entadecane\\-1,1\C,11.8330546196,0.009951039,-7.4246012445\C,10.795597
6122,-0.2033075385,-6.3260364409\C,10.5282093921,1.0808693166,-5.54884
10786\N,9.5189767107,0.8493391314,-4.5372385245\C,9.2847983034,1.77000
16299,-3.5726333506\O,9.9367072468,2.8121376999,-3.456225334\N,8.24469
91693,1.4150415621,-2.7271164605\C,7.7736354545,2.1218871544,-1.637607
1726\C,8.303049777,3.34222411,-1.1847814802\C,6.6841189917,1.556399727
2,-0.9396251314\C,6.1391618648,2.1862726709,0.1701776463\C,6.650417706
,3.3978735605,0.6330333858\C,7.7227444563,3.9339798449,-0.068327709\H,
12.028196473,-0.9177976125,-7.9724531252\H,12.7850829968,0.3587428521,
-7.0070154814\H,11.1363233975,-0.9762989782,-5.6262913997\H,9.85525777
14,-0.5687550188,-6.7562155651\H,10.2110939913,1.877038712,-6.24033889
06\H,11.4474820788,1.4320913893,-5.0649779328\H,8.8919691087,0.0340810
206,-4.6467258297\H,9.1372415325,3.8045330868,-1.6921908855\H,6.282457
8293,0.6110905923,-1.2968552834\H,5.3010339409,1.7257207764,0.68492734
92\N,8.2848054363,5.211997583,0.4012347109\H,6.2412504589,3.9069074227
,1.496223699\O,9.2315252966,5.6867070964,-0.2025001037\O,7.7729102338,
5.738602999,1.3798411959\H,11.493138124,0.7598652381,-8.1485859898\H,7
.7463943189,0.5201386582,-2.9180068181\O,6.7493118338,-0.904735458,-3.
0395136091\O,7.8466471974,-1.4083040717,-4.9294894646\C,6.9698124705,-
1.6220781347,-4.0566976077\C,6.0687044382,-2.8539929452,-4.2183314292\
C,6.3992064168,-3.7253652409,-5.4222667542\H,5.0349192846,-2.489378452
3,-4.2715705882\H,6.1340561469,-3.4286878478,-3.2863356996\H,6.3192991
362,-3.1526686158,-6.3509575985\H,5.7209417331,-4.5847523263,-5.485646
0846\H,7.4255770672,-4.1000426327,-5.3620179196\\Version=ES64L-G09RevE
.01\State=1-A\HF=-1046.2961265\RMSD=9.560e-09\RMSF=5.346e-06\Dipole=-0
.4448889,-1.0272953,-0.2897771\Quadrupole=15.7937069,-19.3359546,3.542
2477,-9.8968473,-3.0360819,-22.8963032\PG=C01 [X(C13H18N3O5)]\\@

3_propanoate.M062X_6-31pGd_opt

1\1\GINC-R4045\FOpt\RM062X\Gen\C13H18N3O5(1-)\ROOT\22-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=26843
54560\\3Nitro_EtO.M062X_6-31pGd_opt\\-1,1\C,11.8422003791,-0.009314000
6,-7.406870633\C,10.866875673,-0.2318581274,-6.253193625\C,10.48961594
27,1.0798747015,-5.5720591867\N,9.5200365692,0.8350186116,-4.529696950
9\C,9.2943101649,1.7621778254,-3.5657444579\O,9.9438561715,2.804393551
1,-3.4554937513\N,8.2612192768,1.4017353285,-2.7120670116\C,7.78803551
22,2.1113103946,-1.6285846348\C,8.3061095686,3.3423983982,-1.187159866
9\C,6.7052929987,1.5390966883,-0.9242337145\C,6.1573847307,2.172966462
4,0.1819231382\C,6.6564138272,3.3935457161,0.6343305718\C,7.7213752671
,3.9360589324,-0.0743008182\H,12.1197804264,-0.9548649909,-7.884304708
1\H,12.7625793791,0.4739804664,-7.0576144492\H,11.3071846469,-0.902176
4164,-5.5050485334\H,9.9560552247,-0.7272056827,-6.6105623226\H,10.094
0713387,1.7866319967,-6.3205037311\H,11.3714738271,1.5556864862,-5.127
9192856\H,8.8748597608,0.0341612278,-4.6465636567\H,9.1341421411,3.808
7168447,-1.7022744142\H,6.3136035437,0.5871695606,-1.2763731265\H,5.32
50312091,1.7077709394,0.7024495606\N,8.2663634102,5.2261437734,0.38674
33337\H,6.2472087104,3.9083488466,1.4938473978\O,9.2040663202,5.710598
9572,-0.22163442\O,7.7473769434,5.750323776,1.3639245924\H,11.40087719
52,0.6362531285,-8.1753604744\H,7.7653037491,0.5044412784,-2.901745918
5\O,6.7768482391,-0.91642851,-3.0355757571\O,7.827446644,-1.3935625599
,-4.9625862393\C,6.9752745343,-1.6158633805,-4.0681978032\C,6.07461581
44,-2.8526776643,-4.220596633\C,6.3410901161,-3.6716931353,-5.47740355
16\H,5.0360703091,-2.5002365146,-4.1914253422\H,6.2075942576,-3.460687
187,-3.3171035449\H,6.1991567076,-3.0600853105,-6.3731270158\H,5.67285
74534,-4.539762253,-5.5356934326\H,7.3761520165,-4.0250581587,-5.49479
75836\\Version=ES64L-G09RevE.01\State=1-A\HF=-1046.2535069\RMSD=5.298e
-09\RMSF=1.829e-06\Dipole=-0.3352079,-0.9156316,-0.2789361\Quadrupole=
16.0621437,-18.533502,2.4713583,-9.6037577,-1.1544174,-24.1217358\PG=C
01 [X(C13H18N3O5)]\\@

3.M062X_6-31pGd_opt

1\1\GINC-R3711\FOpt\RM062X\Gen\C10H13N3O3\ROOT\05-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214748364
8\\3Nitro.M062X_6-31pGd_opt\\0,1\C,11.976345989,0.0061280099,-7.425520
7149\C,10.8599533005,-0.2924071031,-6.4272884814\C,10.5728612723,0.908
0702491,-5.5349502823\N,9.5095481378,0.5967348862,-4.5866521223\C,9.25
30092586,1.4844080597,-3.5681185861\O,9.952752698,2.4537198739,-3.3394
170983\N,8.1350171797,1.1430021223,-2.8121527081\C,7.6333355535,1.8305
06074,-1.6997216586\C,8.0070456154,3.1400457179,-1.3765148363\C,6.6863
913503,1.1702845688,-0.9025678979\C,6.1170359542,1.7948255666,0.200292
6271\C,6.4784965145,3.0946293002,0.5419748871\C,7.4160242875,3.7239169
032,-0.2643959348\H,12.1769164426,-0.8587165088,-8.0638275071\H,12.905
4839288,0.2637654957,-6.9064944111\H,11.1317909462,-1.1477822545,-5.79
74928625\H,9.947339418,-0.5730046714,-6.9716982387\H,10.3074211527,1.7
851039085,-6.1422505364\H,11.4592970175,1.177666817,-4.9545682245\H,8.
7290288318,0.0656375877,-4.9536922562\H,8.7385016168,3.6814458108,-1.9
596330923\H,6.3946268677,0.1526370683,-1.1522600875\H,5.3875463395,1.2
608258081,0.8005345069\N,7.8096120773,5.1086270685,0.0756222932\H,6.05
76182961,3.6087303978,1.3966338025\O,8.6108307305,5.6654731589,-0.6502
661505\O,7.3020524464,5.6082646417,1.0648925181\H,11.7105991917,0.8479
597051,-8.0736411785\H,7.771797585,0.2075823377,-2.9390657686\\Version
=ES64L-G09RevE.01\State=1-A\HF=-778.4465485\RMSD=5.446e-09\RMSF=3.616e
-06\Dipole=-0.9115699,-3.0607712,-1.4438158\Quadrupole=2.5712875,-6.69
18327,4.1205452,2.2393257,-4.2671613,-3.3203394\PG=C01 [X(C10H13N3O3)]
\\@

3_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3876\FOpt\RM062X\Gen\C13H18N3O3(1-)\ROOT\19-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2684354560\\3Nitro_EtO.M062X_6-31pGd_opt_water\\-1,1
\C,11.7946268034,0.0466150654,-7.4270879364\C,10.6517761139,-0.1247145
886,-6.431475741\C,10.6353190445,1.0088510765,-5.4160111499\N,9.54021
1451,0.8297944793,-4.4739927157\C,9.323499262,1.7248786773,-3.49083130
94\O,10.0467820684,2.72588007,-3.3263383629\N,8.2411480312,1.433824355
6,-2.6866058391\C,7.7730016999,2.1603182038,-1.5952295543\C,8.26611779
43,3.4101675986,-1.2023329412\C,6.7194006241,1.5863704815,-0.856530313
\C,6.1733803272,2.2335269136,0.2433730682\C,6.6552401005,3.4753998837,
0.6532634949\C,7.6911926458,4.0201709734,-0.0916336234\H,11.8075466745
,-0.7694641336,-8.1557118272\H,12.7628132218,0.055937794,-6.9141245625
\H,10.7522669337,-1.0816948172,-5.9046121334\H,9.6918611035,-0.1497949
318,-6.9619392784\H,10.5270278455,1.9709212975,-5.9326277763\H,11.5882
379222,1.037813212,-4.8732673979\H,8.9046473829,0.0319123047,-4.604656
8984\H,9.0657562212,3.8944564422,-1.7406801009\H,6.3327474904,0.617767
7669,-1.1610337003\H,5.3634236783,1.7638705712,0.7918644717\N,8.220931
2702,5.3274618043,0.3115939005\H,6.2446433172,3.9929576464,1.511072031
4\O,9.1472806271,5.8066392087,-0.3262151001\O,7.7134496874,5.887974721
9,1.272964786\H,11.696255525,0.9887357563,-7.9778199782\H,7.745780255,
0.547098298,-2.8754752759\O,6.8110885669,-1.0051267568,-3.0936284011\O
,7.8630883329,-1.4744661098,-5.0091031026\C,7.0024040686,-1.7260653568
,-4.1211193008\C,6.1230476594,-2.9655785114,-4.2582003273\C,6.37856010
51,-3.8090202495,-5.4990869406\H,5.0819798968,-2.6219996154,-4.2296615
993\H,6.2676151028,-3.5600363012,-3.348014345\H,6.2084889142,-3.231203
3462,-6.4128466358\H,5.7086631756,-4.6744625168,-5.5170253055\H,7.4085
090555,-4.1783873676,-5.5218204459\\Version=ES64L-G09RevE.01\State=1-A
\HF=-1046.3291487\RMSD=5.952e-09\RMSF=4.329e-06\Dipole=-1.0506236,-1.2
74423,0.1161399\Quadrupole=15.8218801,-22.5551851,6.733305,-10.1054368
,-7.3455213,-22.1841876\PG=C01 [X(C13H18N3O5)]\\@

3.M062X_6-31pGd_opt_water

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13N3O3\ROOT\05-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=h2o) maxdisk=2147483648\\3Nitro.M062X_6-31pGd_opt_water\\0,1\C,11.958
3662522,-0.0398805739,-7.4267135578\C,10.7522815818,-0.2281169012,-6.5
123191543\C,10.665179954,0.8886003743,-5.4829591982\N,9.5112063584,0.6
865335269,-4.6151687795\C,9.237628695,1.5397411494,-3.6057799257\O,9.8
92789743,2.576605003,-3.4186311158\N,8.1711914219,1.170894275,-2.80966
48645\C,7.6579542565,1.8504793734,-1.7021361925\C,7.9662163512,3.17882
03266,-1.3952138614\C,6.7579391537,1.1496515703,-0.8803184671\C,6.1806
444095,1.7532018149,0.229101436\C,6.4828829829,3.0723550146,0.56008911
84\C,7.3712003108,3.7405161619,-0.2703208518\H,12.0176881047,-0.842921
909,-8.1672437787\H,12.8903647103,-0.0421590674,-6.8508852079\H,10.822
3478404,-1.1922777084,-5.9936625521\H,9.8299782281,-0.2451620512,-7.10
55760172\H,10.5724272987,1.8578454845,-5.9855736369\H,11.5801635397,0.

9165315714,-4.8785712962\H,8.9906309808,-0.1799058751,-4.6996858865\H,
8.6379868926,3.7592609009,-2.0089785181\H,6.5151154162,0.1182575982,-1
.1229258904\H,5.4909959841,1.1879936407,0.8471252331\N,7.7038298848,5.
1340095056,0.0465781156\H,6.0489832865,3.5570355363,1.4256926132\O,8.5
202131906,5.7137359645,-0.6540116658\O,7.1486108854,5.6592067101,1.000
871033\H,11.8965588424,0.9121190607,-7.9653109286\H,7.7669034439,0.255
1095229,-2.9800502023\\Version=ES64L-G09RevE.01\State=1-A\HF=-778.4707
003\RMSD=4.352e-09\RMSF=4.333e-06\Dipole=-1.3828861,-5.0146593,-1.5740
941\Quadrupole=2.0411232,-5.8243226,3.7831994,2.5324333,-5.5294194,-3.
8730558\PG=C01 [X(C10H13N3O3)]\\@

3.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3879\FOpt\RM062X\Gen\C10H13N3O3\ROOT\22-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solvent
=n-Pentadecane) maxdisk=2147483648\\3Nitro.M062X_6-31pGd_opt_Pentadeca
ne\\0,1\C,11.9732352486,-0.0220521338,-7.4271575308\C,10.8871040704,-0
.3066766638,-6.3938329815\C,10.5699384465,0.9292137156,-5.5619056109\N
,9.5286825356,0.6305041265,-4.5873330345\C,9.2542075407,1.5205562078,-
3.5860828129\O,9.9286195073,2.5181348066,-3.3785464448\N,8.1548004403,
1.1649889795,-2.8141889642\C,7.6335460166,1.848922254,-1.7121754731\C,
8.0417097897,3.1341093741,-1.3361911202\C,6.6322285468,1.2039024079,-0
.9681002634\C,6.0446842,1.819283102,0.129511224\C,6.4383837845,3.09580
19425,0.5217446068\C,7.4289068369,3.7103717128,-0.2307140116\H,12.1970
436471,-0.9141853752,-8.0194886974\H,12.9012126001,0.299914532,-6.9421
886448\H,11.2037838282,-1.1155646689,-5.7243855441\H,9.9754789796,-0.6
485516888,-6.9032592195\H,10.2637490586,1.7602051771,-6.2128731667\H,1
1.4558677234,1.2583414761,-5.0119643812\H,8.7984666209,-0.007019048,-4
.8818898977\H,8.8119541498,3.6621998588,-1.8794377318\H,6.3143689032,0
.2049439562,-1.2579908882\H,5.2735781246,1.2972733603,0.6868040616\N,7
.8607145625,5.0665176613,0.1623062404\H,5.9996630588,3.5977938906,1.37
47373036\O,8.7177051054,5.6117251316,-0.5089733625\O,7.3308577199,5.56
71439926,1.1406227092\H,11.6638782919,0.7701545783,-8.1177526375\H,7.7
539106623,0.250128134,-2.9815301261\\Version=ES64L-G09RevE.01\State=1-
A\HF=-778.4653178\RMSD=8.776e-09\RMSF=1.411e-05\Dipole=-1.1216815,-3.5
337825,-1.649406\Quadrupole=3.1612106,-6.4324384,3.2712278,2.3648128,-
4.5930142,-3.417306\PG=C01 [X(C10H13N3O3)]\\@

5_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3714\FOpt\RM062X\Gen\C13H18N3O5(1-)\ROOT\09-Apr-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=h2o) maxdisk=2684354560\\4Nitro_EtO_c3.M062X_6-31pGd_opt_water\\-
1,1\C,-3.7351386832,3.9843548265,-1.5202798621\C,-3.952622903,2.696466
9799,-1.0245574362\C,-2.9604271335,2.0953912817,-0.278796061\C,-1.7408
593272,2.7607562492,-0.0145752656\C,-1.5462634468,4.0594710165,-0.5291
512512\C,-2.543187622,4.6637939487,-1.2777311711\N,-0.8174500322,2.063
1925995,0.73878491\C,0.4372799304,2.4790683332,1.1580507041\N,1.090612
0233,1.5559613045,1.894300811\O,0.9005945849,3.602406767,0.9019492867\
C,2.4869569993,1.7455178429,2.2591757926\C,3.4556817927,1.4666315232,1
.1124287828\C,4.901616228,1.6958323013,1.5413115572\H,-3.1129035524,1.
094799476,0.114515573\H,-0.623823213,4.5889047394,-0.3451382483\H,-1.1
034606464,1.1129743164,1.0284767003\H,0.7231884346,0.5963045295,1.9495
431998\H,2.6931508403,1.0693050767,3.0943809553\H,2.6194685207,2.76836
03057,2.625373019\H,3.2041144778,2.1163643272,0.2654284935\H,3.3193590
874,0.4307796144,0.7782237991\H,5.055740011,2.7339190829,1.8570649596\
H,5.596539885,1.4866564513,0.7222897861\H,5.1678200842,1.0460952122,2.
3829036086\H,-4.8842006199,2.1785656633,-1.2213227909\H,-2.3928534682,
5.6618669253,-1.6731421592\N,-4.7665169924,4.6239788542,-2.3002719736\
O,-4.5675954415,5.7576176772,-2.7283257552\O,-5.8111204828,4.013812616
2,-2.511196442\O,-1.6777977766,-0.5516623728,1.4879055769\C,-0.8761812
522,-1.4308085984,1.9162035806\O,0.3457838169,-1.2109446121,2.17209235
1\C,-1.3834490139,-2.8511266385,2.146285821\C,-2.8640720874,-3.0648823
201,1.8670531044\H,-1.1412300119,-3.1122652791,3.1833033252\H,-0.77108
92878,-3.5112384534,1.5199253445\H,-3.4835610307,-2.4276700991,2.50583
5233\H,-3.1416941702,-4.1063182803,2.0580005491\H,-3.1083885214,-2.835
6531882,0.8252315922\\Version=ES64L-G09RevE.01\State=1-A\HF=-1046.3333
889\RMSD=9.153e-09\RMSF=8.902e-06\Dipole=0.9082268,-0.4847987,0.108102
1\Quadrupole=-3.3612231,-3.3961292,6.7573523,17.0409585,-19.2556513,17
.9396419\PG=C01 [X(C13H18N3O5)]\\@

5.M062X.opt

1\1\GINC-R4420\FOpt\RM062X\Gen\C10H13N3O3\ROOT\16-Jul-2018\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman maxd
isk=2147483648\\aryl_urea_nitro.M062X.opt\\0,1\C,-4.128982565,3.513988
4707,-1.183629988\C,-4.1394367067,2.1380556781,-0.980631752\C,-3.03562
00123,1.5473000123,-0.3915244311\C,-1.9239638653,2.3167845953,-0.00403
83317\C,-1.9358355191,3.7051896614,-0.2166303245\C,-3.0439732604,4.296
7312443,-0.8091844109\N,-0.8494364913,1.6312121575,0.5641581443\C,0.30
8824824,2.1728409354,1.1171399472\N,1.1888002006,1.2206407743,1.569444
1465\O,0.5144614668,3.3685438184,1.2209619949\C,2.4936961304,1.6435313
258,2.0637768724\C,3.2051943681,0.4848117514,2.7501874186\C,4.57461540
56,0.9040119455,3.2800831193\H,-3.0294983004,0.4724187398,-0.228228290
2\H,-1.0897004552,4.3048941219,0.0866659614\H,-0.9915740742,0.63770443
47,0.6915892694\H,1.1445721653,0.2963064929,1.1582438455\H,2.326574727
2,2.4641925997,2.7666049834\H,3.1082105742,2.0417376927,1.2439385006\H
,3.3258784696,-0.3454201641,2.0402325705\H,2.5771055313,0.1158543846,3
.5696552029\H,5.2198538338,1.2570295116,2.4686710726\H,5.0801740532,0.
0683053998,3.7714896634\H,4.4795597748,1.7152069562,4.0094514898\H,-5.
0003564541,1.5529591911,-1.2818353504\H,-3.0719931253,5.3664144182,-0.
9817447106\N,-5.2917156323,4.1494177591,-1.8063943022\O,-5.2575694001,
5.3567293852,-1.9739154499\O,-6.2275656631,3.4325567062,-2.1221368611\
\Version=ES64L-G09RevE.01\State=1-A\HF=-778.4499459\RMSD=6.870e-09\RMS
F=4.894e-06\Dipole=2.2256844,-2.5208187,1.018129\Quadrupole=-6.8461647
,7.6056811,-0.7595163,2.5829747,-6.6148256,1.6003784\PG=C01 [X(C10H13N
3O3)]\\@

5_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3723\FOpt\RM062X\Gen\C13H18N3O5(1-)\ROOT\08-Apr-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) maxdis
k=2684354560\\4Nitro_EtO_c3.M062X_6-31pGd_opt\\-1,1\C,-3.7513263626,3.
9287002984,-1.4505395418\C,-3.9455572747,2.6243727976,-0.9846289191\C,
-2.936927777,2.0014055091,-0.2802025115\C,-1.7096688283,2.6659517193,-
0.024422138\C,-1.535695504,3.9850310636,-0.5052467599\C,-2.5539939553,
4.6028171751,-1.2117753213\N,-0.7720089716,1.9608725535,0.6831292376\C
,0.5025559611,2.3834607537,1.0573525174\N,1.1827517827,1.436268654,1.7
431219496\O,0.9586568773,3.4999641801,0.7991663616\C,2.531028656,1.696
0751786,2.1907891791\C,3.5776208211,1.5305754301,1.0868344849\C,4.9865
738083,1.8272058884,1.5959812679\H,-3.0605239941,0.987906215,0.0934343
262\H,-0.6039465985,4.4975466848,-0.3123095345\H,-1.0586934705,0.99557
56732,0.9643172981\H,0.7778337816,0.4951882362,1.9102444592\H,2.740122
0338,0.9995352132,3.0110440818\H,2.5834930226,2.717231094,2.5885710843
\H,3.3180971829,2.2087510005,0.2662506309\H,3.5188100697,0.5068521472,
0.6977189723\H,5.0576846237,2.8563362428,1.9673730322\H,5.7355517073,1
.7044446308,0.8065343199\H,5.2569166191,1.156387375,2.4207390873\H,-4.
8840950827,2.1191367085,-1.1815309314\H,-2.4308307514,5.6134303474,-1.
5843936687\N,-4.8063636602,4.5870895478,-2.1895779655\O,-4.6149556496,
5.7315272307,-2.5882817866\O,-5.8500105627,3.9735506972,-2.3875348715\
O,-1.7268088676,-0.5462757561,1.3134473007\C,-0.9655792279,-1.35944505
96,1.9063291377\O,0.2158334553,-1.1367762144,2.2719443567\C,-1.5213058
226,-2.7585251525,2.2149996278\C,-2.9643848344,-2.9757780895,1.7770555
166\H,-1.4069722479,-2.9182392918,3.2942125986\H,-0.850421965,-3.48194
0197,1.7351049278\H,-3.6285789748,-2.2568840959,2.265498238\H,-3.30515
12128,-3.9892626873,2.0219187841\H,-3.0677088063,-2.8234837015,0.69888
11716\\Version=ES64L-G09RevE.01\State=1-A\HF=-1046.2609461\RMSD=6.397e
-09\RMSF=2.208e-06\Dipole=1.1289521,-0.3191933,0.3132944\Quadrupole=-6
.1728893,-4.3508446,10.5237339,14.5279586,-18.8912194,18.5300414\PG=C0
1 [X(C13H18N3O5)]\\@

5.M062X.SMD.h2o.opt

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H13N3O3\ROOT\16-Jul-2018\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Freq=Noraman SCRF
=(SMD,Solvent=h2o) maxdisk=2147483648\\aryl_urea_nitro.M062X.SMD.h2o.o
pt\\0,1\C,-4.125916005,3.4998430573,-1.206437773\C,-4.128777902,2.1259
278664,-0.9605600196\C,-3.0246350367,1.5584023043,-0.3576118826\C,-1.9
119464806,2.3456821077,0.0059553437\C,-1.9313341496,3.7288291274,-0.25
5360463\C,-3.0400976655,4.2997898532,-0.8608799511\N,-0.8512055527,1.6
766772167,0.5976971031\C,0.3193607839,2.2062546602,1.119767672\N,1.173
9391185,1.2886176225,1.613403176\O,0.5597848137,3.4207456825,1.1436391
442\C,2.4679646225,1.6830276002,2.1574539036\C,3.2188585319,0.46395184
31,2.6707726964\C,4.5824900658,0.8559491883,3.230461217\H,-3.010563251
9,0.4907358273,-0.1583851458\H,-1.0886115892,4.349875342,0.00839646\H,
-0.9664323857,0.6704535873,0.6781382897\H,0.9718771744,0.2991123058,1.
5175175017\H,2.310784151,2.4001941662,2.9706984173\H,3.0542511821,2.18

86527433,1.3804177611\H,3.3428834259,-0.2554520755,1.8519236849\H,2.62
09760398,-0.0281878136,3.447377251\H,5.2007183719,1.3287852149,2.45946
7659\H,5.1200131976,-0.0210156903,3.6029294341\H,4.4763612625,1.564290
3173,4.0594634011\H,-4.9808383039,1.5153116349,-1.2357679338\H,-3.0564
117285,5.3641711626,-1.0648929006\N,-5.2783902402,4.1058908085,-1.8367
558933\O,-5.2670118799,5.3139073691,-2.0490752659\O,-6.2277905702,3.38
95269707,-2.1373528872\\Version=ES64L-G09RevE.01\State=1-A\HF=-778.474
2615\RMSD=9.912e-09\RMSF=9.398e-06\Dipole=2.8426373,-4.0499692,1.68655
44\Quadrupole=-11.9526653,11.6593844,0.2932808,2.84577,-9.5921794,0.48
90728\PG=C01 [X(C10H13N3O3)]\\@

5_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3711\FOpt\RM062X\Gen\C13H18N3O5(1-)\ROOT\09-Apr-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Sol
vent=n-Pentadecane) maxdisk=2684354560\\4Nitro_EtO_c3.M062X_6-31pGd_op
t_Pentadecane\\-1,1\C,-3.7754690421,3.9292772446,-1.4479382126\C,-3.95
88053733,2.6240019118,-0.9812727949\C,-2.9438338958,2.0121398969,-0.27
63035684\C,-1.7229984506,2.6869946707,-0.0215264154\C,-1.5617407644,4.
0065180011,-0.503086808\C,-2.5849605006,4.6152917546,-1.2104691045\N,-
0.777909037,1.9894032278,0.6867074353\C,0.4965768113,2.4153111318,1.05
44576313\N,1.1808652332,1.474144496,1.7423936195\O,0.9482747953,3.5319
002094,0.7869693707\C,2.5351382559,1.7244745502,2.1859180632\C,3.58250
57216,1.4879709924,1.0966059725\C,4.9961777596,1.7548837981,1.60604846
95\H,-3.0616756844,0.9978138377,0.0961339656\H,-0.6359403841,4.5302897
383,-0.3130740521\H,-1.0565897459,1.0228153717,0.9679905929\H,0.773912
2691,0.537371505,1.917516041\H,2.7260725891,1.0599125921,3.0362575498\
H,2.6052710393,2.7585736722,2.5430807284\H,3.3545850013,2.1439687766,0
.2486293095\H,3.4930978892,0.4538207367,0.7418876994\H,5.1018184048,2.
7926921032,1.943896383\H,5.7437698849,1.5812235903,0.8249030749\H,5.24
09121428,1.1021271769,2.4528381402\H,-4.8909511027,2.106000407,-1.1757
948482\H,-2.4665622067,5.626806215,-1.5823592155\N,-4.8363327464,4.577
2146911,-2.1875488101\O,-4.6558148372,5.7225220325,-2.5879815787\O,-5.
8747334344,3.955086474,-2.3850789601\O,-1.7022507337,-0.5296809659,1.3
191478454\C,-0.9511725814,-1.342797,1.9255507864\O,0.2235478663,-1.109
9844459,2.3098304815\C,-1.5063940024,-2.7406189072,2.22765851\C,-2.925
4257614,-2.9823165415,1.7313748169\H,-1.4407725092,-2.884070965,3.3133
521048\H,-0.809086851,-3.4651639148,1.7891344506\H,-3.6235102529,-2.27
14955993,2.1834235382\H,-3.2603934045,-3.9976291313,1.9751928833\H,-2.
9871823615,-2.8502133347,0.6469949048\\Version=ES64L-G09RevE.01\State=
1-A\HF=-1046.302573\RMSD=4.715e-09\RMSF=2.074e-06\Dipole=1.1417111,-0.
3652287,0.2807062\Quadrupole=-5.2490388,-3.9388533,9.1878921,14.957380
7,-18.6858002,18.056195\PG=C01 [X(C13H18N3O5)]\\@

5.M062X.SMD.pentadecane.opt

1\1\GINC-R3717\FOpt\RM062X\Gen\C10H13N3O3\ROOT\25-Feb-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT=CalcFC IOP(2/17=4) SCRF=(SMD,
Solvent=n-Pentadecane) maxdisk=2147483648\\aryl_urea_nitro.M062X_6-31p
Gd_opt_Pentadecane\\0,1\C,-4.15445993,3.6247819097,-1.0853892591\C,-4.
2572485059,2.320112074,-0.6099078225\C,-3.1583054192,1.7491559756,0.00
4822759\C,-1.9559582724,2.4676076469,0.1504614651\C,-1.8758527939,3.78
445036,-0.3350423832\C,-2.9794159439,4.3560329683,-0.9532087861\N,-0.9
005977541,1.8043094513,0.7686633261\C,0.3578115569,2.3058970684,1.0913
448135\N,1.1794119564,1.3763560428,1.6624581202\O,0.6877993509,3.46780
2739,0.9091510278\C,2.5640853314,1.7102058017,1.9691307369\C,3.1700182
37,0.6624847188,2.8940999195\C,4.6238995858,0.9841045311,3.2274809992\
H,-3.2246141799,0.7310783691,0.380210396\H,-0.960446306,4.3472565124,-
0.2225234152\H,-1.1087687601,0.8632374015,1.0801119538\H,0.9626469457,
0.3939959538,1.5425153374\H,2.5694392334,2.693291802,2.4476897215\H,3.
1549212034,1.7937348566,1.0461135692\H,3.1127555576,-0.3252310863,2.41
6322066\H,2.5729519866,0.6104342451,3.8124770761\H,5.2393461437,1.0171
527261,2.3217437607\H,5.0508567619,0.2296808746,3.894814377\H,4.706598
0469,1.9567086817,3.7246560699\H,-5.1840411143,1.7699708816,-0.7231630
009\H,-2.9297946531,5.3702987525,-1.332376085\N,-5.3090564018,4.236044
5226,-1.7365396053\O,-5.1967574501,5.3799199441,-2.1487984625\O,-6.328
884413,3.5701842752,-1.835848675\\Version=ES64L-G09RevE.01\State=1-A\H
F=-778.4688472\RMSD=3.881e-09\RMSF=3.369e-06\Dipole=2.2744712,-2.88254
94,1.5805109\Quadrupole=-8.923933,8.6816601,0.2422729,2.9466523,-7.180
1777,0.2545\PG=C01 [X(C10H13N3O3)]\\@

5_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R51\SP\RM062X\Gen\C13H18N3O5(1-)\ROOT\09-Apr-2019\0\\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671088640\
\4Nitro_EtO_c3.M062X_6-31pGd_bsse\\-1,1\C,0,-3.7513263626,3.9287002984
,-1.4505395418\C,0,-3.9455572747,2.6243727976,-0.9846289191\C,0,-2.936
927777,2.0014055091,-0.2802025115\C,0,-1.7096688283,2.6659517193,-0.02
4422138\C,0,-1.535695504,3.9850310636,-0.5052467599\C,0,-2.5539939553,
4.6028171751,-1.2117753213\N,0,-0.7720089716,1.9608725535,0.6831292376
\C,0,0.5025559611,2.3834607537,1.0573525174\N,0,1.1827517827,1.4362686
54,1.7431219496\O,0,0.9586568773,3.4999641801,0.7991663616\C,0,2.53102
8656,1.6960751786,2.1907891791\C,0,3.5776208211,1.5305754301,1.0868344
849\C,0,4.9865738083,1.8272058884,1.5959812679\H,0,-3.0605239941,0.987
906215,0.0934343262\H,0,-0.6039465985,4.4975466848,-0.3123095345\H,0,-
1.0586934705,0.9955756732,0.9643172981\H,0,0.7778337816,0.4951882362,1
.9102444592\H,0,2.7401220338,0.9995352132,3.0110440818\H,0,2.583493022
6,2.717231094,2.5885710843\H,0,3.3180971829,2.2087510005,0.2662506309\
H,0,3.5188100697,0.5068521472,0.6977189723\H,0,5.0576846237,2.85633624
28,1.9673730322\H,0,5.7355517073,1.7044446308,0.8065343199\H,0,5.25691
66191,1.156387375,2.4207390873\H,0,-4.8840950827,2.1191367085,-1.18153
09314\H,0,-2.4308307514,5.6134303474,-1.5843936687\N,0,-4.8063636602,4
.5870895478,-2.1895779655\O,0,-4.6149556496,5.7315272307,-2.5882817866
\O,0,-5.8500105627,3.9735506972,-2.3875348715\O,0,-1.7268088676,-0.546
2757561,1.3134473007\C,0,-0.9655792279,-1.3594450596,1.9063291377\O,0,
0.2158334553,-1.1367762144,2.2719443567\C,0,-1.5213058226,-2.758525152
5,2.2149996278\C,0,-2.9643848344,-2.9757780895,1.7770555166\H,0,-1.406
9722479,-2.9182392918,3.2942125986\H,0,-0.850421965,-3.481940197,1.735
1049278\H,0,-3.6285789748,-2.2568840959,2.265498238\H,0,-3.3051512128,
-3.9892626873,2.0219187841\H,0,-3.0677088063,-2.8234837015,0.698881171
6\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.7284552\RMSD=4.083e-09\D
ipole=1.1203743,-0.3445599,0.3193793\Quadrupole=-6.2426389,-4.2072351,
10.449874,14.5445351,-18.8761834,18.4243407\PG=C01 [X(C13H18N3O5)]\\@

7_propanoate.M062X_6-31pGd_opt

1\1\GINC-R3713\FOpt\RM062X\Gen\C13H17F1N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=268
4354560\\2Nitro4Fluro_OS_EtO.M062X_6-31pGd_opt\\-1,1\C,-1.1297360717,2
.3964663439,1.119823652\C,0.0220389649,2.2519398472,0.1277236605\C,1.3
723773182,2.5076111547,0.7889029145\N,2.4371352014,2.2922401897,-0.165
5555889\C,3.6849726872,2.7430983417,0.0983367986\O,3.9816855367,3.4666
031099,1.0454266173\N,4.6275253398,2.2757149579,-0.8272584821\C,5.9724
798625,2.515543343,-0.7162276324\C,6.5624079888,3.7237027227,-0.288632
9181\C,6.8501682752,1.4609049261,-1.0520908211\C,8.2076047841,1.629582
6765,-0.9046695791\C,8.7904937954,2.7954342952,-0.4144263475\C,7.93945
79256,3.8451155029,-0.1087361243\H,-2.0975897422,2.224915508,0.6371843
423\H,-1.1468735781,3.4005539422,1.5603711866\H,-0.10045457,2.95667940
22,-0.7035913154\H,0.0245044916,1.2474366228,-0.3128865024\H,1.4890789
871,1.8470734548,1.6641000921\H,1.4389750588,3.5368961175,1.1579551905
\H,2.3096726042,1.5330629141,-0.8588104976\H,6.4339869116,0.5186707578
,-1.4000974964\F,9.0247718742,0.6010078017,-1.2269002991\N,5.800724308
7,4.967410592,-0.1566095338\H,9.8658208157,2.8681825393,-0.3013975589\
O,6.1767234063,5.7746313394,0.6810016511\O,4.8987091014,5.166357629,-0
.9474404129\H,-1.0331709942,1.6762377865,1.9407523237\H,4.3909752855,1
.3844463705,-1.3206750411\H,8.3261834916,4.7920899598,0.2506022672\O,4
.2550600381,-0.1632620162,-2.0456000495\O,2.0288813997,0.0819811224,-1
.876616107\C,3.0632086793,-0.5342100038,-2.2347328328\C,2.8422663648,-
1.8641804944,-2.9733029244\C,4.1233174845,-2.5808007956,-3.3819876591\
H,2.2173696447,-1.6438725652,-3.8476722675\H,2.2272904792,-2.495642009
,-2.3201589564\H,4.7276270009,-1.9470350564,-4.0373168526\H,3.90338233
87,-3.5187366042,-3.9067291366\H,4.7361975098,-2.8073017264,-2.5046977
594\\Version=ES64L-G09RevE.01\State=1-A\HF=-1145.4562657\RMSD=5.523e-0
9\RMSF=7.067e-06\Dipole=0.653526,-0.4650718,0.1381915\Quadrupole=3.992
4685,-10.2778694,6.2854009,-1.8914837,-1.9498735,-12.092034\PG=C01 [X(
C13H17F1N3O5)]\\@

7.M062X_6-31pGd_opt_water

1\1\GINC-R3710\FOpt\RM062X\Gen\C10H12F1N3O3\ROOT\04-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2147483648\\2Nitro4Fluro.M062X_6-31pGd_opt_water\\0,1\
C,-1.0125306187,2.0137799716,0.4981301908\C,0.2883085143,1.5904330624,
-0.1761984722\C,1.4720450154,2.3592671422,0.3899427657\N,2.7064605185,
1.9467995501,-0.2684328883\C,3.8908800932,2.4781745051,0.0827193511\O,
4.0030068211,3.3507302217,0.9516121919\N,4.9767417829,1.9392966714,-0.
6074013019\C,6.2919326308,2.3478020477,-0.516269283\C,7.3809896947,1.5
023087074,-0.8593377436\C,6.6159073498,3.6492842771,-0.0945225818\C,7.

9365242334,4.0345700765,-0.0261704793\C,9.0112985207,3.2146015975,-0.3
561888216\C,8.7101110433,1.9373123361,-0.7777311948\H,-1.8634146095,1.
4605264493,0.0900180407\H,-1.2013657893,3.0824629355,0.3482287602\H,0.
2260604467,1.7678729534,-1.2568328218\H,0.4538579866,0.5157357782,-0.0
327294416\H,1.560508879,2.1793367972,1.4676325626\H,1.3277503484,3.436
3028519,0.2457206468\H,2.6585426065,1.2459060521,-1.0007246647\H,5.839
4383038,4.3570915007,0.1587305259\F,8.1973697765,5.2930073839,0.369617
4246\N,7.1922880824,0.1403816708,-1.3056271005\H,10.0304803066,3.57691
92168,-0.2918303895\O,8.1619395458,-0.6056476948,-1.3423685523\O,6.068
8515175,-0.2352975144,-1.6413168232\H,-0.9735596895,1.8259329859,1.576
7222469\H,4.8109539025,1.08320985,-1.1265749631\H,9.5018827865,1.25426
86167,-1.060057184\\Version=ES64L-G09RevE.01\State=1-A\HF=-877.6784303
\RMSD=3.571e-09\RMSF=6.704e-06\Dipole=-1.1593172,-0.1071962,-0.9661862
\Quadrupole=18.9485783,-14.3365663,-4.612012,9.4325059,3.1287428,-6.74
0761\PG=C01 [X(C10H12F1N3O3)]\\@

7_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3729\FOpt\RM062X\Gen\C13H17F1N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=n-Pentadecane) maxdisk=2684354560\\2Nitro4Fluro_OS_EtO.M062X_6-
31pGd_opt_Pentadecane\\-1,1\C,-1.1278809855,2.4182071301,1.1592007895\
C,0.0377063152,2.1176467908,0.2214931872\C,1.3668642623,2.5705085742,0
.8136278506\N,2.4500516808,2.2535789359,-0.0945725752\C,3.6971202695,2
.7074098094,0.1474672733\O,3.9933509195,3.4694426857,1.0673513719\N,4.
6419401766,2.2051769714,-0.7543176375\C,5.9859375211,2.4732290897,-0.6
688868445\C,6.5562122439,3.7147253862,-0.3191484676\C,6.8809044736,1.4
192920523,-0.9476188029\C,8.23649125,1.6249470876,-0.8267344755\C,8.80
16815386,2.8285508625,-0.4164426252\C,7.9324374508,3.877050815,-0.1632
952152\H,-2.0800144752,2.0958087408,0.7251574965\H,-1.2009421952,3.492
2573195,1.3668753351\H,-0.1103077283,2.6199769021,-0.7422693815\H,0.08
54547059,1.0428893863,0.0084495468\H,1.5272339463,2.0880836115,1.78994
35152\H,1.3571051867,3.6521542347,0.9935836022\H,2.302668564,1.5273494
423,-0.8173526328\H,6.4860855073,0.448141494,-1.2335103528\F,9.0674307
691,0.592677213,-1.0955131966\N,5.7647359655,4.942741414,-0.2440667775
\H,9.8764423127,2.9309559582,-0.3217699005\O,6.1151367771,5.7968868328
,0.5567861422\O,4.8582495588,5.0853090106,-1.0437484743\H,-1.006207826
3,1.9014553324,2.1184397006\H,4.4122079068,1.2964382312,-1.2186537186\
H,8.3077263473,4.8505640092,0.132113475\O,4.2753400691,-0.2474351695,-
1.946905502\O,2.0720888387,0.1697364594,-1.9785202\C,3.0859797819,-0.5
105149324,-2.2793003328\C,2.83965765,-1.7642076787,-3.1294225598\C,4.0
853211786,-2.5854510466,-3.4331675094\H,2.357432554,-1.4297974542,-4.0
566331934\H,2.0889569344,-2.3675915002,-2.6044258568\H,4.8265340612,-1
.9860128013,-3.9698158436\H,3.839000208,-3.4607376501,-4.0463281421\H,
4.5591162853,-2.9348935898,-2.5107090679\\Version=ES64L-G09RevE.01\Sta
te=1-A\HF=-1145.4991168\RMSD=3.164e-09\RMSF=2.434e-06\Dipole=0.7350205
,-0.5221865,0.1673755\Quadrupole=6.9520892,-11.5215369,4.5694478,-0.39
0856,-3.1057428,-11.1801063\PG=C01 [X(C13H17F1N3O5)]\\@

7.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R3720\FOpt\RM062X\Gen\C10H12F1N3O3\ROOT\24-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=n-Pentadecane) maxdisk=2147483648\\2Nitro4Fluro.M062X_6-31pGd_opt_P
entadecane\\0,1\C,-1.0576715397,2.5476750865,1.1585684792\C,0.17948265
07,1.9099230201,0.5331505778\C,1.4191099795,2.7671436394,0.7512900498\
N,2.5841393789,2.1412651614,0.1355399483\C,3.8246689411,2.6526805017,0
.3664750035\O,4.0636983771,3.5516060554,1.1534365781\N,4.8313314207,2.
0160571226,-0.378221566\C,6.1664660255,2.4036670988,-0.3078257641\C,6.
5967935849,3.7410447026,-0.3409287792\C,7.1504699665,1.4149316737,-0.1
928385622\C,8.4815699519,1.7788951932,-0.1091336944\C,8.9101129166,3.0
982280315,-0.097281821\C,7.9395798369,4.0828019744,-0.2081008241\H,-1.
9441658237,1.9265190577,0.9999481378\H,-1.2561926924,3.5331171838,0.72
32147891\H,0.0167311022,1.7717374532,-0.5445802968\H,0.3516284009,0.91
54020951,0.9624535832\H,1.6260746214,2.8778599591,1.8195256171\H,1.267
075794,3.7751759025,0.3421994408\H,2.4355037001,1.6751591796,-0.752399
2115\H,6.8765858823,0.3659640939,-0.1381837729\F,9.3980004171,0.800071
1853,-0.0070769371\N,5.6736956247,4.8474668813,-0.6119689009\H,9.96444
0874,3.3343227453,-0.012294067\O,5.9154031699,5.9209787256,-0.09187403
45\O,4.7583706332,4.6460332449,-1.3915648196\H,-0.9285632537,2.6784869
087,2.2385557452\H,4.6731119323,1.0410814219,-0.6053458361\H,8.2123481
271,5.1321047009,-0.2176890626\\Version=ES64L-G09RevE.01\State=1-A\HF=
-877.6701264\RMSD=7.307e-09\RMSF=4.072e-06\Dipole=-0.4926326,-2.181008
9,-0.5745452\Quadrupole=11.7837334,-5.8217086,-5.9620249,8.0073373,-0.
108409,1.6816334\PG=C01 [X(C10H12F1N3O3)]\\@

7_propanoate.M062X_6-31pGd_opt_water

1\1\GINC-R3744\FOpt\RM062X\Gen\C13H17F1N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=2684354560\\2Nitro4Fluro_OS_EtO.M062X_6-31pGd_opt_
water\\-1,1\C,-1.0535728957,2.269192852,1.1138158709\C,0.1426459507,1.
9177682156,0.2352973397\C,1.4156088431,2.5721999753,0.7520136738\N,2.5
384419747,2.2358897761,-0.1120306198\C,3.7806513875,2.6540754373,0.167
2380084\O,4.0577311567,3.4013275146,1.1217595748\N,4.7512276383,2.1658
365345,-0.7025903991\C,6.0965267833,2.4771720236,-0.5905507543\C,6.603
1567269,3.7586533072,-0.3052993362\C,7.0340771384,1.4497717185,-0.7706
997481\C,8.3800303912,1.7276989092,-0.6436020332\C,8.8831223233,2.9801
483575,-0.3118625848\C,7.9663152749,4.0029180927,-0.136355638\H,-1.966
8790344,1.7948984612,0.7425434032\H,-1.219891122,3.3519828532,1.133669
5293\H,-0.0386749418,2.2454628301,-0.7959548382\H,0.2823185354,0.82997
66842,0.2066843693\H,1.6239247662,2.2353807799,1.7750374517\H,1.291277
1707,3.6614115261,0.785739063\H,2.381512223,1.6286447061,-0.9284229257
\H,6.7018596831,0.4380028899,-0.9815886491\F,9.2521905661,0.7174415671
,-0.8270043925\N,5.7360821102,4.9276151368,-0.2645784958\H,9.950360173
2,3.1409445453,-0.2122076116\O,5.9979591136,5.8098551465,0.5403338009\
O,4.8146833695,4.9997877457,-1.0638271723\H,-0.8942327712,1.9338187283
,2.1446610368\H,4.5323622575,1.2654266615,-1.1683383528\H,8.299199311,
5.0087597485,0.0953080999\O,4.1385157735,-0.3202511227,-1.9036968666\O
,2.1213004859,0.5136688148,-2.3857677284\C,3.0059240648,-0.3908918033,
-2.4631492272\C,2.656048838,-1.6289594917,-3.282389358\C,3.7571963506,
-2.6744979794,-3.3826073551\H,2.3595092456,-1.2790114669,-4.278332454\
H,1.7521004629,-2.0591589691,-2.8342045789\H,4.65545817,-2.2605102015,
-3.8512206181\H,3.4223198218,-3.5239678625,-3.9862236273\H,4.036862683
4,-3.0519326418,-2.3942358566\\Version=ES64L-G09RevE.01\State=1-A\HF=-
1145.5374082\RMSD=6.936e-09\RMSF=5.673e-06\Dipole=1.5658626,-0.9675569
,0.2315619\Quadrupole=14.2827095,-12.4275073,-1.8552022,4.3868576,-6.1
358712,-9.5105758\PG=C01 [X(C13H17F1N3O5)]\\@

7.M062X_6-31pGd_opt

1\1\GINC-R3812\FOpt\RM062X\Gen\C10H12F1N3O3\ROOT\04-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483
648\\2Nitro4FluroNside.M062X_6-31pGd_opt\\0,1\C,-1.0352678055,2.036279
399,0.4335330475\C,0.318954075,1.4442677246,0.049933106\C,1.4302717083
,2.4809518289,0.1538324012\N,2.7106141557,1.8952699927,-0.2171995475\C
,3.8708598619,2.5614737557,0.0526486769\O,3.9042813274,3.6074264633,0.
6892938521\N,4.9972788279,1.9068629247,-0.4557861809\C,6.312317588,2.3
181790852,-0.3910800272\C,7.3644533904,1.5406724905,-0.9512319958\C,6.
6777887645,3.530571848,0.2249560082\C,8.0036734159,3.9049305708,0.2589
34644\C,9.0412181228,3.1515251359,-0.2846028517\C,8.6978265154,1.96182
86222,-0.8908801088\H,-1.8284371654,1.2876699411,0.3567820672\H,-1.298
8014596,2.8735236115,-0.2213985301\H,0.272340478,1.0574717064,-0.97739
77919\H,0.5601221078,0.5956410796,0.7011145145\H,1.5200381887,2.849420
0718,1.1797210141\H,1.2068977087,3.3486737469,-0.4825534905\H,2.706764
9081,1.162758537,-0.9153294545\H,5.9240694621,4.1623674563,0.672677997
5\F,8.3107997157,5.0652093172,0.8537883752\N,7.1400764495,0.2665364015
,-1.6220770058\H,10.0656374367,3.4983385991,-0.2247386039\O,8.09902786
65,-0.3207647954,-2.0843715113\O,5.9917389557,-0.1756668701,-1.7009136
117\H,-1.0219289235,2.4076542079,1.4635753727\H,4.8668511064,1.0035652
741,-0.8977444736\H,9.4537932168,1.3264318737,-1.3347258921\\Version=E
S64L-G09RevE.01\State=1-A\HF=-877.6632646\RMSD=8.727e-09\RMSF=2.068e-0
6\Dipole=-0.8554689,-0.1352166,-0.1707841\Quadrupole=14.6916499,-10.80
73033,-3.8843466,5.7497949,2.2093733,-6.0460769\PG=C01 [X(C10H12F1N3O3
)]\\@

7_propanoate.M062X_6-31pGd_bsse

1\1\GINC-R3747\SP\RM062X\Gen\C13H17F1N3O5(1-)\ROOT\21-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671088
640\\2Nitro4Fluro_OS_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-1.1297360717,2.
3964663439,1.119823652\C,0,0.0220389649,2.2519398472,0.1277236605\C,0,
1.3723773182,2.5076111547,0.7889029145\N,0,2.4371352014,2.2922401897,-
0.1655555889\C,0,3.6849726872,2.7430983417,0.0983367986\O,0,3.98168553
67,3.3466031099,1.0454266173\N,0,4.6275253398,2.2757149579,-0.82725848
21\C,0,5.9724798625,2.515543343,-0.7162276324\C,0,6.5624079888,3.72370
27227,-0.2886329181\C,0,6.8501682752,1.4609049261,-1.0520908211\C,0,8.
2076047841,1.6295826765,-0.9046695791\C,0,8.7904937954,2.7954342952,-0
.4144263475\C,0,7.9394579256,3.8451155029,-0.1087361243\H,0,-2.0975897
422,2.224915508,0.6371843423\H,0,-1.1468735781,3.4005539422,1.56037118
66\H,0,-0.10045457,2.9566794022,-0.7035913154\H,0,0.0245044916,1.24743

66228,-0.3128865024\H,0,1.4890789871,1.8470734548,1.6641000921\H,0,1.4
389750588,3.5368961175,1.1579551905\H,0,2.3096726042,1.5330629141,-0.8
588104976\H,0,6.4339869116,0.5186707578,-1.4000974964\F,0,9.0247718742
,0.6010078017,-1.2269002991\N,0,5.8007243087,4.967410592,-0.1566095338
\H,0,9.8658208157,2.8681825393,-0.3013975589\O,0,6.1767234063,5.774631
3394,0.6810016511\O,0,4.8987091014,5.166357629,-0.9474404129\H,0,-1.03
31709942,1.6762377865,1.9407523237\H,0,4.3909752855,1.3844463705,-1.32
06750411\H,0,8.3261834916,4.7920899598,0.2506022672\O,0,4.2550600381,-
0.1632620162,-2.0456000495\O,0,2.0288813997,0.0819811224,-1.876616107\
C,0,3.0632086793,-0.5342100038,-2.2347328328\C,0,2.8422663648,-1.86418
04944,-2.9733029244\C,0,4.1233174845,-2.5808007956,-3.3819876591\H,0,2
.2173696447,-1.6438725652,-3.8476722675\H,0,2.2272904792,-2.495642009,
-2.3201589564\H,0,4.7276270009,-1.9470350564,-4.0373168526\H,0,3.90338
23387,-3.5187366042,-3.9067291366\H,0,4.7361975098,-2.8073017264,-2.50
46977594\\Version=ES64L-G09RevE.01\State=1-A\HF=-267.7284743\RMSD=4.10
5e-09\Dipole=0.6522519,-0.4939089,0.1235596\Quadrupole=3.9437066,-10.1
848382,6.2411316,-1.8009603,-1.9030818,-11.972177\PG=C01 [X(C13H17F1N3
O5)]\\@

13.M062X_6-31pGd_opt_water
1\1\GINC-R4385\FOpt\RM062X\Gen\C11H12F3N3O3\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=h2o) maxdisk=2684354560\\3TMF4Nitro.M062X_6-31pGd_opt_water\\0,1\C,
-1.9658583651,1.7695463288,-0.0806185923\C,-0.5748401399,1.1463961009,
-0.0305590128\C,0.5063299695,2.216108136,-0.0490110062\N,1.8263642127,
1.5984374705,-0.0000821539\C,2.9454696501,2.3446251474,-0.0058065997\O
,2.9248691756,3.5811891951,-0.0534855861\N,4.124626415,1.6091318544,0.
0466079608\C,5.4266422861,2.0726650522,0.0544016583\C,5.7725297188,3.4
370215379,-0.0002268114\C,6.4509666772,1.1159961964,0.1197849502\C,7.7
722455996,1.5126936927,0.1305456401\C,8.1086522995,2.8643317224,0.0767
05958\C,7.0990477618,3.843902737,0.0101327904\H,-2.7407901678,0.997521
9055,-0.0674054174\H,-2.0964904253,2.3635387404,-0.9918183894\H,-2.131
0648046,2.4285530951,0.7787918005\H,-0.4328059774,0.4754882938,-0.8866
41676\H,-0.4671247412,0.5406127915,0.8775174936\H,0.3889532993,2.88838
78603,0.8087869112\H,0.4237131695,2.8226806228,-0.9582852559\H,1.88682
29705,0.5864361641,0.0399825723\H,4.0270808005,0.5981791982,0.08690422
95\H,4.9872875817,4.1737619263,-0.051189859\H,6.2045612467,0.059321554
1,0.1623503465\C,7.329136288,5.3463141309,-0.0539291145\F,6.1608984364
,6.0127638745,-0.1111521995\F,8.0137372387,5.7235553182,-1.145443386\F
,7.9644922531,5.8239192891,1.0280049278\N,9.5287044493,3.1772535021,0.
093655538\O,10.3272100878,2.249811702,0.1525131333\O,9.8747021929,4.34
76421223,0.0493661491\H,8.5596508371,0.7710427371,0.1814030004\\Versio
n=ES64L-G09RevE.01\State=1-A\HF=-1115.4153608\RMSD=7.192e-09\RMSF=2.13
1e-05\Dipole=-4.1935416,-4.7697022,0.1108934\Quadrupole=-12.3248682,11
.5609379,0.7639304,6.9454957,-0.5307636,-0.3262755\PG=C01 [X(C11H12F3N
3O3)]\\@

13.M062X_6-31pGd_opt_Pentadecane
1\1\GINC-R3884\FOpt\RM062X\Gen\C11H12F3N3O3\ROOT\22-Feb-2019\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,Solve
nt=n-Pentadecane) maxdisk=2684354560\\3TMF4Nitro.M062X_6-31pGd_opt_Pen
tadecane\\0,1\C,-1.9776202957,1.8025031131,-0.0902413331\C,-0.59628399
75,1.1770732272,0.0804641007\C,0.5096733242,2.1871804746,-0.1943910193
\N,1.8174743754,1.5645733385,-0.0308023587\C,2.9428021468,2.3306752562
,0.0037466875\O,2.9194036241,3.5519794142,0.0059301471\N,4.1230667502,
1.5884517518,0.0632940743\C,5.4280725587,2.0641138822,0.0726966238\C,5
.7571775316,3.4314243869,0.0645937364\C,6.4609050716,1.1155917155,0.10
75382134\C,7.7845264951,1.5164537338,0.1091293083\C,8.0975911542,2.869
0113039,0.0580562699\C,7.0863286701,3.8360600248,0.0471380313\H,-2.767
300252,1.0723755889,0.1096355042\H,-2.1179075543,2.1775396555,-1.10991
72785\H,-2.1157780654,2.6429926083,0.5984535757\H,-0.4922080708,0.3248
591225,-0.6050363617\H,-0.4805950593,0.7879852613,1.0993752209\H,0.447
4409518,3.0244578528,0.5064957016\H,0.4075773392,2.6009486145,-1.20697
17068\H,1.8918274198,0.577955157,-0.2469341351\H,4.0304002233,0.581366
0363,-0.1264764381\H,4.9678232697,4.1686211059,0.0861363496\H,6.2241552
612,0.0552940067,0.1284377876\C,7.3552720749,5.3297298827,0.0947552479
\F,6.2605445203,5.9972393958,0.4988900063\F,7.6878165344,5.8372453438,
-1.0981652605\F,8.3283812406,5.6340452721,0.9674506296\N,9.5195993838,
3.209815263,-0.0253700944\O,10.3081659488,2.4624502486,0.5309160954\O,
9.8310142228,4.1915999457,-0.6734378532\H,8.5863732026,0.7872180161,0.
1336676519\\Version=ES64L-G09RevE.01\State=1-A\HF=-1115.4098895\RMSD=9
.956e-09\RMSF=4.284e-06\Dipole=-3.3528451,-3.5115204,-0.1106912\Quadru
pole=-7.5140199,8.8459824,-1.3319625,4.1844033,1.3057368,2.0295117\PG=

C01 [X(C11H12F3N3O3)]\\@

13_propanoate.M062X_6-31pGd_bsse
1\1\GINC-R3741\SP\RM062X\Gen\C14H17F3N3O5(1-)\ROOT\21-Feb-2019\0\\# M0
62X/Gen 6D SCF=Tight INT(grid=ultrafine) Counterpoise=2 maxdisk=671088
640\\3TMF4Nitro_EtO.M062X_6-31pGd_bsse\\-1,1\C,0,-2.1722391602,2.33648
54292,0.0288168634\C,0,-0.8072702157,1.6558326114,-0.0380522485\C,0,0.
3288473265,2.6703114776,0.0241364934\N,0,1.6013033822,1.9862647428,-0.
0418431479\C,0,2.7508738913,2.6905949403,0.0022655287\O,0,2.7988579333
,3.9178098533,0.0974655628\N,0,3.8821447947,1.872672689,-0.0716291428\
C,0,5.1912545365,2.2612686797,-0.0505714259\C,0,5.628347117,3.60588775
84,0.0191291486\C,0,6.1642357428,1.239509341,-0.1226466602\C,0,7.50640
76405,1.5542025436,-0.098785673\C,0,7.9284046706,2.8804285157,0.009577
2806\C,0,6.9795446292,3.9174455414,0.057203102\H,0,-2.9851196651,1.604
4966154,-0.0159193457\H,0,-2.3049408311,3.0364722735,-0.8046108831\H,0
,-2.2838795461,2.9053335352,0.9594718642\H,0,-0.7153377429,1.069821114
8,-0.960100357\H,0,-0.6945927909,0.9399238662,0.7846429553\H,0,0.26693
54063,3.2578300181,0.9513886557\H,0,0.2456411586,3.3888735979,-0.80394
36705\H,0,1.6061389996,0.9508743887,-0.123368046\H,0,3.7286645924,0.83
91002873,-0.1433673094\H,0,4.8848776664,4.3897802354,0.0281236317\H,0,
5.8308519051,0.2069389434,-0.1905046146\C,0,7.3365214364,5.3922129271,
0.070874928\F,0,6.2659346773,6.1513458064,-0.2345721331\F,0,8.27475150
4,5.6980526388,-0.8430817347\F,0,7.7626601259,5.8255526885,1.266573998
3\N,0,9.3618195749,3.1030020141,0.1127336989\O,0,10.1080472359,2.23612
44652,-0.3279026509\O,0,9.7535587102,4.122340404,0.6579032828\H,0,8.25
83740229,0.7752440434,-0.1467498728\O,0,1.4918541706,-0.8029655917,-0.
2573317722\O,0,3.7356564194,-0.8609038907,-0.2595479306\C,0,2.59567443
83,-1.4019775371,-0.2983899165\C,0,2.5373001381,-2.932958525,-0.405853
6117\C,0,3.8984417199,-3.6159985994,-0.4514571662\H,0,1.9469536933,-3.
1686319092,-1.2999091959\H,0,1.9438604769,-3.2910707473,0.4444146069\H
,0,4.4805563127,-3.2608513632,-1.3066804669\H,0,3.792807737,-4.7049356
365,-0.5283289059\H,0,4.4773361651,-3.3844101868,0.4472462808\\Version
=ES64L-G09RevE.01\State=1-A\HF=-267.7283856\RMSD=4.138e-09\Dipole=-0.7
121311,0.0014285,-0.0400603\Quadrupole=-23.0707935,-3.853867,26.924660
5,-19.3131138,-1.6812656,-3.279839\PG=C01 [X(C14H17F3N3O5)]\\@

13.M062X_6-31pGd_opt
1\1\GINC-R4500\FOpt\RM062X\Gen\C11H12F3N3O3\ROOT\30-Oct-2018\0\\# M062
X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354
560\\3TMF4Nitro.M062X_6-31pGd_opt\\0,1\C,-1.9742617108,1.8081430099,-0
.0743695693\C,-0.5979881938,1.1567532736,0.041399076\C,0.5183664618,2.
1733536185,-0.1588726302\N,1.8221393759,1.5290110584,-0.0453994365\C,2
.9457757133,2.3094894675,0.0347638849\O,2.9092410257,3.5221504368,0.13
22635068\N,4.1308980638,1.5715892349,0.029740871\C,5.4356186189,2.0582
333087,0.0620162185\C,5.7519439037,3.4266046246,0.0374284985\C,6.47332
97834,1.1185424186,0.1248147935\C,7.7939255906,1.5308174969,0.14043570
59\C,8.0964148976,2.8846153733,0.0748085108\C,7.0786995758,3.842315559
1,0.0340899126\H,-2.7711822265,1.0741265791,0.0721825569\H,-2.11314200
46,2.2628061725,-1.0609042435\H,-2.098867125,2.594374661,0.6774641467\
H,-0.5069220117,0.3576899585,-0.7076542375\H,-0.481067923,0.6877261511
,1.0255231131\H,0.4720571883,2.9534405162,0.6057165612\H,0.4175323368,
2.6705390481,-1.1337652116\H,1.9044140171,0.605826923,-0.4529969127\H,
4.0433024454,0.5673805647,0.1154476273\H,4.9562756426,4.1574343408,0.0
404785465\H,6.2447774601,0.0564592484,0.1585816452\C,7.331696866,5.342
5798193,0.0568299258\F,6.2160761973,6.0014106888,0.415636203\F,7.68969
67997,5.8224866796,-1.1377286734\F,8.2740748502,5.671815069,0.95089076
84\N,9.5222919386,3.2310767065,0.0117549002\O,10.3009411288,2.47755959
01,0.571921867\O,9.8349201249,4.2181475989,-0.6238281177\H,8.604741189
6,0.8134308036,0.1933765923\\Version=ES64L-G09RevE.01\State=1-A\HF=-11
15.3915663\RMSD=2.107e-09\RMSF=2.631e-06\Dipole=-2.9671422,-2.9888594,
-0.2429525\Quadrupole=-6.3576759,7.3458022,-0.9881263,3.2836212,1.7880
44,2.1060722\PG=C01 [X(C11H12F3N3O3)]\\@

13_propanoate.M062X_6-31pGd_opt_water
1\1\GINC-R3777\FOpt\RM062X\Gen\C14H17F3N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=h2o) maxdisk=3221225472\\3TMF4Nitro_EtO.M062X_6-31pGd_opt_water
\\-1,1\C,-2.1497372383,2.3558095669,0.032056354\C,-0.7965743427,1.6551
470486,-0.0359306698\C,0.3431651485,2.6628645178,-0.0038610415\N,1.627
3696908,1.9788990849,-0.0729785432\C,2.7748068282,2.6767210777,-0.0480
69852\O,2.8100120877,3.917601678,0.0137967615\N,3.9156578568,1.8864562
477,-0.1029935257\C,5.2308060483,2.2937973929,-0.0636854412\C,5.645845
7562,3.6411820475,-0.0053871103\C,6.2129780764,1.2864790419,-0.1013646

387\C,7.5534537693,1.610447077,-0.054026888\C,7.9486152141,2.943013049
2,0.0437543881\C,6.9912157753,3.9696689214,0.0555912517\H,-2.969319053
2,1.6314447663,0.0085375802\H,-2.2795946632,3.0398239587,-0.8140017464
\H,-2.2421812921,2.9398502347,0.9545018304\H,-0.7272177283,1.058650557
9,-0.9539284361\H,-0.6903441463,0.9611097768,0.8068341951\H,0.29095219
11,3.2586974494,0.9160660816\H,0.2534149777,3.3583833369,-0.847111791\
H,1.6365733651,0.9489650259,-0.0688869041\H,3.7693720058,0.8631973325,
-0.1776354732\H,4.9046770937,4.4247699292,-0.0240500946\H,5.9100931097
,0.2453074957,-0.1579254993\C,7.331537824,5.4471038318,0.0511639485\F,
6.2716159994,6.1876011756,-0.3190788055\F,8.3124077104,5.7434563505,-0
.8189925822\F,7.6997127932,5.9079479893,1.2578965535\N,9.370342344,3.1
94109839,0.175261244\O,10.1488671999,2.3644652149,-0.2797795741\O,9.73
43454546,4.206684092,0.7570600473\H,8.3060360328,0.8302267385,-0.06343
73628\O,1.4561824748,-0.8985211766,-0.0241019346\O,3.6658276366,-0.924
952448,-0.3561204744\C,2.5493901004,-1.5054859195,-0.227489709\C,2.486
007491,-3.0271315799,-0.3177781091\C,3.8158058383,-3.720422424,-0.5776
864844\H,1.7616464779,-3.2687172054,-1.1048567827\H,2.0398143437,-3.38
20858851,0.6190795491\H,4.2564437932,-3.3901303527,-1.5234644541\H,3.6
764702217,-4.8048218722,-0.630101281\H,4.5350657335,-3.5102829837,0.21
9945421\\Version=ES64L-G09RevE.01\State=1-A\HF=-1383.2755413\RMSD=7.99
4e-09\RMSF=2.715e-06\Dipole=-0.5132885,-0.3203964,-0.1192825\Quadrupol
e=-21.6140632,-2.679299,24.2933622,-23.1018033,-1.3205378,-2.9452925\P
G=C01 [X(C14H17F3N3O5)]\\@

13_propanoate.M062X_6-31pGd_opt

1\1\GINC-R4165\FOpt\RM062X\Gen\C14H17F3N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=322
1225472\\3TMF4Nitro_EtO.M062X_6-31pGd_opt\\-1,1\C,-2.1722391602,2.3364
854292,0.0288168634\C,-0.8072702157,1.6558326114,-0.0380522485\C,0.328
8473265,2.6703114776,0.0241364934\N,1.6013033822,1.9862647428,-0.04184
31479\C,2.7508738913,2.6905949403,0.0022655287\O,2.7988579333,3.917809
8533,0.0974655628\N,3.8821447947,1.872672689,-0.0716291428\C,5.1912545
365,2.2612686797,-0.0505714259\C,5.628347117,3.6058877584,0.0191291486
\C,6.1642357428,1.239509341,-0.1226466602\C,7.5064076405,1.5542025436,
-0.098785673\C,7.9284046706,2.8804285157,0.0095772806\C,6.9795446292,3
.9174455414,0.057203102\H,-2.9851196651,1.6044966154,-0.0159193457\H,-
2.3049408311,3.0364722735,-0.8046108831\H,-2.2838795461,2.9053335352,0
.9594718642\H,-0.7153377429,1.0698211148,-0.960100357\H,-0.6945927909,
0.9399238662,0.7846429553\H,0.2669354063,3.2578300181,0.9513886557\H,0
.2456411586,3.3888735979,-0.8039436705\H,1.6061389996,0.9508743887,-0.
123368046\H,3.7286645924,0.8391002873,-0.1433673094\H,4.8848776664,4.3
897802354,0.0281236317\H,5.8308519051,0.2069389434,-0.1905046146\C,7.3
365214364,5.3922129271,0.070874928\F,6.2659346773,6.1513458064,-0.2345
721331\F,8.274751504,5.6980526388,-0.8430817347\F,7.7626601259,5.82555
26885,1.2665739983\N,9.3618195749,3.1030020141,0.1127336989\O,10.10804
72359,2.2361244652,-0.3279026509\O,9.7535587102,4.122340404,0.65790328
28\H,8.2583740229,0.7752440434,-0.1467498728\O,1.4918541706,-0.8029655
917,-0.2573317722\O,3.7356564194,-0.8609038907,-0.2595479306\C,2.59567
44383,-1.4019775371,-0.2983899165\C,2.5373001381,-2.932958525,-0.40585
36117\C,3.8984417199,-3.6159985994,-0.4514571662\H,1.9469536933,-3.168
6319092,-1.2999091959\H,1.9438604769,-3.2910707473,0.4444146069\H,4.48
05563127,-3.2608513632,-1.3066804669\H,3.792807737,-4.7049356365,-0.52
83289059\H,4.4773361651,-3.3844101868,0.4472462808\\Version=ES64L-G09R
evE.01\State=1-A\HF=-1383.207903\RMSD=5.516e-09\RMSF=3.717e-06\Dipole=
-0.7117307,0.030075,-0.0379697\Quadrupole=-23.0082046,-4.0509797,27.05
91843,-19.4503144,-1.6907912,-3.3042036\PG=C01 [X(C14H17F3N3O5)]\\@

13_propanoate.M062X_6-31pGd_opt_Pentadecane

1\1\GINC-R4197\FOpt\RM062X\Gen\C14H17F3N3O5(1-)\ROOT\19-Feb-2019\0\\#
M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) SCRF=(SMD,S
olvent=n-Pentadecane) maxdisk=3221225472\\3TMF4Nitro_EtO.M062X_6-31pGd
_opt_Pentadecane\\-1,1\C,-2.1825420614,2.3525563062,0.0189703177\C,-0.
8209839876,1.6653241011,-0.0265687125\C,0.3181487691,2.6754301606,0.04
20352114\N,1.5936649197,1.9891684308,-0.0076758382\C,2.7457533183,2.68
846435,0.0228015021\O,2.7977146021,3.9183089119,0.0968328744\N,3.87623
32281,1.871353562,-0.0381011114\C,5.1876481964,2.2610797961,-0.0279687
77\C,5.6244700807,3.6062611295,0.0082911805\C,6.1605475034,1.238982457
9,-0.0788722845\C,7.5037502775,1.5513751198,-0.0631835808\C,7.92332915
86,2.8794427197,0.0156477044\C,6.9758342188,3.9168770475,0.038385433\H
,-2.9965227278,1.622028601,-0.0301419657\H,-2.3042118591,3.0456006012,
-0.8218727644\H,-2.3049557192,2.9277467129,0.9443313811\H,-0.723191641
3,1.0753426925,-0.9457566036\H,-0.7242462005,0.9571576723,0.8051064436
\H,0.2460843235,3.265760689,0.9660091432\H,0.2445301421,3.3870398269,-