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Heterocycles as Supramolecular Handles for Crystal Engineering: A Case Study with 7-Diethylaminocoumarin Derivatives

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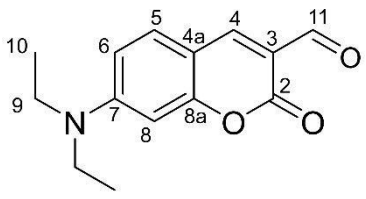
Experimental Section

All reagents used were obtained from commercial suppliers and used without further purification. Solvents were dried using standard methods or distilled prior to use. Reactions were monitored by TLC on precoated silica gel plates (Aldrich Silica gel on TLC plates with 254 nm fluorescent indicator) and revealed by exposure to an UV lamp. Melting points were measured using open glass capillaries in Electrothermal Digital Programmable Melting Point Apparatus (Cole-Parmer) and are uncorrected. IR spectra were recorded using Attenuated Total Reflectance (ATR) as solid samples on a Perkin Elmer FTIR Spectrometer Spectrum Two and units are stated as cm^{-1}. ^{1}H and ^{13}C NMR spectra were recorded using a Bruker 400 MHz spectrometer; chemical shifts (δ, ppm) are reported relative to $CDCl_3$. High-resolution mass spectra were acquired with Bruker micrOTOF-Q II spectrometer.

Synthesis of 7-(diethylamino)coumarin-3- carbaldehyde, compound **2**.

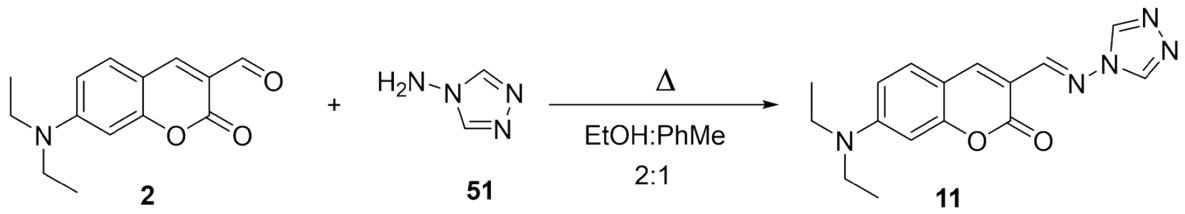
Compound **2** was synthesized from 4-(diethylamino)salicylaldehyde in two steps according to a literature procedure[1,2] to give an orange solid. Rf = 0.2 (hexane/ethyl acetate, 8:2) Yield: 79%.



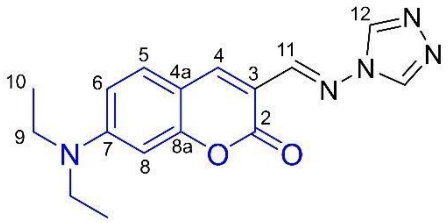
Melting point: 163–165 °C. ^{1}H-NMR (400 MHz, $CDCl_3$, δ, ppm): 10.10 (s, 1H, H-11), 8.23 (s, 1H, H-4), 7.40 (d, J = 9.0 Hz, 1H, H-5), 6.62 (dd, J = 9.0, 2.5 Hz, 1H, H-6), 6.47 (d, J = 2.5 Hz, 1H, H-8), 3.46 (q, J = 7.2 Hz, 4H, H-9), 1.24 (t, J = 7.2 Hz, 6H, H-10). ^{13}C-NMR (75 MHz, $CDCl_3$, δ, ppm): 188.0 (C-11), 162.0 (C-2), 159.0 (C-8a), 153.6 (C-7), 145.5 (C-4), 132.6 (C-5), 114.4 (C-3), 110.3 (C-6), 108.3 (C-4a), 97.2 (C-8), 45.4 (C-9), 12.6 (C-10).

Synthesis of (*E*)-3-(((4*H*-1,2,4-triazol-4-yl)imino)methyl)-7-(diethylamino)-2*H*-chromen-2-one, compound 11:

In a round bottom flask equipped with a Dean-Stark distillation trap, 4-amino-4*H*-1,2,4-triazole (0.017 g, 0.2 mmol) and 7-diethylaminocoumarin-3-aldehyde (0.05 g, 0.2 mmol) were suspended in 5mL of a 2:1 mixture of EtOH and toluene. The mixture was stirred at reflux temperature for 150 h, frequently draining the Dean-Stark trap and adding more solvent mixture accordingly (**Scheme 1**). The product was formed as an orange precipitate. The solution was cooled in an ice bath, the solid was filtered and washed with cold toluene. The crude product was purified by chromatography on silica gel, starting with CH_2Cl_2 100%, followed by a linear gradient of CH_2Cl_2: Acetone until 8:2, to give the product as a bright orange solid that grows crystals from CH_2Cl_2 (0.16 mmol, 50 mg, 80 %). Rf = 0.15 (CH_2Cl_2: Acetone 9:1).



Scheme 1. Synthesis of Compound **11**.



Melting point (*from* CH_2Cl_2): 238–240 °C. FTIR (ATR, ν, cm^{-1}): 3105, 3080, 2968, 2950, 2930, 1701, 1603, 1570, 1516, 1502, 1478, 1424, 1351, 1255, 1188, 1180, 1127. ^{1}H-NMR (400 MHz, $CDCl_3$, δ, ppm): 8.75 (s, 1H, H-11), 8.57 (s, 2H, H-12), 8.40 (s, 1H, H-4), 7.40 (d, J = 9.0 Hz, 1H, H-5), 6.65 (dd, J = 9.0, 2.5 Hz, 1H, H-6), 6.49 (d, J = 2.5 Hz, 1H, H-8), 3.46 (q, J = 7.2 Hz, 4H, H-9), 1.24 (t, J = 7.2 Hz, 6H, H-10). ^{13}C-NMR (75 MHz, $CDCl_3$, δ, ppm): 161.4 (C-2), 158.1 (C-8a), 153.0 (C-7), 151.8 (C-11), 142.2 (C-4), 138.3 (C-12), 131.5 (C-5), 110.3 (C-6), 110.1 (C-3), 108.5 (C-4a), 97.3 (C-8), 45.3 (C-9), 12.6 (C-10). HRMS (ESI): calculated for $C_{16}H_{17}N_5O_2Na$ ($[M+Na]^+$) 334.1274, found $[C_{16}H_{17}N_5O_2+Na]^+$ 334.1283. Error: 2.693583 ppm.

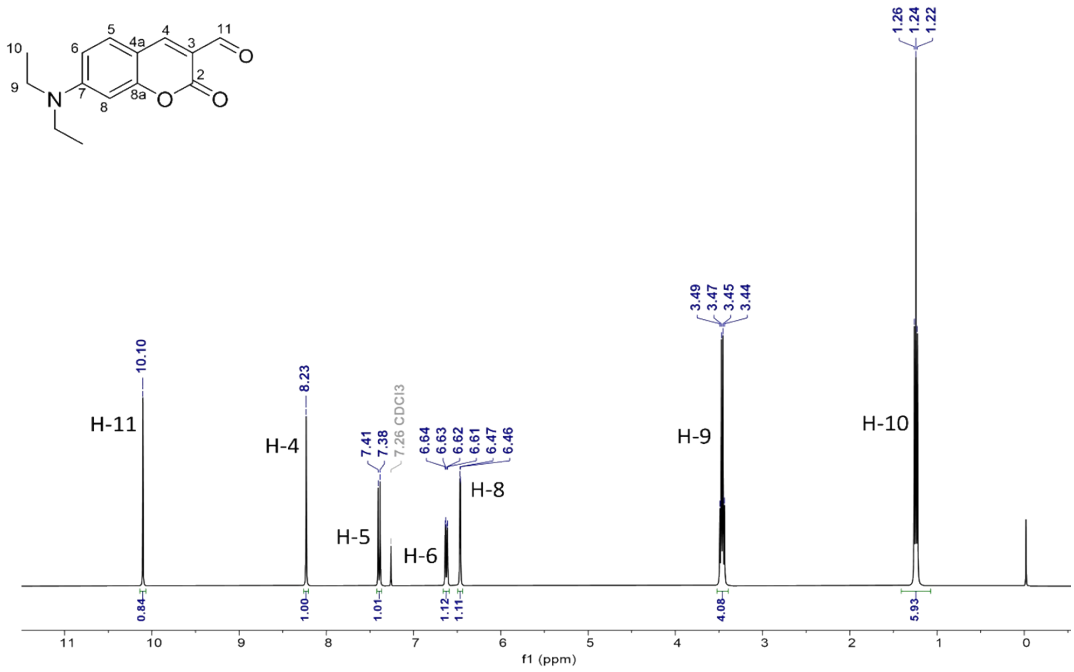


Figure S1. ^{1}H NMR spectrum of **Compound 2** in $CDCl_3$.

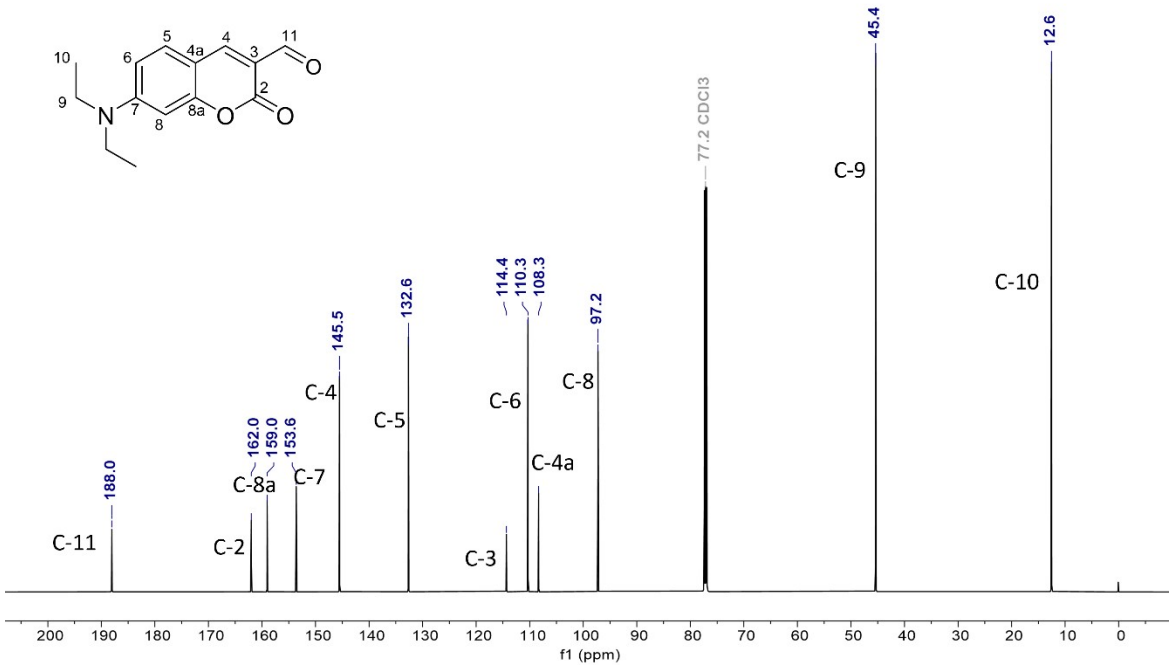


Figure S2. ^{13}C NMR spectrum of **Compound 2** in $CDCl_3$.

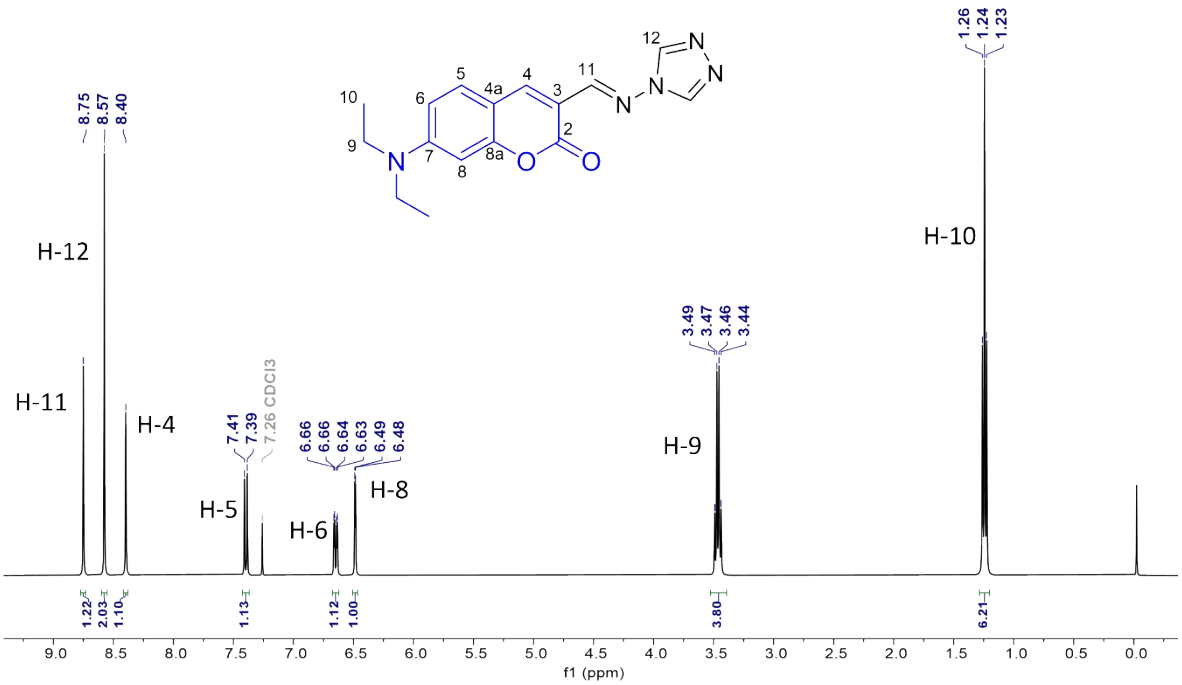


Figure S3. ^{1}H NMR spectrum of **Compound 11** in $CDCl_3$.

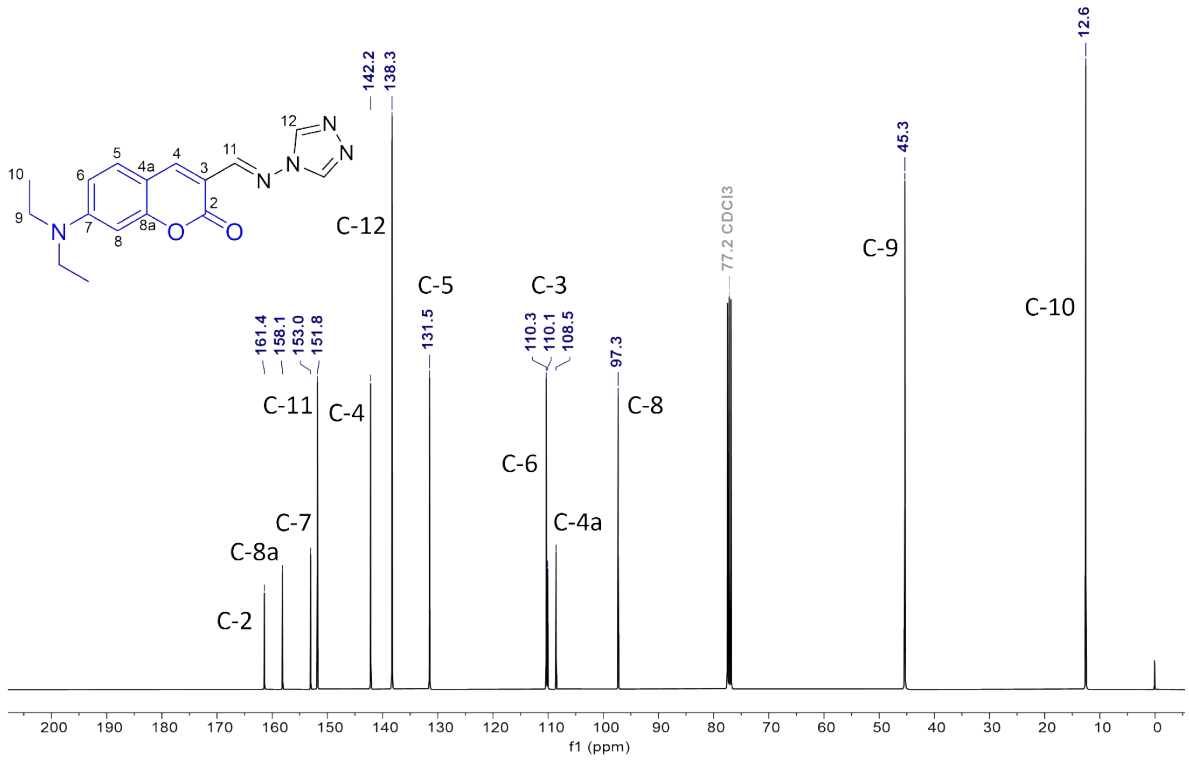


Figure S4. ^{13}C NMR spectrum of **Compound 11** in $CDCl_3$.

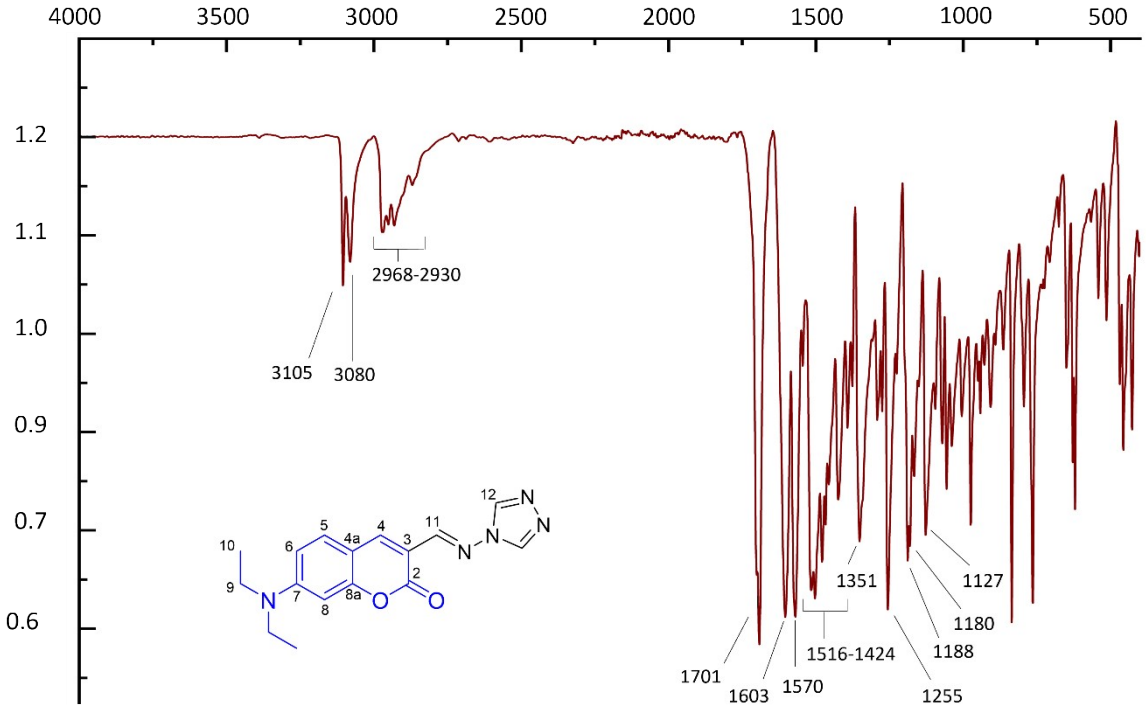


Figure S5. IR spectrum of **Compound 11**.

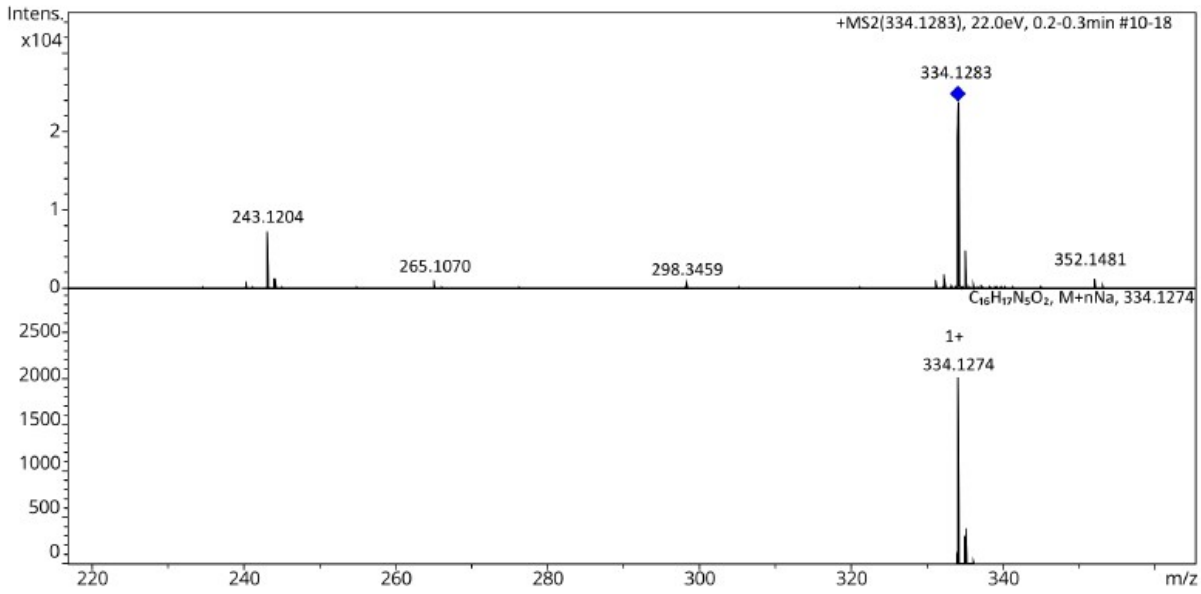


Figure S6. HRMS (ESI) of **Compound 11**.

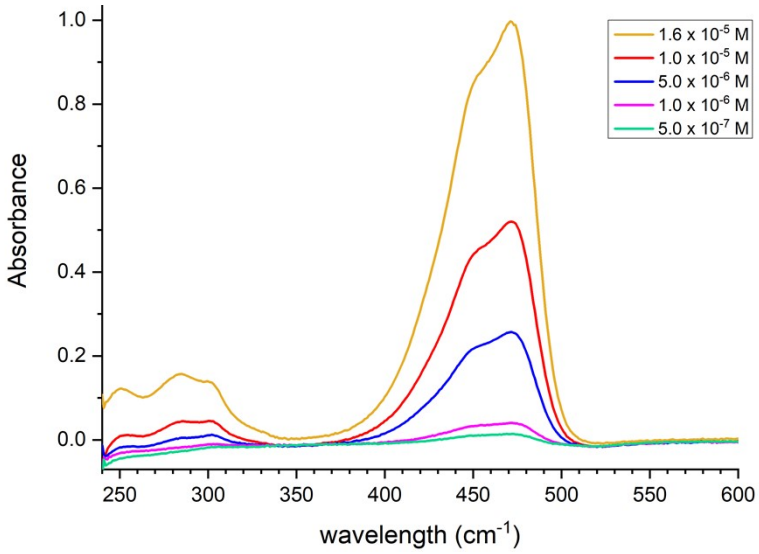


Figure S7. UV-Vis spectra of **Compound 11**.

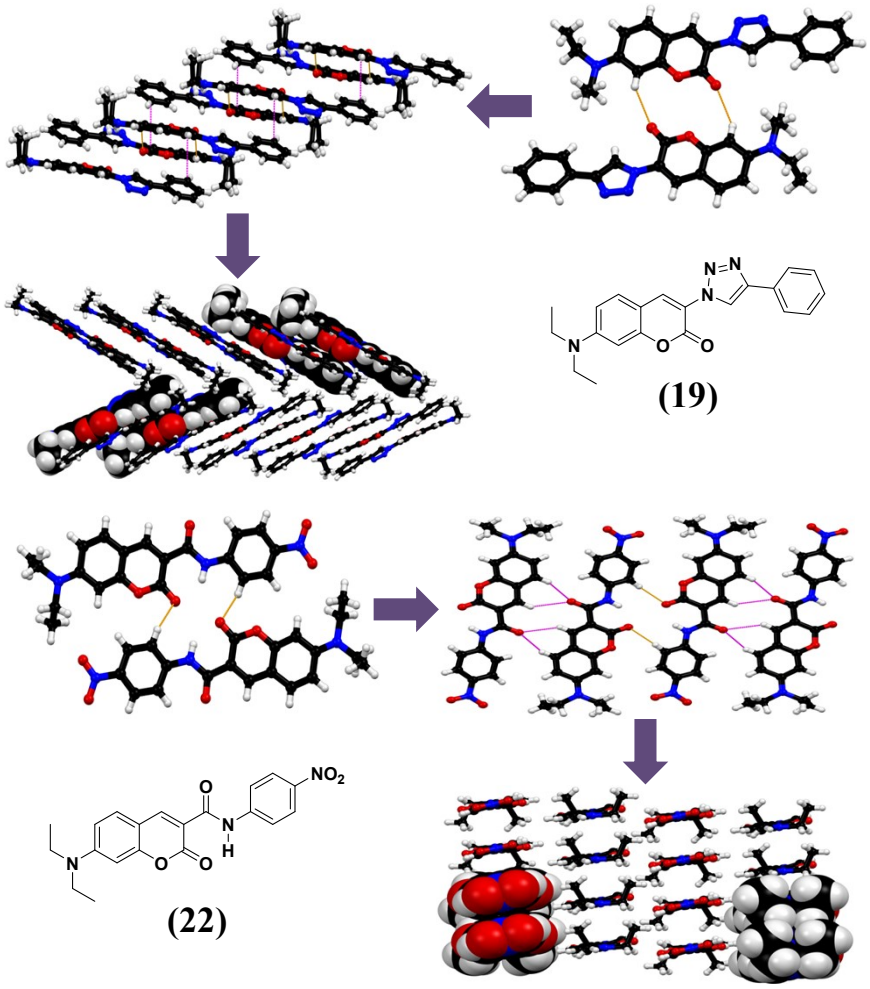


Figure S8. Selected examples (**19** and **22**) illustrate how the coumarin carbonyl group acts as a versatile handle in different supramolecular assemblies, demonstrating a cooperative effect with various substituents in a series of π-extended DAC-derivatives.

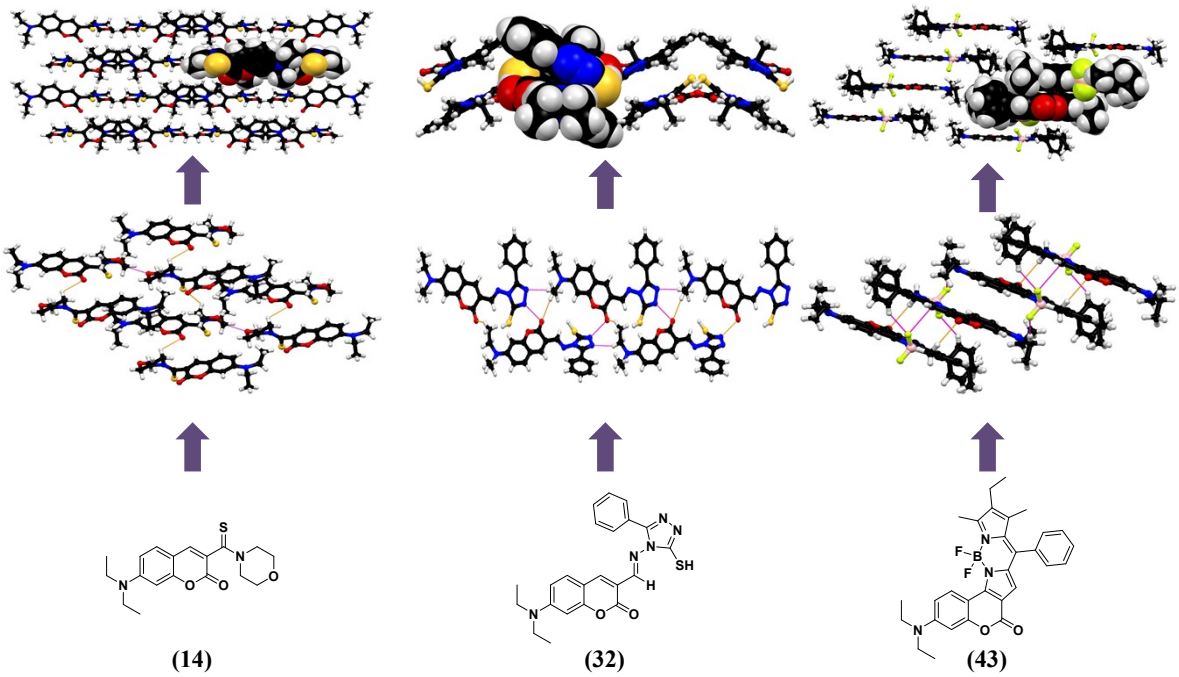


Figure S9. Selected examples where the structural features of substituents influence or override the interactions mediated by the coumarin carbonyl group.

Table S1. Crystallographic data of compound **11**.

Chemical formula: $C_{16}H_{17}N_5O_2$
Formula weight = 311.35
T = 122 K
Crystal system: Monoclinic Space group: P21/c
a = 14.3674(10)Å α = 90°
b = 10.3669(7)Å β = 103.365(7)°
c = 10.6054(6)Å γ = 90°
V = 1538.12(18) Å^3 Z = 4
Dx = 1.344 g/cm^3
Radiation: Mo Ka (l = 0.71073 Å)
μ(Mo Ka) = 0.093 mm^{-1} F(0 0 0) = 656.3
Crystal size = 0.1053 · 0.2728 · 0.4735 mm^3
No. of reflections collected = 4035
No. of independent reflections = 3267
$2\theta_{max}$ = 59.1˚ with Mo Ka
Theta range for data collection: 3.9530 to 29.249°
Index ranges: -18<=h<=19, -14<=k<=14, -14<=l<=14
Completeness to theta = 25.2417° 99.8%
Data/Restraints/Parameters = 3267/0/210
Final R indices [I>2sigma(I)] R1 = 0.0422, wR2 = 0.1308
R indices (all data): R1 = 0.0563, wR2 = 0.1474
Goodness-of-fit on F^2 = 1.0953
Largest diff. peak and hole (eÅ^{-3}): 0.3835, –0.2745
Refinement method: Full-matrix least-squares on F^2
Measurement: Oxford Diffraction Gemini Atlas diffractometer
Data collection & cell refinement program: CrysAlisPro and CrysAlisRED
Structure solving & refinement program: OLEX2
CCDC: 2338583

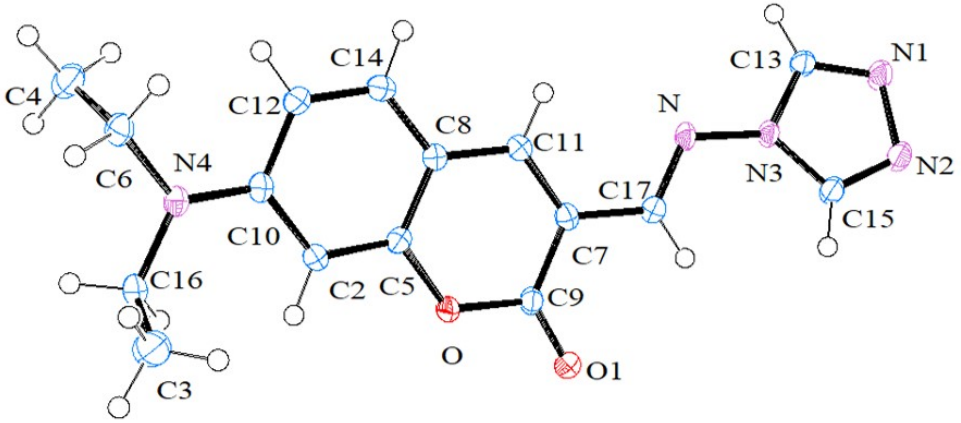


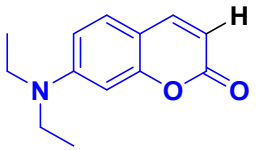
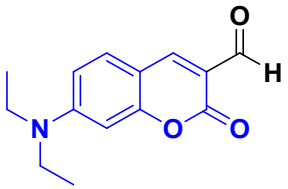
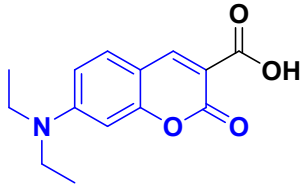
Table S2. Crystallographic data of DAC-derivatives retrieved from the crystallography open database. employed in the comparative study of DAC-derivatives as supramolecular structure-directing groups.

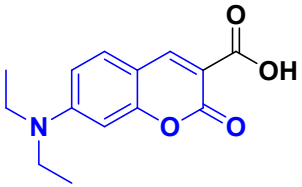
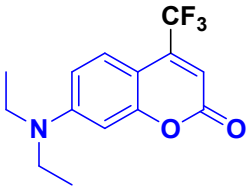
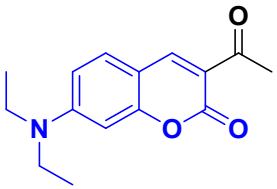
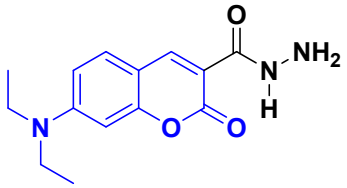
ID	*DAC*	*Space group*	*Z, Z'*	*a* (Å)	*b* (Å)	*c* (Å)	A (degrees)	β (degrees)	γ (degrees)	*ρ* (g/cm^3)	*Crystallized from*	*Reference*
1438103	1	P-1	2, 1	6.8714	8.7065	10.0466	93.938	104.204	106.910	1.31	acetone	J. Mol. Struct. (2017), 1130, 914-921, doi:10.1016/j.molstruc.2016.10.080
2230615	2	C 2/c	8, 1	13.33	13.33	12.60	92.28	92.28	34.21	1.21	dichloromethane/ petroleum	Acta Crystallographica Section E (2011), 67, o1713, doi:10.1107/S160053681102294X
1553722	3	P-1	2, 1	5.08	10.06	12.91	76.26	80.91	81.18	1.38	diethyl ether/ethyl acetate	Materials Chemistry Frontiers (2018), 2, 910, doi:10.1039/C7QM00617A
2209698	3	P 2_1/c	4, 1	14.12	7.75	12.63	90.00	116.48	90.00	1.40	chloroform	Acta Crystallographica Section E (2006), 62, o3076, doi:10.1107/S160053680602321X
2000551	4	P-1	8, 4	14.39	18.84	10.19	90.15	98.72	85.49	1.39	cyclohexane	Acta Crystallographica Section C (1992), 48, 1859, doi:10.1107/S0108270192000623
2208873	5	C 2/c	8, 1	9.42	9.42	22.09	106.93	106.93	47.06	1.27	ethanol	Acta Crystallographica Section E (2006), 62, o2072, doi:10.1107/S1600536806014899
7117321	6	P-1	4, 2	9.21	12.62	12.93	94.78	109.99	105.42	1.37	ethanol	Chem.Commun. (2015), 51, 10435, doi:10.1039/C5cc03972J
2229947	6	P-1	4, 2	9.34	12.77	12.98	95.17	110.13	106.18	1.34	dichloromethane/ petroleum	Acta Crystallographica Section E (2011), 67, o1107, doi:10.1107/S1600536811010944
2206681	7	P $2_12_12_1$	4, 1	6.60	14.36	14.55	90.00	90.00	90.00	1.25	ethanol	Acta Crystallographica Section E (2005), 61, o3041, doi:10.1107/S1600536805026607
1551651	8	P-1	2, 1	7.43	9.09	11.25	105.51	93.33	111.01	1.40	chloroform/ methanol	X-ray Structure Analysis Online (2014), 30, 21, doi:10.2116/xraystruct.30.21
1551552	9	C 2/c	8, 1	11.65	11.65	13.14	115.59	115.59	69.24	1.33	chloroform	X-ray Structure Analysis Online (2018), 34, 3, doi:10.2116/xraystruct.34.3
8102531	10	P 2_1/c	4, 1	6.74	15.85	13.38	90.00	97.36	90.00	1.36	ethanol	Zeitschrift für Kristallographie - New Crystal Structures (2009), 224, 593
2338583	11	P 2_1/c	4, 1	14.36	10.36	10.60	90.00	103.16	90.00	1.34	dichloromethane	**This work**
2243765	12	P 2_1/c	4, 1	13.72	13.05	8.56	90.00	95.52	90.00	1.31	acetone	Acta Crystallographica Section E (2021), 77, 331, doi:10.1107/S2056989021002218
7101415	13	P 2_1/c	8, 2	14.98	16.93	13.55	90.00	99.48	90.00	1.24	methanol	Chem.Commun., (2006), 3886, doi:10.1039/b609861d
4517186	14	C c	4, 1	11.73	11.73	8.62	109.82	109.82	110.45	1.29	hexane/ethyl acetate	ACS Chem. Neuroscience (2019), 10, 4847, doi:10.1021/acschemneuro.9b00554
2003249	15	P-1	2, 1	8.96	11.14	8.92	95.14	104.50	86.74	1.36	ethanol	Acta Crystallographica Section C (1995), 51, 531, doi:10.1107/S0108270194003628

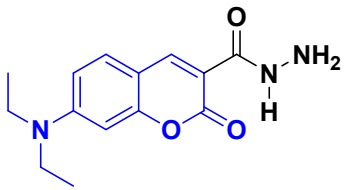
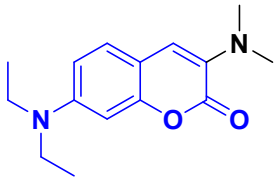
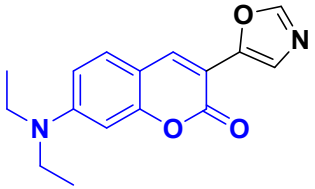
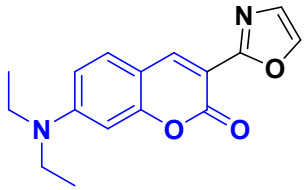
7054002	16	P-1	2, 1	6.95	9.49	13.29	104.26	91.62	100.78	1.41	dichloromethane	New J. Chem., (2014), 38, 260, doi:10.1039/c3nj01176c
2210108	17	P $2_12_12_1$	4, 1	6.33	12.10	22.42	90.00	90.00	90.00	1.36	chloroform	Acta Crystallographica Section E (2006), 62, o3826, doi:10.1107/S1600536806031138
7117322	18	P 2_1/c	4, 1	13.16	6.94	21.08	90.00	109.63	90.00	1.29	dichloromethane/ petroleum/methanol	Chem.Commun. (2015), 51, 10435, doi:10.1039/C5cc03972J
7225474	19	P 2_1/c	4, 1	11.78	19.84	7.64	90.00	98.40	90.00	1.35	ethyl acetate	CrystEngComm, (2016), 18, 5562, doi:10.1039/C6CE01041E
4127666	20	P-1	4, 2	8.96	12.76	17.76	91.17	95.78	99.49	1.34	acetonitrile	J. Am. Chem. Soc., (2019), 141, 16344, doi:10.1021/jacs.9b07175
7054004	21	P-1	2, 1	6.90	7.38	19.54	81.88	82.06	65.32	1.35	dichloromethane	New J. Chem., (2014), 38, 260, doi:10.1039/c3nj01176c
7054005	22	P-1	2, 1	4.94	12.56	14.66	98.17	99.30	92.67	1.43	dichloromethane	New J. Chem., (2014), 38, 260, doi:10.1039/c3nj01176c
4027127	23	P-1	4, 2	9.42	12.51	16.57	88.22	75.86	80.76	1.37	hexane/ethanol	J. Org. Chem., (2012), 77, 3475, doi:10.1021/jo3002722
7023327	24	P 2_1	2, 1	6.32	12.30	12.39	90.00	97.70	90.00	1.32	chloroform/ acetonitrile	Dalton Trans., (2013), 42, 13078, doi:10.1039/c3dt51182k
7116652	25	P 2_1	2, 1	9.14	9.39	12.69	90.00	110.69	90.00	1.43	dichloromethane/ petroleum/ diethyl ether	Chem.Commun., (2015), 51, 4443, doi:10.1039/C5cc00295H
4027128	26	P 2_1/c	4, 1	6.46	20.65	15.10	90.00	101.92	90.00	1.34	hexane/ethanol	J. Org. Chem., (2012), 77, 3475, doi:10.1021/jo3002722
7017064	27	P-1	2, 1	8.36	10.07	11.97	89.95	85.21	67.72	1.36	dichloromethane/ ethanol	Dalton Trans., (2011), 40, 10815, doi:10.1039/c1dt11123j
8102459	28	P 2_1/c	4, 1	10.08	21.95	8.19	90.00	90.25	90.00	1.39	ethanol	Zeitschrift für Kristallographie - New Crystal Structures (2009), 224, 413 doi:10.1524/ncrs.2009.0181
4027133	29	P-1	2, 1	9.57	9.82	11.06	92.91	95.69	94.93	1.33	hexane/ethanol	J. Org. Chem., (2012), 77, 3475, doi:10.1021/jo3002722
2231616	30	P $2_12_12_1$	4, 1	7.94	12.60	20.23	90.00	90.00	90.00	1.44	petroleum/ethyl acetate	Acta Crystallographica Section E (2011), 67, o2344, doi:10.1107/S1600536811031916
7054003	31	P-1	2, 1	8.45	8.95	12.90	92.36	104.60	92.58	1.39	dichloromethane	New J. Chem., (2014), 38, 260, doi:10.1039/c3nj01176c
7106102	32	P 2_1/c	4, 1	9.57	15.53	16.34	90.00	122.09	90.00	1.35	chloroform/ethanol	Chem.Commun., (2011), 47, 3165, doi:10.1039/c0cc05421f
1558692	33	P 2_1/c	4, 1	9.52	19.76	10.80	90.00	103.76	90.00	1.31	petroleum/ethyl acetate	Photochem. Photobiol. Sci., (2020), 19, 1211, doi:10.1039/d0pp00140f
4325585	34	P-1	1, 0.5	8.22	9.32	13.36	97.93	105.24	94.29	2.02	ethanol/DMF	Inorg. Chem., (2011), 50, 6543, doi:10.1021/ic200181p
7154613	35	P-1	2, 1	6.96	10.23	14.78	102.73	97.40	94.66	1.34	methanol	Org. Biomol. Chem., (2015), 13, 8822, doi:10.1039/c5ob01333j

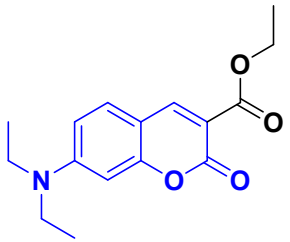
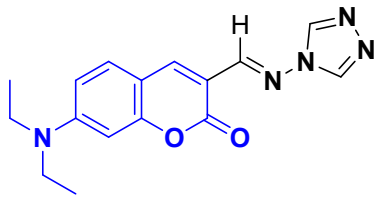
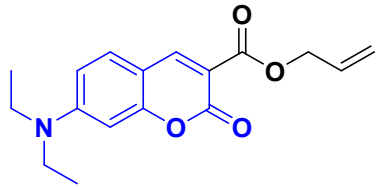
7119168	36	P 2_1/n	4, 1	10.91	7.82	22.43	90.00	97.30	90.00	1.38	dichloromethane	Chem.Commun., (2016), 52, 7387 doi: 10.1039/C6CC02937J
1547843	37	P 2_1/c	4, 1	8.35	12.42	20.68	90.00	97.92	90.00	1.35	acetonitrile/ dichloromethane	Chem. Sci., (2018), 9, 502, doi:10.1039/c7sc03765a
4027132	38	P-1	2, 1	10.16	10.67	11.26	103.42	93.16	90.02	1.33	hexane/ethanol	J. Org. Chem., (2012), 77, 3475, doi:10.1021/jo3002722
1558693	39	P 2_1/c	4, 1	9.68	10.45	12.13	112.87	91.88	103.59	1.35	petroleum/ethyl acetate	Photochem. Photobiol. Sci., (2020), 19, 1211, doi:10.1039/d0pp00140f
1558694	40	P-1	2, 1	9.57	10.63	12.25	113.08	91.15	103.72	1.32	petroleum/ethyl acetate	Photochem. Photobiol. Sci., (2020), 19, 1211, doi:10.1039/d0pp00140f
2237330	41	P-1	2, 1	9.65	10.25	11.12	87.21	86.36	84.35	1.33	chloroform	Acta Crystallographica Section E (2013), 69, o266, doi:10.1107/S1600536813001591
2239004	42	P 2_1/n	4, 1	15.51	8.47	16.88	90.00	97.73	90.00	1.28	Methanol/ dichloromethane	Acta Crystallographica Section E (2014), 70, o176, doi:10.1107/S1600536814001123
7110104	43	P-1	2, 1	10.51	10.78	11.98	84.89	69.76	81.74	1.35	dichloromethane/ petroleum	Chem.Commun., (2013), 49, 11653, doi:10.1039/c3cc46498a
7023928	44	P 2_1/c	4, 1	14.32	9.66	18.97	90.00	91.51	90.00	1.23	dichloromethane/ petroleum	Dalton Trans., (2013), 42, 16302, doi:10.1039/c3dt51953h
7219031	45	P 2_1/n	4, 1	11.57	17.72	14.37	90.00	105.94	90.00	1.16	petroleum/ethyl acetate	RSC Adv., (2014), doi:10.1039/C4RA13445A
2212633	46	P 2_1/c	4, 1	20.84	7.94	13.58	90.00	107.25	90.00	1.32	acetone/toluene	Acta Crystallographica Section E (2007), 63, o1140, doi:10.1107/S1600536807004771
4028361	47	P-1	2, 1	11.25	11.98	12.34	81.87	76.57	63.04	1.21	Ethanol/water	J. Org. Chem., (2013), 78, 6121, doi:10.1021/jo400783x
1544743	48	P 2_1/c	4, 1	11.48	20.46	11.67	90.00	111.06	90.00	1.73	dichloromethane/ hexane	Chem. Sci., (2017), 8, 2352, doi:10.1039/c6sc03775e
7229754	49	P 2_1/n	4, 1	14.06	13.27	15.33	90.00	104.96	90.00	1.27	toluene	Phys. Chem. Chem. Phys., (2018), 20, 6060, doi:10.1039/c7cp07274k
7229755	50	P-1	2, 1	9.83	11.70	12.98	113.25	93.22	93.12	1.25	toluene	Phys. Chem. Chem. Phys., (2018), 20, 6060, doi:10.1039/c7cp07274k

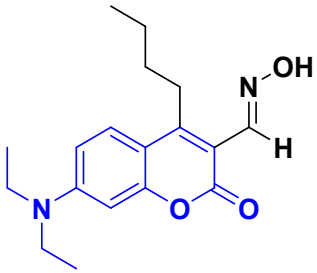
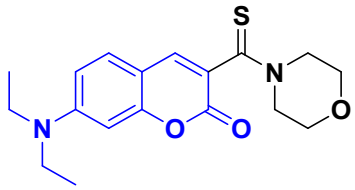
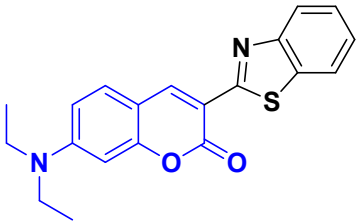
Table S3. Unit cells retrieved from the Crystallography Open Database, employed in the comparative study of DAC-derivatives as supramolecular synthons. The solvent-accessible surface area, A_{SASA} (Å^2), is provided for the molecular unit of all systems **01-50**, measured with a 1.4 Å radius probe. The type of interactions, the coumarin alignment, the distances between the planes of the compounds that present π-stacking and the stacking modes are also provided.

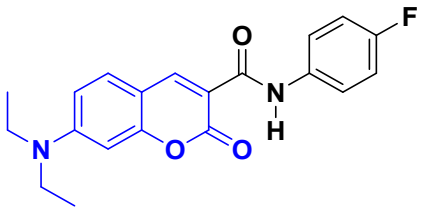
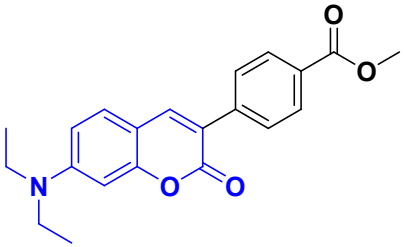
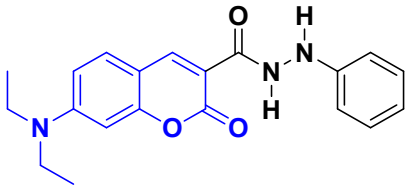
Entry	Structure	ID	A_{SASA} (Å)	Interaction	Structure-directing functional group	Non-directing functional group	Coumarin alignment	π-stacking	Stacking-modes
1		1438103	421.9	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin (Ring)	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Face to face	****	Anti-parallel	Yes (3.030)	1 (2D)
2		2230615	450.4	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Coumarin···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl···Carboyl π-stacking: Offset	****	Anti-parallel	Yes (3.429)	2 (2D)
3		2209698	453.5	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Coumarin···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.441)	2 (2D)

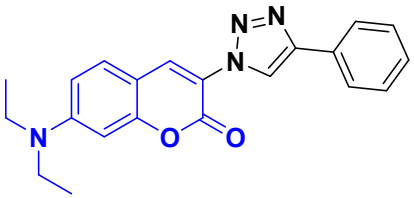
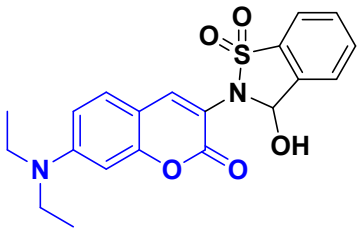
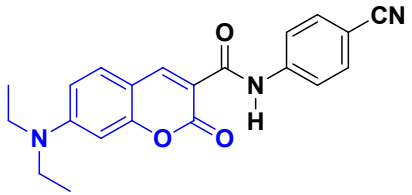
3		1553722	456.6	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.644)	2 (1D)
4		2000551	469.3	C-H···O Ethyl···Coumarin (Ring)	H-bonding: C-H···O Ethyl···Carbonyl π-stacking: Face to face	****	Anti-parallel	Yes (3.616) Two Pairs	2 (1D)
5		2208873	475.0	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Ethyl···Substituent C═O···C═O Coumarin···Coumarin	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl··· Carbonyl π-stacking: Offset Carbonyl···Carbonyl (n →π*)	****	Anti-parallel	Yes (3.450)	2 (2D)
6		7117321	484.1	C-H···O Ethyl···Coumarin (Chain) N-H···O Substituent···Substituent (Ring)	H-bonding: C-H···O Ethyl···Carbonyl N-H···O Hydrazide···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (4.050)	1 (2D)

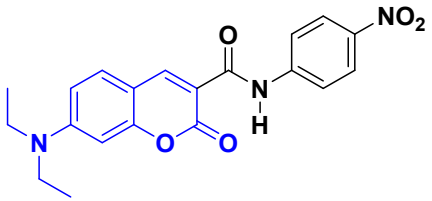
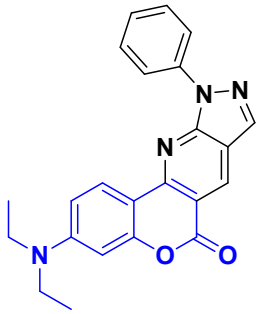
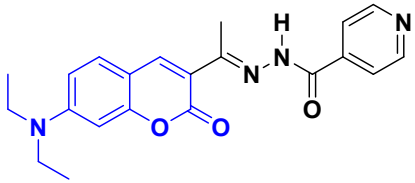
6		2229947	485.2	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin N-H···O Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl··· Carbonyl N-H···O Hydrazide···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.347)	1 (2D)
7		2206681	485.6	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···O Substituent···Coumarin	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Methyl···Carbonyl π-stacking: Edge to face	****	Anti-parallel	Yes (3.415) Pairs	2 (1D)
8		1551651	497.8	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Coumarin ···Substituent (Ring) C═O···C═O Coumarin···Coumarin	H-bonding: C-H···O Ethyl···Carbonyl C-H···O Ethyl···Oxazole π-stacking: Offset Carbonyl···Carbonyl (n →π*)	****	Anti-parallel	Yes (3.810) Pairs	1 (2D)
9		1551552	502.4	C-H···O Coumarin···Coumarin (Ring) C-H···O/N Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O/N Ethyl···Oxazole π-stacking: Offset Face to edge	****	Anti-parallel	Yes (3.394)	2 (1D)

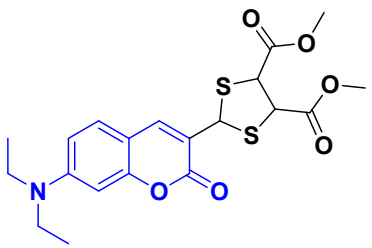
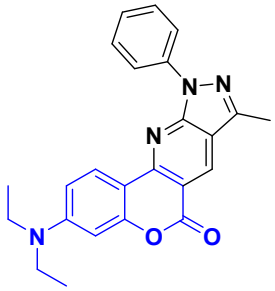
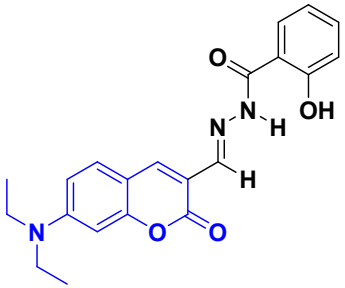
10		8102531	528.5	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···O Ethyl/Substituent···Substituent	H-bonding: C-H···O Aromatic··· Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl···O-Et π-stacking: Offset	****	Anti-parallel	Yes (3.365)	2 (2D)
11		2338583	546.5	C-H···O Coumarin···Coumarin (Ring) C-H···O Substituent···Coumarin C-H···N Coumarin/Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Imine···Carbonyl C-H···N Ethyl···Triazole Triazole···Imine π-stacking: Offset Face to edge	****	Anti-parallel	Yes (3.456)	2 (2D)
12		2243765	549.7	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Substituent···Substituent (Ring)	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl··· Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.356)	2 (1D)

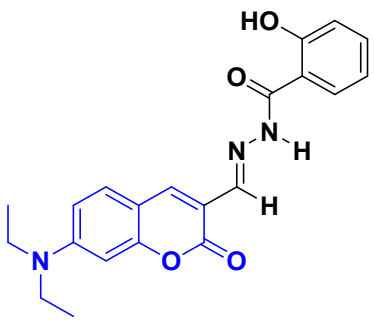
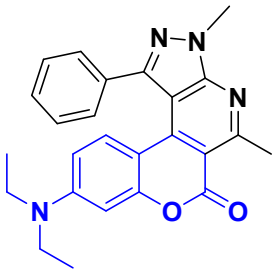
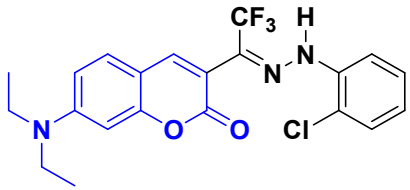
13		7101415	557.5	C-H···O Ethyl···Coumarin O-H···O Substituent···Coumarin C-H···O Ethyl···Substituent	H-bonding: C-H···O Ethyl···Carbonyl C-H···O Ethyl···O-H π-stacking: Offset	****	Anti-parallel	Yes (3.386) Pairs	2 (2D)
14		4517186	567.1	C-H···O Substituent···Coumarin (Ring) C-H···O Substituent···Substituent C-H···S Substituent···Substituent	H-bonding: C-H···O Morpholine···Morpholine C-H···S Morpholine···C=S	H-bonding: C-H···O Aliphatic···Carbonyl	Parallel	No	****
15		2003249	570.6	C-H···O Ethyl···Coumarin (Chain)	H-bonding: C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.388)	1 (1D)

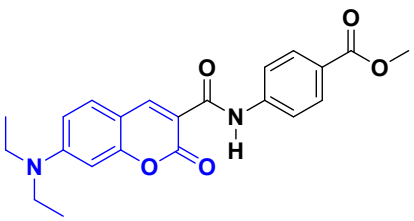
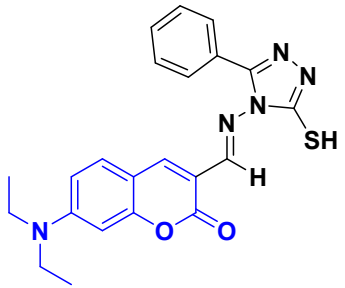
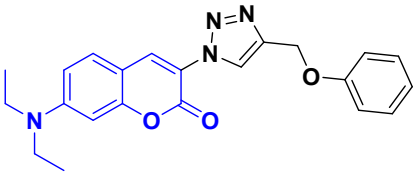
16		7054002	586.8	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Ethyl/Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.463) Pairs	1 (2D)
17		2210108	597.1	C-H···O Coumarin···Coumarin (Chain) C-H···O Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl Ethyl···O-CH_3 π-stacking: Offset	****	Parallel	Yes (3.194) Coumarin-Substituent	2 (2D)
18		7117322	600.7	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···O Coumarin···Substituent (Ring)	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.425) Coumarin-Substituent	1 (2D)

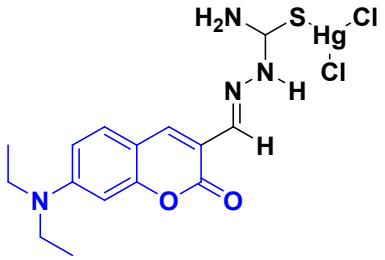
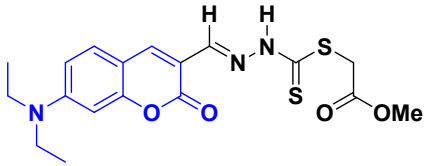
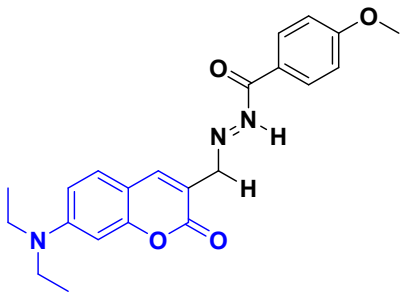
19		7225474	603.1	C-H···O Coumarin···Coumarin (Ring) O···π Coumarin···Substituent	H-bonding: C-H···O Aromatic···Carbonyl O···π Carbonyl···phenyl π-stacking: Offset	****	Anti-parallel	Yes (3.517) Coumarin-Substituent	2 (2D)
20		4127666	606.7	C-H···O Ethyl···Coumarin (Ring) O···H-O Coumarin···Substituent C-H···O Coumarin···Substituent	H-bonding: C-H···O Ethyl···Carbonyl O···H-O Carbonyl···H-O C-H···O Ethyl···O-H π-stacking: Offset	****	Anti-parallel	Yes (3.663) Pairs	2 (1D)
21		7054004	611.8	C-H···O Coumarin···Coumarin (Ring) C-H···O Substituent···Substituent (Chain)	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.497) Pairs	1 (2D)

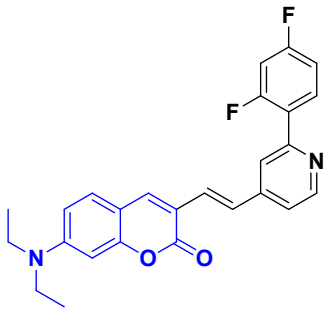
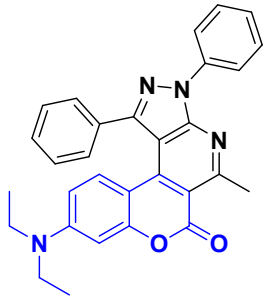
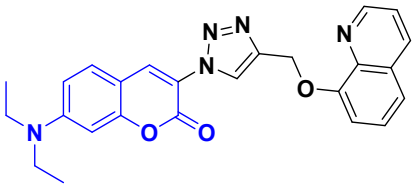
22		7054005	614.9	C-H···O Substituent···Coumarin N-H···O Substituent···Coumarin C-H···O Coumarin···Substituent (Ring)	H-bonding: C-H···O Aromatic···Carbonyl N-H···O Amide··· Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.371) Pairs	1 (2D)
23		4027127	618.2	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···N Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Aromatic···Carbonyl C-H···N Ethyl···N π-stacking: Offset	****	Anti- parallel	Yes (3.352)	1 (2D)
24		7023327	635.5	C-H···O Coumarin···Coumarin C-H···O Coumarin···Substituent (Ring) N-H···O Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.396) Coumarin- Substituent	2 (1D)

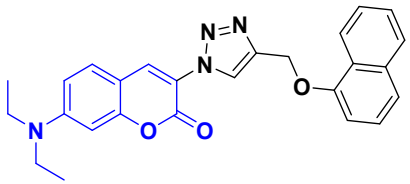
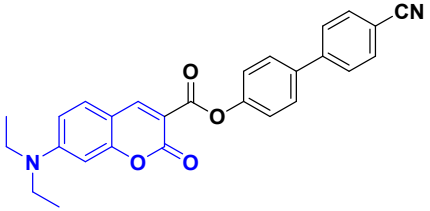
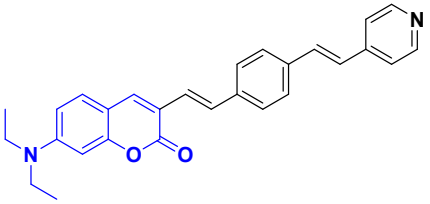
25		7116652	639.6	C-H···O Coumarin···Coumarin C-H···O Ethyl···Coumarin C-H···O Substituent···Substituent C-H···O Coumarin···Substituent π-stacking (C-H···π)	H-bonding: C-H···O S-C-H··· Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Substituent···Coumarin (C-H···π) Edge to face	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl	No	****	****
26		4027128	641.6	C-H···O Substituent···Coumarin (Ring) C-H···O Substituent···Coumarin	H-bonding: C-H···O 7-azaindazole···Carbonyl C-H···O Phenyl···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.995) Pairs	2 (1D)
27		7017064	642.0	C-H···O Substituent-Coumarin (Ring) N-H···O Substituent-Coumarin (Ring) C-H···O Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl Imine···Carbonyl N-H···O Amide··· Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.386) Coumarin- Substituent	1 (2D)

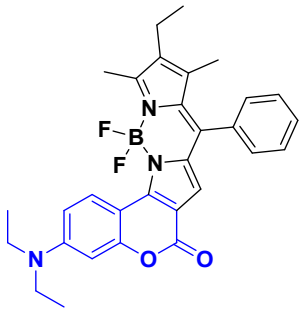
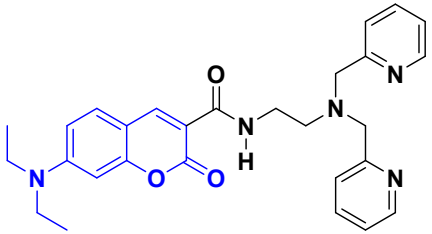
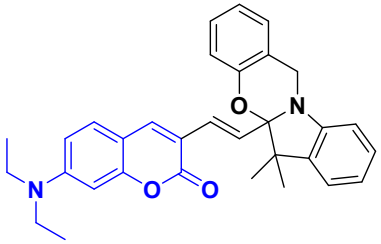
28		8102459	642.6	N-H/C-H···O Substituent···Coumarin (Ring) C-H···O Coumarin···Substituent (Ring) C-H···N Substituent···Substituent	H-bonding: N-H/C-H···O Imine···Carbonyl Amide··· Carbonyl C-H···O Aromatic···Carbonyl Aromatic···O-H C-H···N Aromatic ···Imine π-stacking: Offset	****	Anti- parallel	Yes (3.306)	2 (2D)
29		4027133	642.7	C-H···O Substituent···Coumarin (Ring) C-H···O Ethyl···Coumarin	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.395)	1 (2D)
30		2231616	651.7	C-H···O Substituent···Coumarin C-H···Cl Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···Cl Ethyl···Cl π-stacking: Offset	****	Anti- parallel	Yes (3.753)	2 (2D)

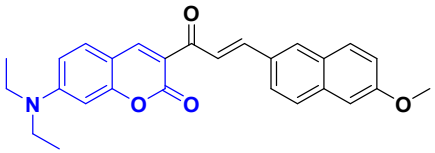
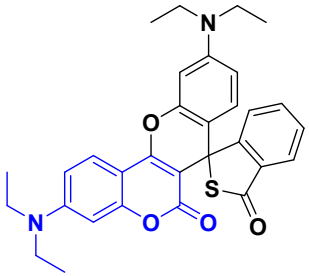
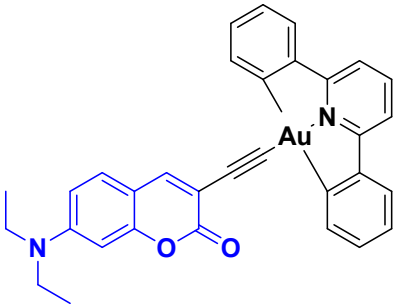
31		7054003	654.5	C-H···O Coumarin···Coumarin C-H···O Substituent···Coumarin C-H···O Coumarin···Substituent (Ring)	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Aromatic···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.483) Pairs	1 (2D)
32		7106102	654.7	C-H···O Ethyl···Coumarin	H-bonding: C-H···O Ethyl···Carbonyl π-stacking: Offset	****	No	Yes (3.673)	2 (2D)
33		1558692	656.2	C-H···O Substituent···Coumarin (Ring)	H-bonding: C-H···O Triazole···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.373)	2 (1D)

34		4325585	658.6	N-H···O Substituent···Coumarin (Ring) N-H···Cl Substituent···Substituent	H-bonding: N-H···O N-H··· Carbonyl N-H···Cl Hydrazone···Cl π-stacking: Offset	****	Anti-parallel	Yes (3.736) Pairs	1 (2D)
35		7154613	664.0	C-H···O Substituent···Coumarin (Ring) N-H···O Substituent···Coumarin C-H···O Coumarin···Substituent	H-bonding: C-H···O Imine··· Carbonyl N-H···O N-H··· Carbonyl C-H···O Aromatic···O-CH_3 π-stacking: Offset	****	Anti-parallel	Yes (3.141)	1 (2D)
36		7119168	683.7	C-H···O Substituent···Coumarin N-H···O Substituent···Coumarin C-H···O/N Ethyl···Substituent	H-bonding: C-H···O Imine··· Carbonyl Aromatic···Carbonyl N-H···O N-H··· Carbonyl C-H···O/N Ethyl···Carbonyl Ethyl··· Hydrazide π-stacking: Offset Face to edge	****	Anti-parallel (Total: stackable surface)	Yes (3.576) Pairs	2 (1D)

37		1547843	699.1	C-H···O Ethyl···Coumarin C-H···N Substituent···Substituent	H-bonding: C-H···O Ethyl··· Carbonyl C-H···N Aromatic···Pyridine π-stacking: Offset	****	Anti-parallel Offset	Yes (3.760)	2 (2D)
38		4027132	706.8	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···N Coumarin···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl··· Carbonyl C-H···N Ethyl···7-azaindazole π-stacking: Offset	****	Anti-parallel	Yes (3.351) Pairs	1 (1D)
39		1558693	718.4	π-stacking (C-H···π)	π-stacking: Coumarin···Substituent C-H···π Offset	****	Anti-parallel	Yes (3.240) Pairs	1 (2D)

40		1558694	720.7	π-stacking (C-H···π)	π-stacking: Coumarin···Substituent C-H···π Offset	****	Anti-parallel	Yes (3.557) Pairs	1 (2D)
41		2237330	722.6	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···O Substituent···Coumarin CN···C-H Substituent···Coumarin	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl··· Carbonyl C-H···O Aromatic···Carbonyl CN···C-H CN··· Aromatic π-stacking: Face to edge	****	Anti-parallel	Yes (3.652) Pairs	2 (1D)
42		2239004	737.2	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin (Ring) C-H···N Ethyl···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···N Ethyl···Pyridine π-stacking: Face to edge Offset	****	Anti-parallel	Yes (3.469) Pairs	2 (2D)

43		7110104	759.4	C-H···O Substituent···Coumarin C-H···F Substituent···Substituent	H-bonding: C-H···O Methyl···Carbonyl C-H···F Ethyl/Methyl···F Aromatic···F π-stacking: Offset	****	Anti-parallel (between BODIPY fragments)	Yes (3.797) Pairs	1 (2D)
44		7023928	760.9	N-H···O Substituent···Coumarin C-H···O Ethyl···Substituent C-H···O Substituent···Substituent	H-bonding: N-H···O Amide···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti-parallel	Yes (3.507) Pairs	2 (1D)
45		7219031	768.0	C-H···O Substituent···Coumarin C-H···N Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···N Methylene···N π-stacking: Offset	****	Anti-parallel	Yes (3.564) Pairs	1 (2D)

46		2212633	772.2	C-H···O Coumarin···Coumarin (Ring) C-H···O Ethyl···Coumarin C-H···O Ethyl···Substituent C-H···O Substituent···Substituent	H-bonding: C-H···O Aromatic···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.719)	1 (2D)
47		4028361	775.6	C-H···O Ethyl···Coumarin (Ring) C-H···O Ethyl···Substituent C-H···O Substituent···Substituent (Ring)	H-bonding: C-H···O Ethyl···Carbonyl C-H···O Ethyl···Carbonyl C-H···O Aromatic···Carbonyl π-stacking: Offset	****	Anti- parallel	Yes (3.488) Pairs	2 (2D)
48		1544743	785.5	C-H···O Substituent···Coumarin Coumarin···Substituent (C-H···π) Substituent···Substituent	π-stacking: Coumarin···Substituent (C-H···π) Edge to face Substituent···Substituent Offset	H-bonding: C-H···O Aromatic···Carbonyl	No	****	****

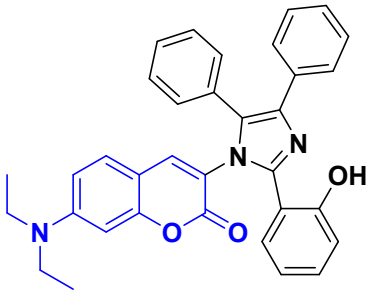
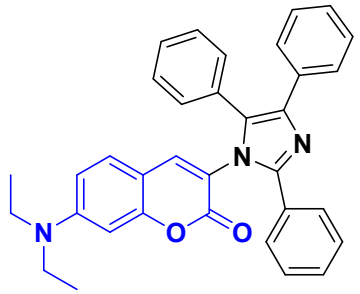
49		7229754	787.9	C-H···O Coumarin···Coumarin (Chain) Substituent···Coumarin (C-H···π)	π-stacking: Phenol···Phenol Offset Phenyl···Coumarin (C-H···π) Edge to face	H-bonding: C-H···O Aromatic···Carbonyl	Parallel Anti-parallel	No	1 (1D)
50		7229755	788.6	C-H···O Ethyl···Coumarin (Chain) C-H···N Substituent···Substituent Substituent···Coumarin (C-H···π)	Phenyl···Coumarin (C-H···π) Edge to face	H-bonding: C-H···O Ethyl···Carbonyl C-H···N Aromatic···pyrazole	Parallel Anti-parallel	No	Phenyl embraces

Table S4. Frontier molecular orbital (FMO) energies, E_{HOMO} and E_{LUMO} for molecules **01**-**50** and FMO energy gap $\Delta E_{HOMO\text{-}LUMO}$, calculated at the MN15(CPCM, ε = 3.5)/def2TZVP level of theory.

	E_{HOMO}		E_{LUMO}		$\Delta E_{HOMO-LUMO}$		
	Ha	**eV**	**Ha**	**eV**	**Ha**	**eV**	**kcal/mol**
1	-0.22879	-6.23	-0.03577	-0.97	0.19302	5.25	121.1
2	-0.23890	-6.50	-0.06545	-1.78	0.17345	4.72	108.8
3	-0.24323	-6.62	-0.06104	-1.66	0.18219	4.96	114.3
4	-0.23575	-6.42	-0.05190	-1.41	0.18385	5.00	115.4
5	-0.23699	-6.45	-0.05958	-1.62	0.17741	4.83	111.3
6	-0.23760	-6.47	-0.05457	-1.48	0.18303	4.98	114.9
7	-0.21420	-5.83	-0.02522	-0.69	0.18898	5.14	118.6
8	-0.22424	-6.10	-0.05112	-1.39	0.17312	4.71	108.6
9	-0.22689	-6.17	-0.05068	-1.38	0.17621	4.79	110.6
10	-0.23665	-6.44	-0.05379	-1.46	0.18286	4.98	114.7
11	-0.23504	-6.40	-0.06909	-1.88	0.16595	4.52	104.1
12	-0.23681	-6.44	-0.05625	-1.53	0.18056	4.91	113.3
13	-0.22726	-6.18	-0.04845	-1.32	0.17881	4.87	112.2
14	-0.22855	-6.22	-0.04377	-1.19	0.18478	5.03	116.0
15	-0.22871	-6.22	-0.05796	-1.58	0.17075	4.65	107.1
16	-0.2368	-6.44	-0.05932	-1.61	0.17748	4.83	111.4
17	-0.22841	-6.22	-0.0568	-1.55	0.17161	4.67	107.7
18	-0.23814	-6.48	-0.05428	-1.48	0.18386	5.00	115.4
19	-0.23253	-6.33	-0.05316	-1.45	0.17937	4.88	112.6
20	-0.22877	-6.23	-0.04471	-1.22	0.18406	5.01	115.5
21	-0.23868	-6.49	-0.06057	-1.65	0.17811	4.85	111.8
22	-0.24114	-6.56	-0.07256	-1.97	0.16858	4.59	105.8
23	-0.22823	-6.21	-0.05318	-1.45	0.17505	4.76	109.8
24	-0.22715	-6.18	-0.05602	-1.52	0.17113	4.66	107.4
25	-0.22791	-6.20	-0.03686	-1.00	0.19105	5.20	119.9
26	-0.23138	-6.30	-0.05038	-1.37	0.18100	4.93	113.6
27	-0.22855	-6.22	-0.06126	-1.67	0.16729	4.55	105.0
28	-0.22759	-6.19	-0.06079	-1.65	0.16680	4.54	104.7
29	-0.22919	-6.24	-0.05197	-1.41	0.17722	4.82	111.2
30	-0.23094	-6.28	-0.06011	-1.64	0.17083	4.65	107.2
31	-0.23906	-6.51	-0.0616	-1.68	0.17746	4.83	111.4
32	-0.23892	-6.50	-0.06978	-1.90	0.16914	4.60	106.1
33	-0.23389	-6.36	-0.05427	-1.48	0.17962	4.89	112.7
34	-0.23083	-6.28	-0.07694	-2.09	0.15389	4.19	96.6
35	-0.22739	-6.19	-0.06284	-1.71	0.16455	4.48	103.3
36	-0.22501	-6.12	-0.0593	-1.61	0.16571	4.51	104.0
37	-0.22349	-6.08	-0.05711	-1.55	0.16638	4.53	104.4
38	-0.23188	-6.31	-0.05280	-1.44	0.17908	4.87	112.4
39	-0.23067	-6.28	-0.05284	-1.44	0.17783	4.84	111.6
40	-0.23271	-6.33	-0.05385	-1.47	0.17886	4.87	112.2
41	-0.24082	-6.55	-0.05957	-1.62	0.18125	4.93	113.7
42	-0.21571	-5.87	-0.05742	-1.56	0.15829	4.31	99.3
43	-0.21551	-5.86	-0.08519	-2.32	0.13032	3.55	81.8
44	-0.23572	-6.41	-0.05162	-1.40	0.18410	5.01	115.5
45	-0.22437	-6.11	-0.04544	-1.24	0.17893	4.87	112.3
46	-0.23330	-6.35	-0.06969	-1.90	0.16361	4.45	102.7
47	-0.22866	-6.22	-0.03810	-1.04	0.19056	5.19	119.6
48	-0.21935	-5.97	-0.05976	-1.63	0.15959	4.34	100.1
49	-0.23148	-6.30	-0.04823	-1.31	0.18325	4.99	115.0
50	-0.23138	-6.30	-0.04718	-1.28	0.18420	5.01	115.6
Average	-0.23090	-6.28	-0.05560	-1.51	0.17530	4.77	110.0
σ	0.00657	0.18	0.01037	0.28	0.01081	0.29	6.781954

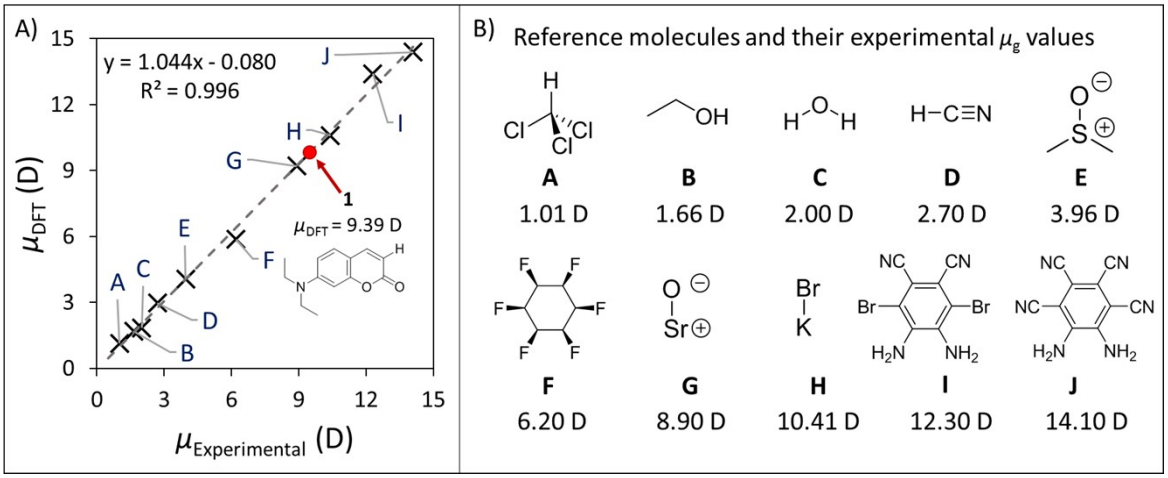


Figure S10. Molecular dipole moments for DAC-H **1** and a series of reference compounds, **A**-**J**. All values were calculated at the MN15(CPCM)/def2TZVP level of theory. Experimental values were obtained from: Weast, Robert C. (1984). CRC Handbook of Chemistry and Physics (65th ed.). CRC Press. ISBN 0-8493-0465-2.

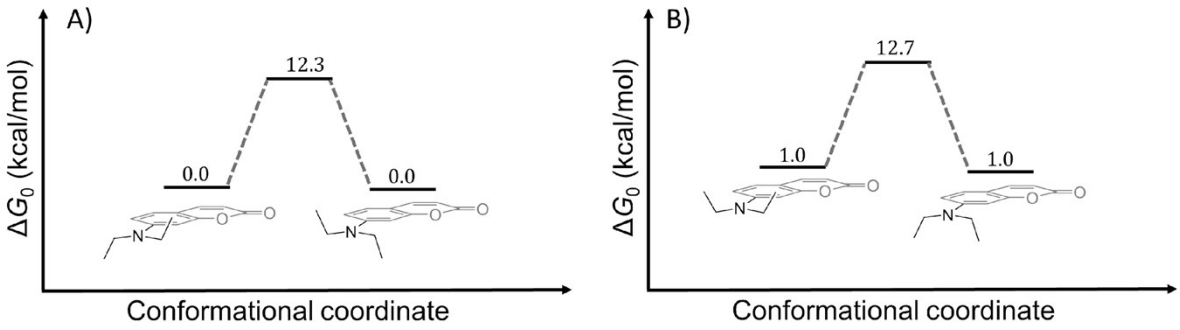


Figure S11. Conformational profiles for rotation around the Et_2N-coumarin bond, calculated using the DFT protocol MN15(CPCM)/def2TZVP

Cartesian coordinates and DFT energies of compounds 1-50

In this section we provide optimized geometries for compounds **1-50**, in XYZ format, and their final electronic potential energies obtained using DFT. All calculations were carried out using the global hybrid *m*-GGA functional MN15 with the triple-zeta polarized basis def2-TZVP, with the CPCM polarizable continuum model and a relative electric permittivity $\varepsilon = 3.5$. All geometries were confirmed as minima by the absence of imaginary eigenvalues upon Hessian diagonalization. The naming convention in all cases is: Molecule (sequential number from **Figure 3**)_(COD deposition code).

Molecule 01_1438103
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

31
c01_1438103.xyz.out Energy: -444933.7678063

C	6.88472	5.32039	-5.30578
C	5.62384	6.01295	-5.42530
H	5.41613	6.46469	-6.38471
C	4.77264	6.07993	-4.37847
H	3.82708	6.60393	-4.47155
C	5.09467	5.46774	-3.13171
C	6.31386	4.79114	-3.02859
C	6.72761	4.16380	-1.87161
H	7.69711	3.68596	-1.87669
C	5.90572	4.18705	-0.72973
C	7.48441	2.75218	0.49560
H	7.60647	2.20063	-0.43889
H	7.31607	1.99816	1.26916
C	8.72972	3.56094	0.81898
H	8.91010	4.32447	0.05968
H	9.60836	2.91557	0.87186
H	8.61886	4.06429	1.78233
C	5.53228	3.70456	1.66029
H	5.12315	4.71394	1.73552
H	6.24511	3.60984	2.48405
C	4.43755	2.65996	1.79824
H	3.71608	2.73849	0.98231
H	3.90342	2.77970	2.74270
H	4.86339	1.65421	1.77392
C	4.66355	4.87227	-0.82226
H	3.99252	4.89727	0.02462
C	4.28243	5.48797	-1.98849
H	3.32689	5.99853	-2.03789
N	6.28563	3.57039	0.42459
O	7.16064	4.73743	-4.09691
O	7.72285	5.20767	-6.17688

Molecule 02_2230615
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

33

c02_2230615.xyz.out Energy: -516001.4716344

O	6.16730	0.04875	-1.65186
O	4.26818	-0.82077	-2.35709
O	3.09411	-1.87354	1.42647
N	10.34500	1.96981	-0.49629
C	4.97458	-0.58206	-1.40212
C	4.68573	-0.89679	-0.01921
C	5.58158	-0.57402	0.96317
H	5.33811	-0.82543	1.99155
C	6.79543	0.06724	0.66294
C	7.06459	0.37578	-0.68239
C	8.22142	0.99900	-1.08598
H	8.35646	1.17778	-2.14316
C	9.19643	1.35444	-0.12945
C	8.93368	1.04883	1.23990
H	9.64583	1.32743	2.00307
C	7.77388	0.42864	1.61053
H	7.58726	0.21097	2.65602
C	3.42573	-1.56437	0.29409
H	2.77182	-1.78158	-0.56371
C	11.42987	2.22320	0.44192
H	11.50229	1.39896	1.15314
H	12.35859	2.20524	-0.13383
C	11.28370	3.55581	1.15554
H	11.25919	4.37598	0.43462
H	12.12226	3.72415	1.83334
H	10.35952	3.59064	1.73619
C	10.58461	2.40023	-1.86631
H	11.25763	3.25981	-1.81902
H	9.65430	2.76891	-2.30146
C	11.19475	1.30352	-2.72180
H	12.15025	0.97827	-2.30416
H	11.37175	1.66129	-3.73736
H	10.53588	0.43449	-2.77410

Molecule 03a_1553722
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

34
c03a_1553722.xyz.out Energy: -563205.0580647

N	1.28752	8.09836	5.69141
O	5.05253	5.36914	6.64950
O	6.72438	4.08481	7.26585
O	8.53122	3.35889	5.52742
H	8.04279	3.44671	6.38619
O	8.31624	4.07461	3.44358
C	6.18822	4.69340	6.34890
C	6.66005	4.75146	4.98825
C	5.96072	5.47181	4.06163
H	6.33162	5.50477	3.04215
C	4.78365	6.16155	4.40657

C	4.34229	6.09183	5.73632
C	3.21151	6.72949	6.18792
H	2.96031	6.62762	7.23348
C	2.43194	7.48829	5.28958
C	2.87661	7.57691	3.93571
H	2.31652	8.15711	3.21759
C	4.00668	6.93066	3.51869
H	4.32293	7.00641	2.48474
C	7.89530	4.04143	4.58142
C	0.87188	8.05350	7.08805
H	-0.19588	8.27384	7.11323
H	0.97532	7.03072	7.45645
C	1.62577	9.02490	7.98347
H	1.40110	10.05868	7.71765
H	1.34042	8.87534	9.02632
H	2.70530	8.88212	7.90343
C	0.56317	8.99944	4.80185
H	0.41469	8.51093	3.83622
H	-0.43258	9.13234	5.22603
C	1.23345	10.35287	4.62137
H	2.25679	10.24524	4.25653
H	0.67807	10.95483	3.89976
H	1.26894	10.90144	5.56340

Molecule 03b_2209698
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

34
c03b_2209698.xyz.out Energy: -563205.0519182

O	6.15501	1.96772	-1.78167
O	4.35571	2.98746	-1.04054
O	2.66267	4.05053	-2.72285
O	3.11173	3.89398	-4.88508
N	10.12017	-0.34363	-3.00480
C	5.00802	2.64986	-2.01977
C	4.66111	2.91458	-3.39353
C	5.48293	2.47713	-4.39332
H	5.20575	2.68578	-5.42161
C	6.66620	1.76948	-4.11193
C	7.56962	1.28753	-5.07905
H	7.35083	1.46214	-6.12619
C	8.70330	0.61285	-4.72203
H	9.36552	0.26154	-5.49942
C	9.01171	0.35982	-3.35129
C	8.11633	0.84702	-2.37586
H	8.28412	0.71982	-1.31646
C	6.98510	1.52230	-2.76832
C	3.42433	3.65471	-3.73703
C	11.13582	-0.68248	-3.99605
H	10.66076	-1.16798	-4.85171
H	11.78029	-1.43669	-3.54375

C	11.97127	0.50480	-4.45056
H	12.66822	0.19608	-5.23187
H	12.55058	0.91668	-3.62330
H	11.34521	1.30371	-4.85244
C	10.44500	-0.57846	-1.60356
H	11.10243	-1.44820	-1.56605
H	9.53521	-0.86711	-1.07345
C	11.11047	0.60753	-0.92221
H	11.23933	0.40770	0.14306
H	10.50968	1.51318	-1.02817
H	12.09509	0.80293	-1.34919
H	3.07601	3.76915	-1.86652

Molecule 04_2000551
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

34
c04_2000551.xyz.out Energy: -656356.8541574

O	8.94023	16.20596	8.87942
C	8.94161	17.11263	9.89739
C	10.23331	17.58441	10.34834
C	11.36609	17.13267	9.77272
C	12.44652	15.63559	8.03344
C	12.29864	14.72442	7.01958
C	11.01255	14.28495	6.60214
C	9.89712	14.82179	7.26985
C	10.07603	15.73863	8.28294
C	11.33694	16.17890	8.70504
O	7.87196	17.45695	10.34872
N	10.86820	13.38438	5.59446
C	12.00628	12.71711	4.98209
C	12.59237	13.50410	3.82238
C	9.56021	13.01412	5.07812
C	8.92571	11.87359	5.85605
C	12.69832	17.64238	10.26683
F	13.38269	18.24565	9.28641
F	12.57292	18.52339	11.25720
F	13.46239	16.64160	10.72303
H	10.22683	18.30202	11.15503
H	13.44717	15.94237	8.30871
H	13.18630	14.35687	6.52501
H	8.88371	14.52880	7.03478
H	11.65749	11.74125	4.63463
H	12.76407	12.51079	5.73997
H	12.94512	14.48348	4.15239
H	13.43221	12.96857	3.37605
H	11.83916	13.66156	3.04707
H	9.69672	12.72538	4.03287
H	8.90929	13.89070	5.06464
H	9.56163	10.98604	5.81985
H	7.95307	11.61255	5.43550

H 8.78449 12.14434 6.90433

Molecule 05_2208873
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

36
c05_2208873.xyz.out Energy: -540653.3619905
C 4.11643 3.48859 20.67016
C 4.14694 4.14072 21.96499
C 3.03898 4.81812 22.39812
H 3.08336 5.29928 23.37028
C 0.69094 5.58334 22.02260
H 0.68010 6.09333 22.97919
C -0.41513 5.61513 21.21968
H -1.28533 6.16503 21.54775
C -0.42146 4.95815 19.95268
C 0.74906 4.28130 19.55183
H 0.81546 3.74261 18.61741
C 1.84618 4.26996 20.38218
C 1.86280 4.90604 21.63240
C 5.33789 4.10464 22.84871
C 6.58522 3.39633 22.42256
H 6.96065 3.81004 21.48546
H 6.38047 2.34174 22.23169
H 7.32786 3.50303 23.21102
C -2.78520 5.55921 19.59797
H -2.93315 5.35569 20.65956
H -3.57790 5.01772 19.07552
C -2.88751 7.04582 19.30459
H -3.85483 7.43669 19.62478
H -2.78246 7.23359 18.23366
H -2.10300 7.60171 19.82222
C -1.51034 4.43482 17.81322
H -0.54439 4.63002 17.34410
H -2.24674 4.99465 17.23157
C -1.84298 2.95287 17.78987
H -1.83793 2.57321 16.76685
H -2.83440 2.77650 18.21319
H -1.12045 2.37830 18.37271
N -1.51961 4.98846 19.15917
O 2.94593 3.59856 19.95480
O 5.00124 2.85429 20.13843
O 5.28944 4.66435 23.93686

Molecule 06a_2229947
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

37
c06a_2229947.xyz.out Energy: -585425.8500230
C 6.21392 9.14834 -5.62210
C 5.22242 8.09528 -5.68229

C	5.04607	7.21906	-6.87166
C	4.40806	7.88114	-4.60970
H	3.67318	7.08537	-4.67620
C	4.49838	8.65805	-3.43547
C	5.45924	9.67530	-3.39537
C	5.64212	10.49416	-2.30368
H	6.41855	11.24285	-2.36070
C	4.83099	10.32837	-1.16328
C	3.85878	9.28524	-1.18664
H	3.22635	9.11427	-0.32813
C	3.70152	8.48912	-2.28870
H	2.95139	7.70650	-2.28718
C	4.23252	10.87349	1.15312
H	4.27450	11.78261	1.75408
H	3.17553	10.71340	0.92754
C	4.79182	9.70235	1.94695
H	5.80426	9.91116	2.29479
H	4.16749	9.50638	2.82082
H	4.82493	8.79288	1.34387
C	5.99071	12.17100	-0.04689
H	6.00019	12.69882	-1.00318
H	5.69092	12.90834	0.69897
C	7.37590	11.63384	0.28139
H	7.65788	10.82480	-0.39543
H	8.12026	12.42713	0.19049
H	7.41607	11.24997	1.30169
N	4.95487	11.14735	-0.08321
N	5.86100	7.42645	-7.92225
H	6.56390	8.15699	-7.88936
N	5.76709	6.64297	-9.07447
H	5.88572	5.66549	-8.81227
H	4.82357	6.72831	-9.44958
O	6.26830	9.88073	-4.47035
O	7.01040	9.45709	-6.48945
O	4.18435	6.33705	-6.88463

Molecule 06b_7117321
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

37
c06b_7117321.xyz.out Energy: -585425.8467317

N	0.79699	6.20650	2.20560
N	1.74747	2.59630	-5.67957
H	2.45375	3.32261	-5.63007
N	1.65781	1.83192	-6.84487
H	0.71725	1.92768	-7.22480
H	1.77031	0.84980	-6.59772
O	2.14351	4.99299	-2.18642
O	2.89930	4.59539	-4.20572
O	0.06089	1.49619	-4.66969
C	1.83725	7.22460	2.26452

H	1.85707	7.76522	1.31549
H	1.53456	7.95314	3.01782
C	3.21714	6.67636	2.59686
H	3.50080	5.87510	1.91155
H	3.96605	7.46710	2.52272
H	3.24715	6.27859	3.61217
C	0.60686	4.73872	4.21673
H	1.61587	4.93986	4.57882
H	-0.02814	4.53399	5.08085
H	0.64410	3.83674	3.60273
C	0.06056	5.92133	3.43098
H	0.09993	6.82313	4.04303
H	-0.99461	5.76840	3.19236
C	0.67958	5.40192	1.11407
C	-0.29710	4.36371	1.06804
H	-0.93741	4.18324	1.91874
C	-0.44892	3.58422	-0.04660
H	-1.20282	2.80540	-0.06255
C	0.35833	3.76553	-1.18418
C	1.32434	4.77673	-1.12129
C	1.50211	5.57890	-0.01646
H	2.28316	6.32390	-0.05605
C	0.27335	3.00637	-2.37039
H	-0.46534	2.21578	-2.45408
C	1.09726	3.23189	-3.43335
C	2.09415	4.27824	-3.34949
C	0.92548	2.37488	-4.63737

Molecule 07_2206681
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

39
c07_2206681.xyz.out Energy: -528926.2437533

O	1.18017	2.62625	1.83270
O	0.30940	4.20652	3.08263
N	2.79747	5.38842	3.61757
N	2.62144	-0.78347	-1.15935
C	1.32162	3.73025	2.61611
C	2.68011	4.24585	2.81587
C	3.70557	3.65425	2.15041
C	3.49612	2.53478	1.28619
C	4.50033	1.87569	0.56435
C	4.22264	0.79067	-0.23420
C	2.90035	0.29070	-0.35989
C	1.88803	0.94411	0.36311
C	2.20457	2.03163	1.15346
C	2.34784	5.22774	4.99657
C	4.09067	6.03437	3.57518
C	1.25859	-1.22476	-1.39541
C	0.76122	-2.19712	-0.33797
C	3.66748	-1.56309	-1.79694

C	4.07260	-1.01170	-3.15427
H	4.71802	4.02523	2.25922
H	5.51979	2.23891	0.63629
H	5.03143	0.33211	-0.78563
H	0.85747	0.61843	0.34209
H	3.06125	4.62301	5.57619
H	2.27043	6.20918	5.46602
H	1.37106	4.75428	5.03437
H	4.37103	6.26461	2.54627
H	4.88688	5.42190	4.02749
H	4.03372	6.96972	4.13263
H	1.23590	-1.70019	-2.37993
H	0.59935	-0.35680	-1.46792
H	0.78478	-1.74251	0.65450
H	-0.26352	-2.50935	-0.54795
H	1.39069	-3.08991	-0.31401
H	3.28924	-2.58310	-1.90781
H	4.53052	-1.63737	-1.13188
H	4.44869	0.00968	-3.06559
H	3.21545	-0.99575	-3.83152
H	4.85199	-1.62732	-3.60766

Molecule 08_1551651
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

37
c08_1551651.xyz.out Energy: -598496.4122413

O	-1.37735	6.23233	-0.12568
O	-2.94615	4.69222	-0.24645
O	-1.73748	3.59222	-4.12378
N	1.86714	9.64851	0.48690
N	-3.41842	2.21032	-3.73941
C	-2.02007	5.23947	-0.80507
C	-1.53357	4.92833	-2.13834
C	-0.48318	5.62699	-2.65193
C	0.15214	6.65505	-1.91168
C	1.23554	7.42449	-2.36809
C	1.79916	8.40299	-1.59077
C	1.30474	8.67952	-0.28508
C	0.21813	7.91434	0.17971
C	-0.32319	6.93674	-0.62664
C	1.46426	9.85895	1.86792
C	0.28065	10.80305	1.99653
C	2.89745	10.54172	-0.01851
C	4.29811	9.97837	0.15270
C	-2.20407	3.87245	-2.86534
C	-2.51498	2.59140	-4.57365
C	-3.23703	3.02316	-2.62937
H	-0.12027	5.39713	-3.64802
H	1.63427	7.22765	-3.35704
H	2.64459	8.95375	-1.97736

H -0.23202 8.07518 1.14907
H 1.25228 8.89670 2.33849
H 2.32865 10.26809 2.39737
H -0.59336 10.41201 1.47188
H 0.01430 10.94854 3.04488
H 0.52167 11.77881 1.56838
H 2.69582 10.78300 -1.06378
H 2.80334 11.48349 0.52861
H 4.50741 9.78752 1.20771
H 4.41038 9.03615 -0.38771
H 5.04616 10.68022 -0.22052
H -2.31124 2.21620 -5.56365
H -3.85099 2.94362 -1.75077

Molecule 09_1551552
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

37
c09_1551552.xyz.out Energy: -598494.2572006
O 1.41447 12.06705 4.52285
O 2.76962 13.51839 3.58092
O 4.05371 15.34103 5.16000
N -1.59991 8.77836 6.15152
N 4.19719 14.89868 7.31925
C 2.33746 13.07681 4.62104
C 2.69496 13.49395 5.96706
C 2.13578 12.86459 7.04005
C 1.19874 11.81880 6.88658
C 0.57500 11.13205 7.94322
C -0.33673 10.13692 7.70997
C -0.69188 9.76288 6.38169
C -0.06861 10.44428 5.31772
C 0.84737 11.43713 5.58660
C -1.89167 8.29986 4.80929
C -2.97263 9.11503 4.11943
C -2.35860 8.15342 7.22414
C -1.63865 6.96255 7.83325
C 3.65730 14.56368 6.18444
C 5.00769 15.97782 7.02117
C 4.91829 16.24282 5.70315
H 2.41635 13.18206 8.03882
H 0.83396 11.39844 8.96175
H -0.77290 9.62129 8.55331
H -0.29600 10.23421 4.28239
H -2.20867 7.25796 4.90141
H -0.97412 8.28290 4.21812
H -2.67414 10.16076 4.02226
H -3.17486 8.72211 3.12157
H -3.90187 9.08186 4.69292
H -3.31330 7.83517 6.79764
H -2.60509 8.89615 7.98490

H -0.67970 7.26137 8.26151
H -2.24098 6.50794 8.62181
H -1.44510 6.20274 7.07270
H 5.59617 16.47896 7.77158
H 5.35940 16.96357 5.03745

Molecule 10_8102531
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

40
c10_8102531.xyz.out Energy: -612484.1835615
O 7.24846 14.03988 4.73606
O 8.32696 12.41107 5.73762
O 4.58974 10.88978 7.07297
O 6.79791 10.60651 7.25168
N 5.31940 17.69104 2.39929
C 3.64750 19.46954 2.80455
H 4.42774 20.19767 3.03735
H 2.80643 20.00318 2.35855
H 3.31351 19.02263 3.74330
C 4.17646 18.40915 1.85422
H 4.50601 18.87223 0.92080
H 3.39349 17.70205 1.57618
C 7.21190 17.59123 0.80935
H 6.55293 17.74869 -0.04752
H 8.18534 18.02458 0.57397
H 7.33887 16.51529 0.94415
C 6.62631 18.23190 2.05595
H 6.49837 19.30622 1.90254
H 7.30169 18.12813 2.90695
C 3.75656 15.01758 4.36433
H 2.76964 14.69579 4.67761
C 3.89403 16.13411 3.58613
H 3.00970 16.68756 3.30530
C 5.18257 16.58282 3.16882
C 6.30715 15.84058 3.58441
H 7.31419 16.10259 3.29312
C 6.13479 14.72254 4.36862
C 4.87413 14.27144 4.78284
C 4.81756 13.11475 5.58608
H 3.84939 12.75760 5.91765
C 7.24764 12.90151 5.51409
C 5.94282 12.43561 5.95987
C 5.86010 11.23465 6.81270
C 4.41312 9.73642 7.90628
H 4.90031 8.88266 7.43153
H 4.90820 9.91495 8.86274
C 2.93150 9.52160 8.06893
H 2.45627 9.35191 7.10160
H 2.75196 8.64858 8.69755
H 2.46348 10.38678 8.54099

Molecule 11_GLCH169-953
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

40
c11_GLCH169-953.xyz.out Energy: -654658.1684797

O	2.04937	10.32523	3.18230
O	0.89556	10.89872	1.39502
N	-3.41409	8.57142	1.57136
N	-2.33651	8.59897	2.42760
N	-5.47782	8.19557	0.95740
N	4.80783	9.31101	6.90607
N	-4.77724	8.65841	-0.13157
C	2.22193	9.64048	4.34712
C	3.41025	9.82681	5.01331
C	-0.13401	9.36726	2.88834
C	1.21267	8.78248	4.81149
C	0.92335	10.23992	2.41302
C	3.65051	9.14005	6.22200
C	0.03304	8.66777	4.05073
C	2.63455	8.26167	6.70287
C	-4.64499	8.14224	1.95652
C	-1.32735	9.29805	2.06771
C	5.80040	10.29710	6.50379
C	1.46381	8.09680	6.01550
C	-3.55057	8.87972	0.24785
C	5.13093	8.54215	8.09948
C	4.59252	9.18321	9.36684
C	6.78766	9.74994	5.48748
H	0.70065	7.43064	6.40180
H	2.77345	7.72958	7.63276
H	4.14003	10.48889	4.56993
H	-0.75945	8.01021	4.39389
H	-4.85651	7.81935	2.96261
H	-1.31241	9.88186	1.14938
H	6.32759	10.60866	7.40885
H	5.29830	11.18929	6.12519
H	-2.75206	9.22214	-0.38842
H	6.22042	8.47054	8.14732
H	4.76899	7.51894	7.99016
H	3.50399	9.26265	9.33278
H	4.99980	10.18923	9.48990
H	4.86782	8.59549	10.24418
H	6.27807	9.42692	4.57763
H	7.32240	8.89012	5.89743
H	7.52253	10.51000	5.21723

Molecule 12_2243765
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

41

c12_2243765.xyz.out Energy: -636357.0080479

O	5.75607	0.74355	0.72286
O	4.09680	-0.13809	-0.40939
O	2.16235	3.63319	-0.48449
O	2.06117	1.50086	-1.12997
N	9.54028	2.21439	3.17752
C	4.53517	0.86837	0.09378
C	3.94291	2.19566	0.12368
C	4.59103	3.21345	0.76542
H	4.12266	4.19228	0.77652
C	5.83339	3.03042	1.40095
C	6.55236	4.03370	2.07808
H	6.13401	5.03280	2.12332
C	7.76106	3.77338	2.66258
H	8.28972	4.57807	3.15306
C	8.33810	2.46950	2.60481
C	7.62259	1.45850	1.93112
H	7.98148	0.44138	1.86543
C	6.40851	1.75263	1.35347
C	2.65164	2.51825	-0.51498
C	0.81274	1.80051	-1.77050
H	0.09812	2.16274	-1.02873
H	0.98301	2.59971	-2.49744
C	0.33463	0.55462	-2.43254
H	1.04520	0.06325	-3.09072
C	-0.88786	0.06995	-2.26720
H	-1.60002	0.54986	-1.60330
H	-1.22192	-0.81829	-2.78953
C	10.21647	0.93599	3.01321
H	10.04177	0.55600	2.00502
H	11.28984	1.13124	3.08003
C	9.80490	-0.08275	4.06215
H	8.73364	-0.28748	4.01211
H	10.34044	-1.02241	3.91697
H	10.03152	0.28663	5.06494
C	10.24150	3.19839	3.98912
H	9.52220	3.77504	4.57277
H	10.84083	2.64442	4.71609
C	11.13481	4.10721	3.16268
H	10.55316	4.66634	2.42700
H	11.65724	4.82047	3.80253
H	11.88360	3.52166	2.62450

Molecule 13_7101415
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

47
c13_7101415.xyz.out Energy: -649263.5483209

O	12.91204	-1.36803	12.18651
C	13.28429	-2.37866	11.35543
C	13.58125	-2.04803	9.96966

C	13.51256	-0.74672	9.53476
C	13.08930	0.27310	10.45321
C	12.93117	1.63484	10.13289
H	13.12616	1.97198	9.12252
C	12.51524	2.56006	11.05661
H	12.39053	3.58633	10.74123
C	12.22516	2.18402	12.39603
C	12.37483	0.82694	12.72973
H	12.19661	0.45070	13.72726
C	12.78894	-0.07680	11.77388
O	13.34257	-3.49137	11.83948
C	13.98083	-3.21427	9.18582
H	14.37039	-4.07041	9.73440
N	13.86077	-3.28384	7.91831
O	14.33731	-4.49374	7.44176
C	13.84127	-0.35407	8.12841
H	14.32533	0.62599	8.12464
H	14.54608	-1.07038	7.70938
C	12.57996	-0.29874	7.25973
H	12.07458	-1.26867	7.30834
H	11.89064	0.43827	7.68446
C	12.88052	0.04927	5.80605
H	11.93770	0.25757	5.29248
H	13.46264	0.97713	5.76937
C	13.61848	-1.05452	5.06132
H	13.78397	-0.78232	4.01694
H	13.03944	-1.98177	5.07789
H	14.59469	-1.26568	5.50320
N	11.81456	3.09961	13.31506
C	11.39189	2.70684	14.64931
H	10.66836	3.45112	14.99213
H	10.84752	1.76179	14.59684
C	12.54990	2.61532	15.62898
H	12.19590	2.32694	16.62034
H	13.05553	3.57990	15.71549
H	13.28474	1.87796	15.29960
C	11.78352	4.52479	13.02958
H	11.94551	5.04573	13.97695
H	12.62944	4.79241	12.39366
C	10.47029	4.97056	12.40894
H	10.47438	6.04618	12.22302
H	9.63566	4.74407	13.07638
H	10.29112	4.45797	11.46150
H	14.18210	-4.46105	6.48784

Molecule 14_4517186
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

46
c14_4517186.xyz.out Energy: -898352.2506032

S	4.65603	16.11681	2.90600

C	4.90271	11.86360	4.41697
C	3.77092	11.46025	5.13388
C	5.74709	10.84778	3.93697
H	6.63434	11.12828	3.38052
C	3.46688	10.13886	5.37738
H	2.55634	9.92026	5.91695
C	4.32077	9.12681	4.89663
C	5.47597	9.52427	4.16431
H	6.16474	8.77976	3.79180
O	2.90681	12.39710	5.61487
C	5.11176	13.25080	4.22660
H	5.96957	13.58259	3.65036
C	4.26554	14.17961	4.74742
C	3.08166	13.74487	5.46526
C	4.45097	15.62944	4.48046
N	4.44066	16.45902	5.52974
C	4.59143	16.04727	6.92295
H	4.50427	14.96984	7.02785
H	5.59680	16.34007	7.24893
C	3.57477	16.75757	7.79322
H	3.73888	16.50268	8.84012
H	2.56127	16.45697	7.50304
C	3.49507	18.54876	6.32952
H	2.47688	18.26672	6.02953
H	3.58828	19.63360	6.28292
O	3.72075	18.15786	7.66775
C	4.49525	17.90723	5.38720
H	5.50849	18.25183	5.62290
H	4.27086	18.17333	4.35688
N	4.05339	7.81397	5.12551
C	4.85079	6.74488	4.54446
H	5.15758	7.01931	3.53365
H	4.19325	5.87897	4.43203
C	2.95228	7.39389	5.97771
H	2.85524	8.08469	6.81766
H	3.23015	6.43009	6.41206
O	2.22581	14.46555	5.93502
C	6.05077	6.37994	5.40192
H	6.61937	5.56690	4.94702
H	6.71614	7.23648	5.52903
H	5.72727	6.05544	6.39368
C	1.64114	7.26567	5.22070
H	1.73326	6.52963	4.41872
H	0.83990	6.94293	5.88775
H	1.35123	8.21762	4.77168

Molecule 15_2003249
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

43
c15_2003249.xyz.out Energy: -897466.6483784

S	4.06057	6.24092	-4.28648
O	7.49161	3.71886	-2.85189
O	5.81485	4.09914	-4.22505
N	4.87265	7.72971	-2.34704
N	11.20083	2.58326	-0.10527
C	6.45564	4.49998	-3.27584
C	5.12228	6.60974	-2.96043
C	6.21605	5.73352	-2.55470
C	7.01962	6.05916	-1.50025
C	3.27198	9.60262	-2.48413
C	8.94737	5.48597	-0.01607
C	2.18302	10.12603	-3.15203
C	9.95377	4.62104	0.32125
C	1.60575	9.44837	-4.23644
C	10.17249	3.42091	-0.41606
C	2.11176	8.23610	-4.66800
C	9.30165	3.14486	-1.48893
C	3.21174	7.70697	-3.99457
C	8.29935	4.03550	-1.80239
C	3.79626	8.37703	-2.90777
C	8.08242	5.22326	-1.09368
C	11.36551	1.31910	-0.80970
C	12.01058	2.80123	1.08636
C	10.40148	0.23197	-0.35784
C	11.31234	2.42612	2.38525
H	6.83332	6.98361	-0.96436
H	3.72516	10.11735	-1.64582
H	8.80327	6.39552	0.55601
H	1.76550	11.07427	-2.83615
H	10.58716	4.86626	1.16098
H	0.75165	9.88090	-4.74284
H	1.66562	7.71313	-5.50495
H	9.38149	2.24928	-2.08772
H	12.39458	0.99349	-0.65163
H	11.26904	1.49516	-1.88346
H	12.33785	3.84314	1.11412
H	10.59675	-0.06044	0.67481
H	10.50977	-0.65441	-0.98575
H	9.36506	0.56908	-0.42306
H	11.11011	1.35501	2.42683
H	11.94018	2.68514	3.24004
H	10.36117	2.95158	2.49130
H	12.91746	2.20690	0.96842

Molecule 16_7054002
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

45
c16_7054002.xyz.out Energy: -757846.9941980

O	2.47323	5.09224	4.58615
N	3.30377	8.86653	6.32777

F	5.59189	13.26318	8.74153
O	3.98671	6.34645	5.55073
N	-0.49595	2.01684	2.51536
C	1.81435	7.29851	5.25692
O	1.14294	9.46618	5.90408
C	0.23128	5.80271	4.18230
C	-0.24603	3.24983	3.03299
C	1.02523	3.58400	3.54217
H	1.85970	2.89843	3.51841
C	0.56508	7.03918	4.77138
H	-0.18493	7.81951	4.84882
C	1.23002	4.82506	4.10029
C	-1.03071	5.46834	3.65761
H	-1.82336	6.20668	3.69830
C	2.83162	6.27286	5.16501
C	2.05410	8.64154	5.85858
C	5.15991	9.97810	7.32100
H	5.73244	9.07558	7.13803
C	-1.26845	4.24269	3.09733
H	-2.25011	4.03735	2.69638
C	-1.78793	1.70025	1.92038
H	-2.58253	2.04808	2.58373
H	-1.87267	0.61310	1.89881
C	3.81688	10.02399	6.93587
C	5.76585	11.06341	7.92916
H	6.80514	11.03397	8.22968
C	3.68568	12.27726	7.78124
H	3.12798	13.18560	7.97070
C	5.01227	12.20097	8.14988
C	3.07968	11.18568	7.17044
H	2.04318	11.23954	6.87955
C	0.58611	1.05904	2.32549
H	0.12723	0.07958	2.18548
H	1.16883	0.98858	3.24717
C	-1.97376	2.26278	0.51937
H	-1.81246	3.34262	0.50208
H	-2.98625	2.06414	0.16274
H	-1.27352	1.80706	-0.18198
C	1.49093	1.38009	1.14504
H	0.94459	1.31224	0.20335
H	2.32308	0.67478	1.10534
H	1.90491	2.38721	1.22260
H	3.94934	8.08297	6.21740

Molecule 17_2210108
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

47
c17_2210108.xyz.out Energy: -732698.4594264

O	1.39390	9.62834	4.63001
O	-0.52313	8.80098	5.31017

O	-4.93535	12.64765	9.89714
O	-4.88050	10.44470	10.25984
N	5.57652	11.07971	2.88969
C	0.27283	9.70995	5.40943
C	0.13929	10.88395	6.26312
C	1.11240	11.83362	6.22789
C	2.25771	11.71463	5.39723
C	3.29791	12.65341	5.31371
C	4.37295	12.46133	4.48361
C	4.48402	11.29098	3.68175
C	3.43953	10.35021	3.75432
C	2.37197	10.57544	4.59754
C	-1.05014	11.01888	7.12500
C	-1.60292	9.92160	7.79346
C	-2.69274	10.08286	8.63217
C	-3.25612	11.34437	8.81501
C	-2.71735	12.44277	8.14953
C	-1.62899	12.27922	7.31212
C	-4.42559	11.56428	9.69560
C	-6.01121	10.59948	11.11500
C	5.63839	9.91806	2.01489
C	4.80114	10.04860	0.75076
C	6.56951	12.12694	2.69496
C	6.10650	13.26076	1.79140
H	1.03109	12.70604	6.86938
H	3.24189	13.55086	5.91967
H	5.14372	13.21734	4.45130
H	3.43172	9.44360	3.16674
H	-1.16931	8.93994	7.66139
H	-3.10769	9.22802	9.14987
H	-3.17087	13.41648	8.28812
H	-1.23422	13.13305	6.77371
H	-6.25044	9.60521	11.48201
H	-5.77128	11.26233	11.94629
H	-6.85385	11.01090	10.55953
H	6.68652	9.76546	1.75294
H	5.33999	9.03239	2.58058
H	3.76429	10.29682	0.98627
H	4.80649	9.10949	0.19408
H	5.19450	10.82887	0.09768
H	6.87894	12.51698	3.66774
H	7.45510	11.65300	2.26918
H	6.86085	14.04935	1.75657
H	5.93961	12.90825	0.77278
H	5.17384	13.69931	2.15186

Molecule 18_7117322
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

47
c18_7117322.xyz.out Energy: -730279.4689324

O	5.70671	8.93578	19.07373
O	2.10177	8.54208	21.25326
O	1.73336	6.60841	20.29146
N	0.57371	2.36293	18.50470
N	4.33996	9.94564	20.57565
H	3.52779	9.83457	21.18198
N	5.19306	11.01168	20.73929
H	4.78256	11.90830	20.51363
C	6.52702	9.79539	22.37401
H	6.09474	8.85578	22.05273
C	7.48682	9.81523	23.37799
H	7.78770	8.88040	23.83632
C	8.06378	11.00812	23.79356
H	8.81176	11.01427	24.57628
C	7.66645	12.19572	23.18670
H	8.10419	13.13725	23.49710
C	6.70807	12.19094	22.18684
H	6.39901	13.11850	21.71605
C	6.12807	10.98875	21.77353
C	4.67780	8.93244	19.73931
C	3.72702	7.78724	19.67216
C	2.51171	7.71752	20.45529
C	2.03342	5.58054	19.45155
C	3.20578	5.63021	18.68777
C	4.03601	6.76126	18.82666
H	4.95262	6.83181	18.24999
C	3.45625	4.54003	17.83397
H	4.35447	4.55022	17.22721
C	2.59320	3.48094	17.75701
H	2.82757	2.66894	17.08451
C	1.40822	3.43626	18.55026
C	1.14429	4.53129	19.39759
H	0.25972	4.58828	20.01482
C	-0.66517	2.35475	19.27113
H	-0.45677	2.70429	20.28472
H	-0.97576	1.31389	19.37071
C	-1.78373	3.17250	18.64298
H	-1.46439	4.19838	18.44887
H	-2.10685	2.73490	17.69747
H	-2.64669	3.20671	19.31061
C	0.76611	1.30375	17.52198
H	1.80771	0.97535	17.54406
H	0.17659	0.44888	17.85523
C	0.35911	1.69454	16.10914
H	-0.71254	1.88839	16.04867
H	0.88224	2.59456	15.78005
H	0.59732	0.88940	15.41146

Molecule 19_7225474
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

47
c19_7225474.xyz.out Energy: -740931.3450679

C	1.64237	20.04384	5.10643
C	3.02305	20.27461	5.48191
C	4.04448	19.82422	4.71485
H	5.06762	20.00776	5.02207
C	4.76879	18.61682	2.64559
H	5.81208	18.77359	2.89478
C	4.43665	17.93248	1.50519
H	5.23212	17.55810	0.87783
C	3.07648	17.71249	1.14622
C	2.08515	18.20484	2.01699
H	1.02941	18.06921	1.83240
C	2.55468	21.08549	7.80708
H	1.63427	20.54825	7.94570
C	3.28726	21.91631	8.61966
C	3.02099	22.35993	9.98943
C	3.99086	23.06326	10.70508
H	4.94223	23.27895	10.23476
C	3.73897	23.47986	12.00446
H	4.50052	24.02487	12.54925
C	2.51832	23.19951	12.60748
H	2.32359	23.52530	13.62198
C	1.54743	22.50024	11.89931
H	0.59130	22.28158	12.35935
C	1.79582	22.08493	10.59948
H	1.02886	21.55110	10.04931
C	3.77207	16.46778	-0.85107
H	3.32551	16.30457	-1.83299
H	4.57594	17.19079	-1.00648
C	4.32905	15.15883	-0.31107
H	4.70930	15.27957	0.70540
H	3.56208	14.38339	-0.29285
H	5.14888	14.80758	-0.94074
C	1.35709	16.73836	-0.29840
H	0.73950	17.62565	-0.13951
H	1.29398	16.51725	-1.36456
C	0.81816	15.56482	0.50668
H	0.94456	15.72658	1.57894
H	-0.24668	15.42835	0.30865
H	1.33189	14.63944	0.24286
C	3.78455	19.12179	3.51069
C	2.45293	18.88988	3.15403
N	3.26451	21.02218	6.65686
N	4.37364	21.77339	6.74720
N	4.39047	22.30733	7.92252
N	2.74593	17.06675	-0.00868
O	1.44642	19.34438	3.95682
O	0.66493	20.41039	5.72220

Molecule 20_4127666

Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

48
c20_4127666.xyz.out Energy: -1039734.2751926

S	5.96521	11.35102	5.50111
O	5.46073	9.13968	1.15655
C	5.74592	10.24063	0.40130
O	5.41617	8.00017	3.03779
C	6.36705	11.33954	0.99555
N	5.34418	11.29505	-3.08609
C	5.69851	11.28775	-1.76663
O	7.90586	8.23895	4.67332
H	7.55336	7.61382	4.02129
C	5.41438	10.18823	-0.93605
H	4.95150	9.28407	-1.30417
C	6.35015	12.40703	-1.17716
H	6.59698	13.26933	-1.77930
C	6.66426	12.42626	0.15763
H	7.14923	13.29662	0.58466
C	6.30187	10.20385	3.13097
C	6.66067	11.28037	2.38397
H	7.16665	12.11568	2.85269
N	6.52611	10.15297	4.52645
C	5.69450	9.05064	2.49004
C	4.70126	10.13515	-3.68418
H	3.93408	9.76553	-3.00066
H	4.16851	10.48104	-4.57167
C	5.84921	12.32211	-3.98734
H	5.27186	12.24592	-4.90984
H	5.62672	13.31021	-3.57629
O	6.52390	12.61374	5.11952
C	7.16761	9.38951	6.64356
C	6.83757	8.91083	5.25914
H	5.95969	8.26217	5.28994
O	4.53757	11.30697	5.62760
C	6.73403	10.67428	6.90633
C	5.66471	9.01866	-4.05975
H	5.11397	8.13670	-4.39253
H	6.28568	8.73117	-3.20859
H	6.32536	9.32765	-4.87117
C	7.81539	8.66952	7.63329
H	8.17429	7.66740	7.43412
C	7.55037	10.56673	9.12285
H	7.71168	11.01274	10.09588
C	6.90275	11.29320	8.13331
H	6.55603	12.30432	8.30560
C	7.33418	12.19948	-4.29737
H	7.65831	13.03084	-4.92654
H	7.54980	11.27012	-4.82619
H	7.93400	12.21253	-3.38532
C	8.00414	9.27171	8.87171

H 8.51642 8.72849 9.65601

Molecule 21_7054003
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

51
c21_7054003.xyz.out Energy: -838497.4306606
O 0.31048 7.71851 11.58954
O 5.74688 13.05094 14.88085
O 7.35557 11.57179 15.34296
O 3.91141 5.92907 12.91384
N 2.78202 7.90447 12.71722
N -2.36077 1.71026 9.38293
O -0.40769 5.75697 10.93172
C 0.56182 6.52807 11.49980
C -1.36965 3.77534 10.15077
H -2.21465 4.37901 9.85341
C -0.30571 4.41202 10.74802
C 0.90573 2.35625 10.93068
H 1.79130 1.81072 11.23573
C 1.88074 4.50781 11.74900
H 2.79432 4.02215 12.07611
C 0.85570 3.74484 11.15646
C 1.76965 5.85715 11.93006
C -1.31622 2.38315 9.93580
C 3.68376 8.81775 13.26799
C 2.91874 6.56044 12.56484
C 5.33879 10.80334 14.32758
C 4.95081 8.48294 13.75659
H 5.29384 7.46174 13.72565
C -3.56434 2.41769 8.96703
H -4.37772 1.69076 8.94931
H -3.83002 3.14386 9.73772
C 6.25183 11.81417 14.89755
C 3.25903 10.15216 13.31591
H 2.27593 10.40567 12.93496
C -2.21886 0.32131 8.96033
H -1.83484 -0.27622 9.79069
H -3.22371 -0.05319 8.76228
C 5.76022 9.47779 14.27935
H 6.74339 9.22891 14.65986
C -0.13363 1.69353 10.33831
H -0.05184 0.62744 10.18664
C 4.07439 11.13442 13.83836
H 3.73304 12.16070 13.86912
C 6.58808 14.06752 15.42014
H 7.52134 14.12636 14.86011
H 6.03447 14.99807 15.32861
H 6.81086 13.86188 16.46712
C -3.44119 3.09472 7.61045
H -3.33590 2.35817 6.81254

H	-4.33207	3.69013	7.40231
H	-2.57359	3.75712	7.57689
C	-1.34856	0.13983	7.72566
H	-0.35176	0.55936	7.87423
H	-1.23785	-0.92174	7.49658
H	-1.79230	0.62963	6.85801
H	1.89348	8.28232	12.38245

Molecule 22_7054005
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

47
c22_7054005.xyz.out Energy: -823846.5848718

O	4.64569	10.18661	-0.15971
N	1.29421	9.68716	-2.69779
O	2.99933	11.18154	-1.20662
O	1.72784	7.44418	-2.72328
N	8.36601	8.44867	2.23179
N	-3.25576	10.36339	-5.89465
O	-3.74283	9.39331	-6.45137
O	-3.70571	11.49340	-5.99329
C	3.17292	8.81206	-1.45726
C	5.03571	7.83316	-0.24729
C	3.91159	7.72314	-1.08645
H	3.60973	6.74962	-1.45873
C	7.27057	8.25867	1.45051
C	6.46478	9.33984	1.03805
H	6.64588	10.35597	1.35667
C	5.83769	6.75670	0.17877
H	5.58957	5.75723	-0.15953
C	5.39006	9.10881	0.21091
C	2.00572	8.57765	-2.34795
C	3.55339	10.12012	-0.97052
C	0.16451	9.77592	-3.50470
C	6.91202	6.95190	1.00132
H	7.50158	6.09720	1.29895
C	-0.39447	11.05538	-3.64616
H	0.06538	11.89034	-3.13082
C	-1.54519	8.89071	-4.94756
H	-2.00991	8.06283	-5.46467
C	-1.51198	11.25689	-4.42514
H	-1.94730	12.23978	-4.53739
C	-2.07687	10.16413	-5.06971
C	-0.42200	8.68919	-4.16505
H	-0.00196	7.70195	-4.06694
C	9.04570	7.32058	2.85998
H	9.32856	6.59107	2.09692
H	9.98084	7.70469	3.26846
C	8.74759	9.78451	2.67006
H	9.81989	9.76542	2.87193
H	8.61237	10.47949	1.83966

C	7.99304	10.26204	3.90099
H	8.25089	9.66255	4.77553
H	8.24411	11.30133	4.12056
H	6.91328	10.19630	3.75027
C	8.23842	6.65464	3.96406
H	7.27452	6.29779	3.59692
H	8.78487	5.79859	4.36414
H	8.04798	7.34949	4.78301
H	1.64721	10.55986	-2.29744

Molecule 23_4027127
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

49
c23_4027127.xyz.out Energy: -788743.9153665

O	2.56914	10.33096	2.07262
O	4.42632	9.64612	1.11935
N	3.99803	5.42117	5.66817
N	2.70370	7.31088	4.91791
N	5.16765	4.81353	5.31326
N	-1.44851	12.12944	3.83618
C	3.98338	4.42595	7.87282
H	5.06351	4.38083	7.83160
C	3.28971	3.95877	8.97917
H	3.83878	3.54284	9.81492
C	1.90221	4.03063	9.02159
H	1.36455	3.66938	9.88939
C	1.20888	4.56349	7.94231
H	0.12707	4.61219	7.96181
C	1.89004	5.02349	6.82338
H	1.35187	5.41873	5.97347
C	3.27898	4.95913	6.79849
C	3.73115	6.47397	4.84250
C	2.68163	8.27519	3.99699
C	1.60463	9.23754	3.99757
C	0.55032	9.23862	4.92045
H	0.54303	8.47862	5.69221
C	-0.45181	10.17658	4.87643
H	-1.22903	10.14212	5.62670
C	-0.45986	11.19279	3.88468
C	0.59608	11.19720	2.95562
H	0.65930	11.92002	2.15460
C	1.58713	10.24071	3.03091
C	3.61488	9.47407	2.00053
C	3.68270	8.40447	2.99689
C	4.75190	7.52358	2.94691
H	5.51294	7.64077	2.18509
C	4.78740	6.52245	3.90369
C	5.64174	5.44629	4.27327
H	6.56402	5.12626	3.81341
C	-2.61395	12.06804	4.70251

H	-2.91022	11.02749	4.84784
H	-3.44050	12.54180	4.16611
C	-2.39346	12.76338	6.03564
H	-3.29191	12.71179	6.65349
H	-2.14702	13.81649	5.88166
H	-1.57035	12.30303	6.58608
C	-1.39910	13.24636	2.90774
H	-0.36879	13.59433	2.80733
H	-1.95076	14.07246	3.36431
C	-1.99545	12.91004	1.55093
H	-1.94948	13.77194	0.88279
H	-3.04258	12.61664	1.65592
H	-1.46005	12.08283	1.08066

Molecule 24_7023327
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

50
c24_7023327.xyz.out Energy: -788865.6297638

O	2.43250	10.03088	7.12813
O	3.68875	9.09227	5.59206
N	5.48827	10.95936	4.37898
N	6.36300	11.16723	3.36020
H	6.16570	11.85849	2.64372
C	3.47994	11.47254	5.50398
C	3.25622	10.12911	6.03339
C	1.93447	12.36265	7.16113
C	0.98259	10.81256	8.78709
H	0.90810	9.78629	9.11743
N	-0.52620	11.62654	10.48329
C	7.57699	10.54346	3.35619
C	2.80256	12.51826	6.05015
H	2.94312	13.51902	5.65213
O	7.96973	9.81324	4.24724
C	0.27289	11.85883	9.40685
C	1.78364	11.08093	7.69815
C	4.42234	11.67256	4.38934
C	8.42874	10.84720	2.16169
C	0.42045	13.16937	8.87096
H	-0.08762	14.00412	9.33222
C	1.22555	13.40172	7.78539
H	1.33071	14.41017	7.40054
C	-1.37520	12.65774	11.05760
H	-2.24093	12.15409	11.49565
H	-1.77080	13.29523	10.26472
C	7.92026	11.19323	0.91469
H	6.85548	11.24277	0.72097
C	9.80655	10.74795	2.30808
H	10.23001	10.46329	3.26250
N	10.13521	11.36291	0.01690
C	-0.66231	13.48112	12.11699

H	-0.31445	12.83915	12.92957
H	-1.33211	14.23194	12.54021
H	0.20677	13.99177	11.69704
C	10.61328	11.02140	1.21539
H	11.69211	10.96219	1.30671
C	8.81196	11.43646	-0.12035
H	8.44009	11.69731	-1.10516
C	-0.59110	10.32280	11.12402
H	-0.83766	10.49240	12.17547
H	0.39872	9.86222	11.11872
C	4.11946	12.71782	3.35360
H	4.84098	13.53915	3.39408
H	3.12158	13.13015	3.47846
H	4.16248	12.28321	2.35063
C	-1.62346	9.40723	10.48772
H	-1.65283	8.44359	10.99925
H	-1.39507	9.22952	9.43493
H	-2.61885	9.85376	10.54623

Molecule 25_7116652
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

52
c25_7116652.xyz.out Energy: -1303545.8363131

S	-0.96929	10.77068	3.44752
S	1.24080	12.66698	3.02632
N	4.85640	5.26769	0.06580
O	-0.80989	9.22161	0.87735
O	1.03629	8.02649	0.68849
O	-1.46306	10.01462	6.25733
O	0.07817	11.36004	7.16912
O	1.62057	9.76239	5.25891
O	3.28520	11.21586	4.91937
C	-0.37822	11.68475	4.89054
H	-0.94297	12.61614	4.98661
C	1.08676	12.04951	4.70759
H	1.37670	12.86617	5.37209
C	0.31547	11.32849	2.26981
H	-0.21170	11.75805	1.41545
C	1.14569	10.16354	1.80149
C	0.37847	9.13998	1.11224
C	2.37939	7.84707	0.85232
C	3.14336	8.84089	1.46872
C	2.48240	10.01408	1.93551
H	3.07836	10.79581	2.39787
C	2.91608	6.66580	0.38543
H	2.24233	5.94466	-0.05480
C	4.29589	6.42436	0.51826
C	5.08703	7.43232	1.13474
H	6.15501	7.29987	1.23305
C	4.51920	8.59595	1.59083

H	5.14436	9.35514	2.04972
C	-0.64963	10.89742	6.15228
C	-0.08301	10.65682	8.40268
H	-1.11489	10.72344	8.74588
H	0.58458	11.13549	9.11357
H	0.18907	9.60972	8.26853
C	2.00321	10.87595	4.98917
C	4.21321	10.15123	5.14396
H	4.14054	9.80142	6.17359
H	5.19972	10.56519	4.95458
H	4.00541	9.31914	4.46970
C	6.24803	4.93125	0.31636
H	6.31402	3.84064	0.35452
H	6.54049	5.28143	1.30823
C	7.18511	5.47053	-0.75135
H	6.91473	5.07393	-1.73266
H	8.21762	5.18452	-0.54215
H	7.13385	6.56010	-0.80422
C	4.08707	4.28343	-0.67741
H	4.78536	3.75540	-1.33241
H	3.38282	4.79218	-1.33890
C	3.37018	3.29318	0.22542
H	4.08869	2.74993	0.84369
H	2.81139	2.56505	-0.36523
H	2.67135	3.80302	0.89153

Molecule 26_4027133
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

55
c26_4027133.xyz.out Energy: -838037.0646074

O	0.40316	3.55807	-1.60912
O	0.65228	3.68751	-3.77402
N	5.27435	7.58848	-0.46994
N	5.37715	7.25743	-1.77127
N	4.19186	5.95566	-3.37577
N	-0.15437	2.34275	2.94201
C	4.26146	6.91239	0.03958
C	4.40520	6.39182	-2.12885
C	3.12775	5.19233	-3.54733
C	2.32117	4.76380	-2.44462
C	1.11828	3.97449	-2.69361
C	0.85738	3.66264	-0.32715
C	0.14039	2.96891	0.62509
H	-0.72824	2.42160	0.28855
C	0.56404	2.97091	1.96631
C	1.77868	3.64675	2.25681
H	2.20428	3.60849	3.24902
C	2.45307	4.34472	1.28602
H	3.39373	4.80898	1.54685
C	1.99035	4.42406	-0.03785

C	2.65455	5.10881	-1.11788
C	3.67344	6.07914	-0.97010
C	3.83338	7.21822	1.41422
C	2.48137	7.40975	1.69989
H	1.75036	7.31545	0.90406
C	2.07387	7.71621	2.99003
H	1.02175	7.86407	3.20114
C	3.01397	7.83729	4.00756
H	2.69604	8.07466	5.01557
C	4.36366	7.65834	3.72635
H	5.09991	7.75505	4.51517
C	4.77278	7.35200	2.43524
H	5.82273	7.20583	2.21055
C	6.36129	7.88743	-2.61808
H	6.28188	7.45407	-3.61198
H	7.35986	7.70930	-2.22139
H	6.18109	8.96087	-2.67398
C	2.86090	4.78105	-4.96083
H	3.67675	5.14922	-5.58026
H	1.91726	5.19428	-5.31898
H	2.78132	3.69839	-5.05894
C	-1.30373	1.51886	2.59767
H	-1.95108	2.07693	1.91637
H	-1.88207	1.37521	3.51171
C	-0.94180	0.16783	1.99714
H	-1.84345	-0.35571	1.67331
H	-0.42951	-0.46182	2.72571
H	-0.28731	0.28095	1.13069
C	0.35121	2.26556	4.30434
H	-0.50135	2.05576	4.95249
H	0.71902	3.24981	4.60293
C	1.42867	1.21011	4.50777
H	1.83725	1.27489	5.51825
H	2.24949	1.34201	3.79979
H	1.02595	0.20550	4.37179

Molecule 27_8102459
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

49
c27_8102459.xyz.out Energy: -801349.6610777

O	4.40607	20.07952	7.62821
O	4.00803	20.79165	5.58239
O	10.10574	23.58663	4.60396
O	11.46153	25.23858	3.19742
H	11.19728	24.68474	3.97610
N	4.90705	18.41934	12.05550
N	7.77853	22.33752	5.10275
N	8.05945	22.92447	3.90918
H	7.33295	22.96552	3.19991
C	5.42879	19.02647	10.95251

C	6.77832	19.48242	10.94128
H	7.40716	19.33045	11.80645
C	7.29642	20.13303	9.85360
H	8.32278	20.48155	9.87113
C	6.52570	20.36631	8.70026
C	6.98866	21.02053	7.53637
H	8.00868	21.39013	7.50244
C	6.18010	21.19585	6.45223
C	4.81622	20.70102	6.48410
C	5.20470	19.90117	8.71827
C	4.65344	19.24610	9.79733
H	3.63237	18.90393	9.70848
C	3.51684	17.98998	12.08103
H	3.20386	17.96587	13.12655
H	2.90412	18.75646	11.60313
C	3.28029	16.63289	11.43618
H	3.75940	15.83799	12.01019
H	2.21160	16.41512	11.38967
H	3.67905	16.60536	10.41975
C	5.77378	17.93785	13.12453
H	6.39025	18.75987	13.49800
H	5.12296	17.65109	13.95151
C	6.64761	16.75759	12.72603
H	7.28344	17.00002	11.87265
H	7.29430	16.47126	13.55766
H	6.03960	15.89346	12.45488
C	6.60074	21.85815	5.22858
H	5.86344	21.92403	4.42604
C	9.26249	23.51996	3.70262
C	9.50711	24.09564	2.36366
C	8.69893	23.82296	1.25176
H	7.87129	23.12819	1.33333
C	8.94683	24.39896	0.02214
H	8.31334	24.16823	-0.82413
C	10.02640	25.27253	-0.11701
H	10.22839	25.73421	-1.07603
C	10.85067	25.54549	0.95572
H	11.70122	26.20967	0.86510
C	10.61235	24.95293	2.19735

Molecule 28_7017064
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

49
c28_7017064.xyz.out Energy: -801350.1096780

C	3.45942	18.11628	4.02098
C	2.62360	19.10667	4.54089
H	2.76367	20.12287	4.19372
C	1.64471	18.78253	5.45807
H	0.99869	19.56060	5.84656
C	1.47370	17.46188	5.87580

H	0.69216	17.20412	6.57827
C	2.30734	16.48214	5.37538
H	2.14003	15.45900	5.69116
C	3.32202	16.78374	4.45669
C	4.25164	15.77087	3.91294
C	5.09295	12.49382	4.76638
H	4.47066	12.38180	5.65647
C	5.91321	11.35380	4.39391
C	6.74613	11.33784	3.31336
H	6.81309	12.21922	2.68334
C	7.51994	10.19900	2.99851
C	7.41636	9.07626	3.83104
C	5.81418	10.18181	5.24336
C	8.39776	10.09858	1.90365
H	8.50697	10.95380	1.24640
C	9.11478	8.95738	1.66162
H	9.79367	8.93578	0.82125
C	8.99646	7.82172	2.51393
C	8.12139	7.91408	3.61467
H	7.96057	7.09118	4.29629
C	10.50932	6.51310	1.07348
H	10.52393	5.44271	0.85230
H	10.01270	6.98672	0.22491
C	11.92824	7.03017	1.23689
H	12.43097	6.51467	2.05843
H	12.50725	6.86421	0.32672
H	11.93307	8.09952	1.45776
C	9.69381	5.56534	3.19822
H	10.64779	5.04456	3.08413
H	9.67442	5.93471	4.22535
C	8.54317	4.60744	2.93915
H	8.60399	4.20220	1.92647
H	8.57053	3.77264	3.64156
H	7.58027	5.11149	3.04288
N	4.28774	14.56607	4.53794
N	5.09937	13.57392	4.08319
N	9.70675	6.68911	2.27455
O	4.37848	18.48980	3.11604
H	4.82853	17.66684	2.79542
O	4.97712	16.00943	2.94081
O	5.11014	10.07589	6.22697
O	6.58052	9.10275	4.90716
H	3.76961	14.41440	5.39876

Molecule 29_4027128
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

52
c29_4027128.xyz.out Energy: -813393.9699756

O	2.65018	19.81574	4.54705
O	4.32109	20.56742	5.75993

N	6.85115	15.26095	3.72003
N	8.03976	15.50648	4.35754
N	4.74244	16.40054	3.45358
N	-1.19150	18.53502	2.06662
C	6.70974	14.10037	2.92288
C	5.47225	13.47707	2.79656
H	4.61213	13.87260	3.31788
C	5.36043	12.33969	2.00825
H	4.39669	11.85483	1.91142
C	6.47231	11.81547	1.36147
H	6.37927	10.92507	0.75217
C	7.70660	12.43804	1.50666
H	8.58049	12.03601	1.00878
C	7.83039	13.58184	2.28109
H	8.78540	14.07686	2.39570
C	9.04350	17.20460	5.80434
H	8.73898	17.32915	6.84556
H	9.90589	16.54079	5.76904
H	9.33997	18.18653	5.42959
C	7.93375	16.64381	4.99358
C	6.63489	17.20204	4.77755
C	5.97015	16.27621	3.94242
C	5.95158	18.34393	5.15166
H	6.38063	19.10668	5.79114
C	4.65990	18.49290	4.66449
C	3.90486	19.68730	5.04032
C	2.06952	18.88542	3.71776
C	2.74827	17.73262	3.33138
C	4.09143	17.50785	3.81473
C	2.06359	16.86029	2.47601
H	2.56865	15.95965	2.14904
C	0.78682	17.12253	2.04273
H	0.31192	16.41557	1.37810
C	0.09733	18.29284	2.45579
C	0.78702	19.17974	3.30145
H	0.35376	20.10636	3.64929
C	-1.83424	17.69531	1.06625
H	-1.71099	16.64541	1.34378
H	-2.90566	17.89406	1.12130
C	-1.33911	17.92934	-0.35403
H	-1.79393	17.20960	-1.03767
H	-1.59651	18.93163	-0.69906
H	-0.25470	17.81996	-0.41890
C	-1.84443	19.78569	2.42192
H	-2.91924	19.63258	2.31190
H	-1.67880	19.98397	3.48372
C	-1.40215	20.97785	1.58504
H	-1.71026	20.86363	0.54478
H	-1.84784	21.89746	1.96940
H	-0.31661	21.09382	1.60417

Molecule 30_2231616
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

49
c30_2231616.xyz.out Energy: -1182860.7320671

C	3.66597	12.36737	17.06006
C	4.11503	12.99321	18.26038
H	4.43682	14.02451	18.24565
C	4.17060	12.30086	19.43924
H	4.51900	12.79456	20.33941
C	3.79178	10.94768	19.51375
C	3.81331	10.16777	20.69020
H	4.14259	10.64538	21.60700
C	3.44167	8.85141	20.69503
C	2.96915	8.25948	19.45933
C	3.36108	10.34366	18.32688
C	3.29060	11.01050	17.12499
H	2.92087	10.46913	16.26590
C	3.42562	8.05818	21.93804
C	4.72501	4.79115	21.52312
C	5.10377	3.91935	20.49943
C	5.52201	2.62743	20.77130
H	5.80508	1.98310	19.94852
C	5.56991	2.17765	22.08229
H	5.89588	1.16793	22.29528
C	5.19532	3.03572	23.11022
H	5.22704	2.69696	24.13834
C	4.77883	4.32842	22.83818
H	4.48745	4.99727	23.63629
C	2.97569	8.76989	23.19661
C	3.83996	14.49347	15.82676
H	3.44069	14.97497	16.72113
H	3.24678	14.87525	14.99198
C	5.30538	14.83782	15.62423
H	5.91453	14.46234	16.44898
H	5.44302	15.91856	15.55934
H	5.67917	14.39142	14.70005
C	3.26392	12.41338	14.63542
H	3.70477	11.41543	14.60439
H	3.75136	12.98256	13.83977
C	1.76470	12.35813	14.39605
H	1.26068	11.79742	15.18572
H	1.54393	11.87878	13.44088
H	1.34333	13.36581	14.37636
Cl	5.04565	4.46045	18.85563
F	1.95349	9.60298	22.95444
F	3.96111	9.52902	23.72289
F	2.59063	7.93438	24.15402
N	3.60577	13.05849	15.89401
N	3.82159	6.85984	22.16182
N	4.33342	6.09079	21.21140

H 4.13535 6.30823 20.23617
O 2.97432 9.03889 18.34231
O 2.56115 7.11962 19.33009

Molecule 31_7054004
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

46
c31_7054004.xyz.out Energy: -753433.4857152
O 4.69062 7.95859 14.26962
N 5.45737 7.87076 10.10545
C 4.11584 7.31309 12.03415
C 3.58152 7.35139 14.77354
O 6.04794 8.57040 12.66366
C 2.69370 6.70210 13.90468
C 2.25221 6.81044 16.70565
C 1.56177 6.09675 14.48432
H 0.86150 5.57939 13.83859
C 3.38906 7.41863 16.13345
H 4.11594 7.95942 16.72221
O 3.53996 6.65784 9.84281
C 2.99776 6.70270 12.53089
H 2.33270 6.20749 11.83089
C 5.01705 7.98180 12.94670
C 4.33782 7.24748 10.56479
N 2.03166 6.85389 18.04178
C 1.34087 6.14309 15.83275
H 0.47030 5.64655 16.23626
C 5.92296 7.97307 8.79519
C 5.26430 7.44921 7.67805
H 4.33129 6.92239 7.79332
C 7.13480 8.65561 8.62212
H 7.64063 9.05862 9.49208
C 7.02447 8.29190 6.25273
C 7.58403 8.45226 4.94736
C 7.68332 8.81606 7.36859
H 8.61975 9.34431 7.24390
C 3.00327 7.42486 18.96345
H 2.86907 6.92058 19.92341
H 4.01326 7.17654 18.63243
C 0.81505 6.33170 18.64833
H 0.64210 6.90565 19.56205
H -0.03853 6.53760 18.00085
C 5.81848 7.61222 6.42002
H 5.31027 7.20756 5.55391
C 0.91656 4.85135 18.97253
H 1.74312 4.66709 19.66254
H -0.00250 4.49454 19.44043
H 1.09437 4.26323 18.06985
C 2.83392 8.92483 19.13319
H 1.83746 9.15712 19.51540

H	3.56855	9.31786	19.83790
H	2.95929	9.44473	18.18135
N	8.03664	8.58261	3.89390
H	6.02420	8.31449	10.83147

Molecule 32_7106102
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

51
c32_7106102.xyz.out Energy: -1049329.6202930

C	7.97389	13.74534	13.52846
N	7.09187	14.63207	12.95490
C	6.52754	15.30402	13.99832
C	6.31201	12.93993	8.64866
C	6.64886	14.12716	9.41138
C	6.87505	15.31302	8.76721
H	7.13940	16.19097	9.34825
C	6.77605	15.41221	7.36717
C	6.98322	16.59232	6.62641
H	7.23746	17.50117	7.15982
C	6.86636	16.61182	5.26437
H	7.02805	17.54325	4.74244
C	6.54210	15.42797	4.53581
C	6.32191	14.24437	5.27187
H	6.05415	13.30969	4.80159
C	6.44487	14.25705	6.64093
C	6.07638	14.24061	2.44707
H	6.62662	13.38506	2.84470
H	6.41901	14.36508	1.41926
C	4.57923	13.97208	2.46703
H	4.19857	13.91989	3.48895
H	4.36002	13.02286	1.97480
H	4.03333	14.75784	1.94306
C	6.55896	16.68777	2.43278
H	6.76244	16.42467	1.39442
H	7.43076	17.24963	2.77537
C	5.30333	17.54265	2.51383
H	4.45686	17.04090	2.04333
H	5.46078	18.49330	2.00095
H	5.03420	17.75646	3.55015
C	5.52449	16.36425	13.89787
C	5.49610	17.33889	14.89767
H	6.22639	17.29480	15.69603
C	4.54796	18.34887	14.86064
H	4.53612	19.10305	15.63787
C	3.61862	18.39642	13.82705
H	2.87903	19.18731	13.79771
C	3.63781	17.42422	12.83519
H	2.90792	17.44952	12.03536
C	4.58446	16.40926	12.86757
H	4.57678	15.64353	12.10327

N	7.92879	13.87491	14.83001
N	7.02037	14.84093	15.12619
N	6.95892	14.96619	11.61922
C	6.73303	13.96816	10.84664
H	6.56074	12.96709	11.23927
N	6.46831	15.43838	3.17993
O	6.22733	13.08074	7.29271
O	6.10038	11.83763	9.10780
S	9.14442	12.78376	12.68187
H	8.32049	11.83762	12.22106

Molecule 33_1558692
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

51
c33_1558692.xyz.out Energy: -812746.0866924

C	1.13531	15.97449	6.29706
C	-0.22675	15.92956	5.99815
H	-0.53273	16.04359	4.96519
C	-1.15077	15.74212	7.01049
H	-2.20631	15.70862	6.76825
C	-0.73237	15.59718	8.33176
H	-1.45676	15.45067	9.12298
C	0.62222	15.64168	8.62043
H	0.96281	15.52891	9.64290
C	1.56580	15.82952	7.61257
H	2.61714	15.85686	7.86485
C	3.36382	16.24207	5.49883
H	3.56359	17.06429	6.19309
H	3.71958	15.30914	5.94647
C	4.07031	16.46075	4.21242
C	4.22493	17.60970	3.48308
H	3.89844	18.62197	3.63977
C	5.72070	19.36252	1.50591
C	5.35640	17.97868	1.27910
C	5.46122	17.41452	0.05258
H	5.18413	16.37564	-0.08542
C	5.93732	18.17205	-1.04767
C	6.27427	19.51156	-0.83237
C	6.74217	20.34066	-1.82813
H	6.98942	21.35707	-1.55876
C	6.88933	19.84555	-3.13805
C	6.56146	18.47896	-3.36659
H	6.66915	18.05279	-4.35326
C	6.09692	17.68080	-2.35378
H	5.84787	16.64530	-2.55555
C	7.64799	20.08989	-5.45903
H	6.82339	19.46680	-5.81397
H	7.71165	20.92561	-6.15717
C	8.95164	19.30526	-5.47253
H	9.11320	18.85808	-6.45532

H	9.80140	19.95208	-5.25079
H	8.93962	18.50198	-4.73316
C	7.68522	22.03186	-3.89981
H	7.62494	22.56563	-4.84943
H	6.93337	22.48821	-3.25201
C	9.07521	22.19334	-3.30186
H	9.84501	21.88939	-4.01258
H	9.25490	23.23704	-3.03709
H	9.19117	21.58916	-2.39971
N	4.68887	15.45124	3.54574
N	5.21151	15.91150	2.45770
N	4.93461	17.22559	2.39864
N	7.30832	20.64938	-4.15714
O	1.97053	16.16442	5.23871
O	6.14803	20.05224	0.41496
O	5.67373	19.94659	2.56689

Molecule 34_4325585
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

43
c34_4325585.xyz.out Energy: -1520324.2429103

Cl	3.46985	7.67434	5.02864
Hg	3.71865	8.61511	2.92583
Cl	3.32128	9.83248	0.97624
S	6.20557	7.35771	2.49454
O	6.00253	11.03041	-5.25494
O	4.38024	10.13904	-4.06203
N	9.22894	13.05811	-8.07894
N	6.84501	9.03251	-0.98700
N	6.23705	8.45843	0.09075
H	5.21974	8.46555	0.16660
N	8.28323	8.06612	1.02017
H	8.70591	8.44331	0.18129
H	8.85593	7.74350	1.78552
C	11.48600	12.58330	-8.97517
H	12.46500	13.02487	-9.16936
H	11.62237	11.71341	-8.32933
H	11.07492	12.23565	-9.92559
C	10.55634	13.59812	-8.33270
H	10.43062	14.46104	-8.99149
H	10.97880	13.98864	-7.40555
C	7.44583	14.55272	-8.91971
H	6.72557	14.69298	-9.72741
H	6.89992	14.52421	-7.97462
H	8.10914	15.42057	-8.90066
C	8.24493	13.27759	-9.12838
H	8.78974	13.32537	-10.07451
H	7.58820	12.40898	-9.20325
C	8.91482	12.41822	-6.92483
C	7.59016	12.02334	-6.64838

H	6.77283	12.22936	-7.32441
C	7.30186	11.37754	-5.46863
C	8.27349	11.08450	-4.50041
C	9.59389	11.47936	-4.78665
H	10.37028	11.25955	-4.06253
C	9.91431	12.12079	-5.95264
H	10.94577	12.38468	-6.13761
C	7.86121	10.43239	-3.31868
H	8.59848	10.20753	-2.55446
C	6.55602	10.08990	-3.11223
C	5.56289	10.39717	-4.12741
C	6.06148	9.43439	-1.91662
H	4.98154	9.29897	-1.84589
C	6.95808	8.00356	1.12644

Molecule 35_7154613
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

48
c35_7154613.xyz.out Energy: -1229292.7673021

S	9.70239	10.57627	5.65836
S	12.46918	11.21044	6.68442
O	6.44690	7.08165	11.13663
N	9.36202	9.41353	8.15071
O	12.54572	11.44849	3.13936
O	8.48517	7.64971	11.74968
N	2.01439	5.69886	10.15545
N	10.60167	9.94155	7.99636
H	11.28826	9.87926	8.74879
O	11.78381	9.43724	3.75582
C	7.82602	8.24366	9.54780
C	5.42020	7.02154	10.24278
C	5.57007	7.58398	8.96695
C	6.80199	8.19270	8.64633
H	6.93935	8.62809	7.66137
C	3.16502	6.31187	9.77842
C	4.46720	7.49155	8.09767
H	4.55597	7.90953	7.10125
C	11.67954	10.63976	3.74366
C	4.26346	6.40229	10.65737
H	4.22834	6.01779	11.66672
C	1.89829	4.99884	11.42561
H	2.83960	4.49460	11.65240
H	1.15735	4.20679	11.28958
C	0.82074	5.70289	9.32317
H	-0.03833	5.64518	9.99643
H	0.73269	6.66101	8.80850
C	0.79094	4.54664	8.33840
H	0.83042	3.59198	8.86783
H	-0.12454	4.56810	7.74462
H	1.64390	4.58909	7.65797

C	9.11430	8.85097	9.27331
H	9.86327	8.80511	10.06557
C	10.53370	11.42557	4.33429
H	10.87670	12.41213	4.64090
H	9.77758	11.55395	3.55400
C	3.30314	6.88075	8.47894
H	2.49094	6.81493	7.76929
C	7.65288	7.66329	10.86672
C	10.96851	10.55718	6.85744
C	1.47944	5.91624	12.56178
H	2.20668	6.71745	12.70780
H	0.51145	6.37464	12.34670
H	1.39139	5.35861	13.49571
C	13.67769	10.80391	2.55429
H	14.23596	10.26645	3.32139
H	13.36107	10.10513	1.78026
H	14.28771	11.59402	2.12564

Molecule 36_7119168
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

52
c36_7119168.xyz.out Energy: -825981.6786300

O	-0.99243	3.88155	2.18655
O	-0.20229	4.54686	4.13180
O	2.57812	8.28759	-1.58905
O	1.00372	7.18490	-7.63044
N	1.29410	5.70469	8.48705
N	1.19746	6.62627	0.06100
N	1.07198	6.61515	-1.29032
H	0.51007	5.88619	-1.72229
C	-0.24824	4.64337	2.77031
C	0.58643	5.33285	4.91791
C	0.53096	5.11571	6.27662
H	-0.11866	4.33020	6.63609
C	1.32963	5.89030	7.14117
C	2.17433	6.87811	6.55855
H	2.78837	7.50593	7.18811
C	2.20668	7.06837	5.20251
H	2.85141	7.83082	4.78008
C	1.41177	6.30145	4.33199
C	1.38988	6.43640	2.92513
H	2.02080	7.18171	2.45108
C	0.59458	5.64712	2.14821
C	0.53345	5.73989	0.69787
H	-0.10414	5.01869	0.18257
C	0.34963	4.79179	9.11098
H	-0.60332	4.83109	8.57995
H	0.14956	5.17218	10.11592
C	0.87491	3.36815	9.18698
H	1.80085	3.33238	9.76552

H	1.08450	2.97355	8.19075
H	0.14729	2.71301	9.66914
C	2.20211	6.39292	9.39169
H	3.18312	6.49396	8.92431
H	2.34910	5.74038	10.25632
C	1.66887	7.74230	9.84233
H	2.36450	8.22177	10.53333
H	0.71006	7.62409	10.35229
H	1.51645	8.40785	8.99014
C	1.78590	7.48645	-2.06456
C	1.54614	7.38224	-3.52832
C	0.39819	6.81822	-4.09480
H	-0.40550	6.44122	-3.47281
C	0.24302	6.76894	-5.46514
H	-0.64629	6.34648	-5.91608
C	1.23700	7.28087	-6.30241
C	2.38256	7.85405	-5.75213
H	3.16186	8.26060	-6.38191
C	2.52039	7.90377	-4.37291
H	3.40217	8.35167	-3.93124
C	1.97683	7.69654	-8.52017
H	2.93266	7.17985	-8.39900
H	2.12005	8.77045	-8.37346
H	1.59863	7.51966	-9.52415

Molecule 37_1547843
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

54
c37_1547843.xyz.out Energy: -917755.1143872

F	4.67443	7.25500	-4.54894
F	4.55913	8.47019	-9.04519
O	0.94804	4.84384	2.43359
O	0.94985	7.00104	2.03546
C	2.81648	8.59785	-2.82385
H	2.76749	7.56981	-3.15499
N	0.76135	0.26660	3.69227
C	1.19485	3.54274	2.12164
N	3.21505	10.88724	-3.39764
C	3.56692	9.26638	-5.12283
C	3.19808	9.58638	-3.72269
C	1.78357	3.22675	0.89292
C	1.85391	5.59965	0.32785
C	1.08849	1.23059	2.79020
C	2.05472	7.97265	-0.49878
H	1.62832	8.39008	0.40415
C	2.10041	4.29171	0.01739
H	2.55949	4.05717	-0.93909
C	2.20811	6.64400	-0.61661
H	2.66944	6.25326	-1.52124
C	0.85119	2.59246	3.05848

H	0.42262	2.93434	3.98972
C	3.22479	10.14614	-6.15266
H	2.68861	11.04893	-5.89012
C	2.45791	8.94210	-1.51846
C	3.54570	9.89461	-7.47613
H	3.26896	10.57586	-8.26950
C	4.23764	8.73437	-7.77059
C	4.26973	8.12324	-5.49053
C	2.85975	11.22021	-2.15901
H	2.87912	12.27881	-1.92130
C	2.48260	10.30013	-1.19557
H	2.20846	10.63107	-0.20109
C	4.61758	7.83348	-6.79654
H	5.17597	6.93910	-7.03765
C	1.68008	0.89416	1.53894
H	1.85596	-0.14097	1.28321
C	0.05509	0.57656	4.92503
H	-0.51282	-0.31469	5.20386
H	-0.68530	1.35674	4.73800
C	2.01386	1.86492	0.63114
H	2.45954	1.58441	-0.31673
C	1.11864	-1.13012	3.50005
H	1.24101	-1.56961	4.49333
H	2.09700	-1.19888	3.02109
C	0.99259	0.97197	6.05368
H	1.69377	0.16265	6.26976
H	0.43151	1.18779	6.96458
H	1.57232	1.85885	5.79006
C	0.06992	-1.90077	2.71649
H	-0.89291	-1.86801	3.23153
H	0.36040	-2.94704	2.60548
H	-0.06731	-1.47408	1.72075
C	1.23668	5.90187	1.61334

Molecule 38_4027132
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

62
c38_4027132.xyz.out Energy: -958247.8353306

O	1.48688	4.35332	-0.29087
O	0.69208	5.78804	1.15277
N	2.78852	1.82570	-4.10159
N	4.54816	6.54622	2.71619
N	6.76212	5.61903	2.72087
N	7.42659	4.61552	2.09756
C	4.36292	-0.11359	-3.95208
H	5.11891	-0.65627	-4.52315
H	3.57514	-0.81598	-3.67601
H	4.83114	0.24505	-3.03241
C	3.80546	1.03339	-4.78352
H	4.61669	1.68328	-5.12373

H	3.33954	0.63828	-5.68737
C	0.80396	0.38234	-3.65671
H	-0.26337	0.28989	-3.86668
H	0.92931	0.52043	-2.58044
H	1.28303	-0.55741	-3.93724
C	1.39847	1.54978	-4.43003
H	1.35052	1.35022	-5.50229
H	0.81192	2.45588	-4.26880
C	3.10938	2.55240	-2.99089
C	2.12660	3.09112	-2.14189
H	1.06802	2.97079	-2.32306
C	2.50121	3.81241	-1.02636
C	3.82839	3.99445	-0.63840
C	4.79864	3.53738	-1.54595
H	5.83983	3.76911	-1.37105
C	4.46352	2.84193	-2.67870
H	5.25386	2.52778	-3.34563
C	1.68770	5.26540	0.70463
C	3.05936	5.46152	1.16837
C	4.09358	4.70119	0.58699
C	3.33393	6.39741	2.21291
C	5.47997	5.69927	2.26882
C	5.33723	4.73721	1.25752
C	2.29131	7.30283	2.78751
H	2.77976	7.99064	3.47526
H	1.52900	6.73349	3.32121
H	1.77069	7.86273	2.01062
C	6.60236	4.05942	1.23670
C	7.01224	2.82373	0.54912
C	8.25664	2.73229	-0.07077
H	8.92686	3.58344	-0.04255
C	8.62200	1.56792	-0.73374
H	9.58746	1.50685	-1.22118
C	7.75083	0.48495	-0.77587
H	8.03634	-0.42144	-1.29604
C	6.51584	0.56512	-0.14130
H	5.83873	-0.28046	-0.15942
C	6.14836	1.72896	0.51817
H	5.18287	1.79835	1.00747
C	7.42563	6.39520	3.70542
C	6.74698	6.84365	4.83274
H	5.70314	6.60053	4.96844
C	7.42877	7.59607	5.77974
H	6.90102	7.94579	6.65848
C	8.77683	7.88708	5.61432
H	9.30300	8.47064	6.35954
C	9.44804	7.42076	4.48994
H	10.49977	7.64042	4.35355
C	8.77606	6.67838	3.53057
H	9.28617	6.31387	2.64866

Molecule 39_1558693
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

56
c39_1558693.xyz.out Energy: -919135.4128799

C	5.58526	7.24569	-0.20749
H	5.39067	6.31862	-0.71570
C	6.17937	8.41065	-0.60694
C	6.74488	8.76713	-1.93509
H	6.12575	9.52578	-2.42783
H	7.75471	9.17665	-1.82006
C	7.21919	7.65070	-3.96973
C	7.67941	8.79719	-4.56893
H	7.70276	9.73284	-4.02688
C	8.13234	8.76983	-5.90763
H	8.48936	9.69035	-6.35306
C	8.12435	7.61343	-6.63281
H	8.47068	7.59014	-7.65946
C	7.65512	6.41688	-6.03699
C	7.19717	6.41992	-4.69801
C	7.61905	5.18611	-6.72968
H	7.96271	5.15000	-7.75762
C	7.15371	4.06858	-6.09617
H	7.11093	3.10985	-6.59636
C	6.72159	4.18173	-4.75900
H	6.34852	3.30393	-4.24028
C	3.65231	5.68752	1.56055
C	4.66476	6.60882	2.03635
C	4.99939	6.67117	3.34687
H	5.76246	7.36893	3.67230
C	4.35368	5.83727	4.29529
C	3.37906	4.94536	3.83628
C	2.69498	4.08497	4.66645
H	1.97519	3.41541	4.21765
C	2.96739	4.08533	6.04808
C	3.95781	4.98817	6.52802
H	4.18359	5.03358	7.58368
C	4.62263	5.82919	5.67384
H	5.36739	6.51393	6.06328
C	1.21142	2.40987	6.44401
H	0.62199	2.94352	5.69592
H	0.54587	2.25711	7.29756
C	1.68929	1.07039	5.90869
H	0.84451	0.45922	5.58630
H	2.36034	1.20441	5.05783
H	2.23121	0.52100	6.68204
C	2.65659	3.13985	8.30351
H	3.73897	3.21738	8.42123
H	2.39338	2.12659	8.61774
C	1.93758	4.15720	9.17305
H	2.20849	4.02940	10.22265

H	2.18964	5.17677	8.87429
H	0.85524	4.03883	9.08432
N	5.25426	7.47492	1.08746
N	5.61914	8.71034	1.45796
N	6.18041	9.27559	0.43699
N	6.73868	5.30378	-4.07920
N	2.30485	3.25465	6.89677
O	6.76874	7.58230	-2.70026
O	3.28336	5.56404	0.41374
O	3.07795	4.89393	2.50599

Molecule 40_1558694
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

57
c40_1558694.xyz.out Energy: -909073.7926893

C	7.01166	7.85680	-4.18511
C	6.77351	9.00548	-4.89704
H	6.29503	9.85904	-4.43694
C	7.16085	9.08333	-6.25526
H	6.96349	9.99953	-6.79880
C	7.77100	8.03360	-6.87876
H	8.06631	8.09645	-7.91984
C	8.02943	6.83653	-6.16264
C	8.66068	5.72580	-6.77184
H	8.94956	5.80400	-7.81441
C	8.90316	4.57834	-6.06478
H	9.38774	3.73649	-6.54462
C	8.52417	4.48717	-4.70914
H	8.72106	3.57612	-4.15716
C	7.91047	5.54444	-4.08943
H	7.61916	5.47992	-3.04909
C	7.65001	6.73817	-4.80053
C	6.00624	8.74412	-2.22056
H	5.07490	8.97298	-2.74829
H	6.63420	9.63991	-2.20955
C	5.73402	8.32710	-0.82288
C	4.79507	7.45644	-0.33597
H	4.02792	6.87109	-0.80994
C	4.37707	6.68655	2.01118
C	2.96542	6.40679	1.84918
C	5.05400	6.27968	3.11180
H	6.11086	6.50255	3.20401
C	4.38913	5.57108	4.14338
C	4.99842	5.10784	5.32158
H	6.05145	5.31191	5.47840
C	4.28876	4.42066	6.27123
H	4.79457	4.10529	7.17275
C	2.90233	4.14627	6.09717
C	2.28473	4.60632	4.91803
H	1.24334	4.41836	4.69926

C	3.02644	5.29676	3.98558
C	2.83855	2.85146	8.19249
H	3.81452	2.45656	7.90469
H	2.23502	1.98343	8.47016
C	2.95783	3.80085	9.37218
H	3.55405	4.67772	9.11159
H	3.42939	3.30435	10.22215
H	1.97047	4.14727	9.68595
C	0.75860	3.28779	6.94208
H	0.30491	4.19158	6.53066
H	0.37571	3.19680	7.96183
C	0.37293	2.06345	6.12928
H	0.75236	2.13361	5.10788
H	-0.71215	1.95536	6.08495
H	0.78625	1.15856	6.58068
N	6.46206	8.79254	0.22523
N	6.02576	8.26313	1.32018
N	5.01316	7.44023	0.99789
N	2.19857	3.46568	7.03972
O	6.67622	7.68180	-2.88265
O	2.37722	5.70880	2.85763
O	2.27728	6.73309	0.90617

Molecule 41_2237330
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

55
c41_2237330.xyz.out Energy: -910747.4703640

O	7.38791	-0.12507	0.74651
O	6.08948	1.61550	1.07779
O	10.00677	1.39554	3.73382
O	9.74954	-0.26130	2.23524
N	3.01241	5.21128	1.48588
N	19.71586	-2.27420	7.43219
C	1.88165	5.94783	3.58665
H	2.61051	5.42840	4.21157
H	1.54954	6.83842	4.12349
H	1.02188	5.28918	3.45755
C	2.47775	6.33818	2.24255
H	3.25661	7.09363	2.37278
H	1.71214	6.80237	1.62002
C	2.16536	4.64098	0.44624
H	1.58525	5.45917	0.01702
H	2.79945	4.26854	-0.36048
C	1.23348	3.54762	0.94579
H	0.49197	3.95015	1.63749
H	0.70052	3.09322	0.10864
H	1.78792	2.76159	1.46276
C	5.74006	2.77946	1.68225
C	4.56248	3.37039	1.28440
H	3.98175	2.86829	0.52460

C	4.14932	4.57991	1.88027
C	4.97699	5.13557	2.90203
H	4.69230	6.05656	3.38880
C	6.14318	4.52643	3.27343
H	6.76236	4.97007	4.04480
C	6.56628	3.32427	2.67513
C	7.74803	2.63427	3.00474
H	8.39671	3.04782	3.76813
C	8.09701	1.46397	2.38862
C	7.22884	0.89693	1.36656
C	9.33674	0.75491	2.73303
C	13.50933	0.31243	3.75308
H	14.34997	0.23564	3.07355
C	12.29228	0.76769	3.27364
H	12.16491	1.03035	2.23146
C	11.22708	0.88594	4.15275
C	11.36179	0.56695	5.49244
H	10.50705	0.66191	6.15022
C	12.58797	0.12153	5.96270
H	12.68906	-0.15073	7.00679
C	13.67714	-0.01632	5.10106
C	14.98059	-0.50134	5.60265
C	15.43439	-0.14113	6.87510
H	14.83654	0.52122	7.48948
C	16.65136	-0.59395	7.35105
H	17.00120	-0.30542	8.33401
C	17.44036	-1.42202	6.55103
C	17.00270	-1.79073	5.27794
H	17.61547	-2.44073	4.66659
C	15.78317	-1.33163	4.81438
H	15.43423	-1.64248	3.83710
C	18.70044	-1.89432	7.03848

Molecule 42_2239004
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

58
c42_2239004.xyz.out Energy: -841769.0010010

N	0.42289	7.53566	10.06017
N	19.62264	7.17930	14.40391
O	12.96946	5.21788	14.56959
O	15.03632	5.93467	14.41821
C	1.43320	8.33853	9.70991
H	1.18075	9.17553	9.06729
C	2.74214	8.15789	10.11652
H	3.49728	8.85941	9.78558
C	3.06133	7.07750	10.94584
C	2.00431	6.24132	11.31105
H	2.18312	5.38633	11.95278
C	0.72434	6.50560	10.85098
H	-0.09725	5.85581	11.13402

C	4.40692	6.78661	11.43868
H	4.47253	5.92081	12.09165
C	5.51264	7.48621	11.14911
H	5.43302	8.34870	10.49210
C	6.86560	7.21944	11.62894
C	7.19358	6.16179	12.48485
H	6.42585	5.47911	12.82915
C	8.49627	5.97235	12.90476
H	8.73068	5.14790	13.56948
C	9.53524	6.82101	12.49535
C	9.20534	7.87724	11.63771
H	9.96985	8.56348	11.29389
C	7.90236	8.06716	11.21775
H	7.66922	8.89347	10.55428
C	10.88506	6.55401	12.98959
H	10.97423	5.71179	13.66421
C	11.98139	7.26218	12.66999
H	11.87833	8.10104	11.98544
C	13.35078	7.07314	13.11537
C	13.71731	6.02469	14.06091
C	16.01551	6.75602	13.95103
C	15.69027	7.77120	13.04682
C	14.33677	7.89655	12.65010
H	14.07532	8.68278	11.94731
C	17.29589	6.54102	14.41441
H	17.44694	5.74747	15.13250
C	18.34613	7.36592	13.96927
C	18.02995	8.40110	13.04470
H	18.81089	9.04215	12.66111
C	16.74449	8.58959	12.60667
H	16.52865	9.38177	11.89827
C	19.98648	6.05726	15.25342
H	21.03696	5.82948	15.05459
H	19.42552	5.17066	14.95123
C	20.69699	8.10298	14.07699
H	21.41207	8.06991	14.90334
H	20.31269	9.12449	14.05645
C	19.78769	6.35195	16.73098
H	20.39723	7.20581	17.03588
H	20.07712	5.49319	17.33923
H	18.74414	6.58931	16.94719
C	21.39450	7.75457	12.77301
H	21.81937	6.74944	12.82366
H	22.20497	8.45624	12.56735
H	20.69485	7.78124	11.93507

Molecule 43_7110104
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

68
c43_7110104.xyz.out Energy: -1066405.0426211

F	7.28355	9.73870	3.44243
F	8.77388	11.39631	2.95081
O	12.00661	7.97851	7.69076
N	12.27246	6.09948	1.03234
C	11.68742	6.89196	1.97345
C	10.65281	7.80114	1.63674
H	10.29341	7.86622	0.61942
C	10.06499	8.59837	2.58720
H	9.27796	9.26726	2.27621
C	10.44943	8.56011	3.93866
C	9.92987	9.32770	5.03211
N	8.96300	10.27340	5.09337
N	7.09272	11.85226	4.59777
C	6.22484	12.60663	3.92206
C	5.61670	13.54517	4.79632
C	6.13586	13.33093	6.05831
C	7.07192	12.25221	5.93596
C	7.91950	11.65717	6.84398
C	8.85394	10.68319	6.42296
C	9.76611	9.97985	7.20124
H	9.90815	10.06531	8.26701
C	10.44867	9.13566	6.32781
C	11.50083	8.19971	6.61180
O	11.95956	7.50157	5.53507
C	11.47310	7.65086	4.25943
C	12.08033	6.84165	3.32141
H	12.87333	6.19416	3.66852
C	11.97964	6.23888	-0.38422
H	11.82828	7.29232	-0.62703
H	12.87554	5.93168	-0.93062
C	10.78985	5.40204	-0.82326
H	10.60614	5.51940	-1.89293
H	9.88624	5.69488	-0.28470
H	10.97189	4.34351	-0.62356
C	13.24448	5.07932	1.38608
H	13.17708	4.29202	0.63036
H	12.95884	4.61273	2.33109
C	14.66394	5.61806	1.45135
H	15.36769	4.82560	1.71249
H	14.74802	6.41119	2.19700
H	14.96091	6.03185	0.48480
C	5.98092	12.47669	2.46496
H	6.28704	11.50455	2.08682
H	6.53949	13.24477	1.92213
H	4.92197	12.62564	2.24760
C	4.58429	14.55054	4.39747
H	4.63513	14.71913	3.31903
H	4.80891	15.51331	4.86507
C	3.17678	14.10836	4.78969
H	2.43090	14.85089	4.50045
H	3.10716	13.95977	5.87027

H	2.91862	13.16159	4.30926
C	5.78820	14.12855	7.26910
H	5.32984	15.07322	6.97258
H	6.66369	14.35063	7.88142
H	5.07429	13.60389	7.90866
C	7.86960	11.99603	8.28361
C	6.73970	11.67075	9.03161
H	5.91235	11.16251	8.54899
C	6.67991	11.99372	10.37959
H	5.80229	11.73167	10.95771
C	7.74479	12.65070	10.98599
H	7.69535	12.90751	12.03705
C	8.87627	12.97044	10.24494
H	9.70887	13.47856	10.71550
C	8.94459	12.63597	8.89875
H	9.82339	12.88384	8.31441
B	8.03471	10.79097	3.96965

Molecule 44_7023928
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

67
c44_7023928.xyz.out Energy: -993861.2423103

C	9.05579	9.02604	1.67843
H	8.95280	9.13875	2.74813
C	10.04274	9.70829	0.93941
C	10.07183	9.51476	-0.47299
H	10.82738	10.00394	-1.07067
C	9.16921	8.69242	-1.09110
H	9.21329	8.55151	-2.16499
C	8.18049	8.00781	-0.36082
C	8.16321	8.20630	1.02500
C	7.21571	7.14036	-0.91493
H	7.20212	6.96041	-1.98496
C	6.28283	6.50638	-0.14788
C	6.26751	6.73923	1.27899
C	5.31555	5.60679	-0.83884
C	3.47015	4.04221	-0.71686
H	3.95445	3.43019	-1.48002
H	2.72048	4.64616	-1.23812
C	2.84159	3.13877	0.32623
H	2.07709	2.50645	-0.15328
H	3.61570	2.46805	0.71068
C	1.05792	4.56708	1.13959
H	0.19834	3.87987	1.10273
H	1.14880	5.01719	0.14655
C	0.75481	5.66209	2.13018
C	1.76079	6.53133	2.55074
H	2.76932	6.41108	2.17168
C	1.44438	7.53879	3.44586
H	2.20752	8.22732	3.78807

C	0.13368	7.65138	3.89347
H	-0.16023	8.42134	4.59489
C	-0.79993	6.74623	3.41759
H	-1.83319	6.80187	3.74417
C	2.14058	3.02136	2.62330
H	1.60269	2.09183	2.38200
H	1.54235	3.56355	3.36335
C	3.47451	2.67825	3.23004
C	4.33160	3.70877	3.60868
H	4.01625	4.73684	3.48242
C	5.57399	3.39499	4.12933
H	6.26187	4.18179	4.41549
C	5.91467	2.05475	4.27381
H	6.87410	1.75543	4.67554
C	4.99163	1.09672	3.88845
H	5.22295	0.04153	3.99091
C	11.87634	11.34915	0.80337
H	12.07504	12.23616	1.41040
H	11.39941	11.71196	-0.10857
C	13.17641	10.62747	0.49297
H	13.66921	10.31225	1.41549
H	13.86064	11.28046	-0.05159
H	12.99498	9.73691	-0.11224
C	11.01943	10.63005	2.99949
H	12.05299	10.88602	3.24607
H	10.83610	9.65266	3.45034
C	10.07453	11.67895	3.56082
H	10.30167	12.66182	3.14178
H	10.16944	11.74212	4.64615
H	9.03618	11.44231	3.32043
N	10.94082	10.52201	1.55075
N	4.45441	4.90040	-0.09204
H	4.41988	5.04091	0.91482
N	2.29721	3.87830	1.45467
N	-0.50442	5.76740	2.55797
N	3.79553	1.39123	3.36900
O	7.22220	7.57873	1.78160
O	5.49049	6.27289	2.09344
O	5.32983	5.51792	-2.07149

Molecule 45_7219031
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

69
c45_7219031.xyz.out Energy: -986795.9045896

O	5.73086	3.61703	7.38725
O	8.02636	-1.00942	11.33375
O	6.37193	-1.01356	9.89241
N	4.79720	1.78136	6.23529
N	11.52668	-1.43136	14.51910
C	1.89479	3.89302	6.28505

H	1.30488	4.38143	7.05410
C	1.55190	4.02584	4.93569
H	0.69181	4.61907	4.65063
C	2.31978	3.40569	3.95963
H	2.05268	3.52133	2.91574
C	3.44061	2.64126	4.29185
H	4.03323	2.17096	3.51661
C	3.76290	2.51463	5.63280
C	3.00034	3.14255	6.62186
C	3.57899	2.79540	7.97458
C	5.01297	2.38573	7.53694
C	6.01952	1.46574	5.52466
H	6.47558	0.58565	5.98985
H	5.78283	1.18792	4.49686
C	6.97159	2.62784	5.56352
C	8.05331	2.73575	4.69397
H	8.20690	1.95407	3.95648
C	8.91920	3.81685	4.75095
H	9.75274	3.88489	4.06315
C	8.70050	4.81804	5.69399
H	9.36461	5.67242	5.74543
C	7.63157	4.72883	6.56989
H	7.43862	5.49683	7.30964
C	6.77343	3.63341	6.50816
C	5.73441	1.45460	8.46094
H	5.35863	0.44009	8.48407
C	6.76388	1.83800	9.22210
H	7.09477	2.87182	9.14736
C	7.53761	1.04903	10.17239
C	8.56665	1.62747	10.85615
H	8.79349	2.67451	10.67583
C	9.35491	0.91625	11.79445
C	10.42698	1.45365	12.52639
H	10.68491	2.49708	12.38275
C	11.14004	0.69332	13.41710
H	11.94315	1.15703	13.97191
C	10.82033	-0.67694	13.63323
C	9.74788	-1.22308	12.90308
H	9.45522	-2.25975	12.99069
C	9.05003	-0.42955	12.01765
C	7.24435	-0.35615	10.41847
C	3.57485	3.93305	8.98074
H	2.55450	4.11028	9.32975
H	4.18257	3.67007	9.85217
H	3.95941	4.85796	8.55264
C	2.83188	1.59242	8.55272
H	1.78165	1.85752	8.69329
H	2.87932	0.73080	7.88361
H	3.24551	1.30502	9.52300
C	12.71740	-0.93210	15.18786
H	13.35738	-1.79460	15.39210

H	13.28386	-0.29499	14.50620
C	12.40038	-0.20142	16.48178
H	13.31517	0.14624	16.96527
H	11.75919	0.66275	16.29607
H	11.87890	-0.86335	17.17696
C	11.13856	-2.79396	14.84469
H	11.48189	-2.99255	15.86328
H	10.04960	-2.86744	14.87584
C	11.72781	-3.81675	13.88761
H	11.42301	-4.82728	14.16534
H	11.40106	-3.62927	12.86284
H	12.81928	-3.77343	13.90643

Molecule 46_2212633
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

57
c46_2212633.xyz.out Energy: -877535.9583367

N	13.08828	7.07492	0.89289
O	4.80922	7.73226	0.38151
C	5.41630	7.48839	-0.66077
C	4.70362	7.18626	-1.91025
H	5.28294	6.85528	-2.75925
C	3.36967	7.32881	-1.96393
H	2.86889	7.68695	-1.06731
C	6.90085	7.44799	-0.62505
C	7.72656	7.54675	-1.81443
O	7.36453	7.71363	-2.95935
O	9.08643	7.46783	-1.62570
C	9.68742	7.34097	-0.41451
C	11.06190	7.27390	-0.39378
H	11.58572	7.30874	-1.33824
C	11.73476	7.13916	0.83787
C	10.94849	7.07639	2.02665
H	11.42974	6.99584	2.99059
C	9.58341	7.14281	1.97122
H	9.00248	7.10042	2.88555
C	8.90349	7.27751	0.74574
C	7.50481	7.34132	0.59758
H	6.87040	7.29513	1.47718
C	13.91365	7.26280	-0.29077
H	13.47075	8.03173	-0.92645
H	14.87189	7.66502	0.04695
C	14.13095	5.97186	-1.06161
H	13.18159	5.55199	-1.39991
H	14.75988	6.14645	-1.93615
H	14.62322	5.22805	-0.43093
C	13.80677	6.81290	2.13122
H	13.24806	6.09857	2.73782
H	14.73873	6.31020	1.86051
C	14.10556	8.08121	2.91185

H	13.18384	8.59612	3.19035
H	14.66097	7.85229	3.82302
H	14.70611	8.76760	2.31058
C	2.50719	7.06352	-3.10498
C	1.14814	7.26037	-2.96935
H	0.75141	7.60641	-2.01957
C	0.25459	7.02504	-4.03340
C	-1.14400	7.22640	-3.90257
H	-1.53567	7.57020	-2.95167
C	-1.98443	6.99482	-4.94979
H	-3.05400	7.14466	-4.86688
C	-1.47030	6.54648	-6.19249
C	-0.12216	6.33866	-6.35694
H	0.28917	5.99630	-7.29800
C	0.76234	6.57530	-5.27842
C	2.16237	6.37774	-5.40425
H	2.55443	6.03665	-6.35623
C	3.00604	6.61255	-4.35801
H	4.07059	6.45914	-4.48640
O	-2.40086	6.35340	-7.15749
C	-1.95652	5.90818	-8.42267
H	-1.46917	4.93192	-8.34774
H	-2.84130	5.82083	-9.04878
H	-1.26537	6.62668	-8.87238

Molecule 47_4028361
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

68
c47_4028361.xyz.out Energy: -1259158.6353427

C	9.81770	14.32870	5.85421
C	10.32867	15.34555	6.79007
C	10.64634	16.64975	6.42745
H	10.53421	16.96147	5.39579
C	11.09196	17.51722	7.41117
H	11.34482	18.53975	7.16044
C	11.21225	17.07764	8.73122
H	11.55979	17.76584	9.49229
C	10.89336	15.77230	9.08273
H	10.99010	15.43169	10.10816
C	10.44646	14.90644	8.09602
C	10.07325	13.45850	8.36392
C	8.94279	13.33806	9.34744
C	7.74191	14.10314	9.09968
C	6.75221	13.16319	11.07392
C	5.63316	13.13461	11.88029
H	4.80138	13.76707	11.60453
C	5.61442	12.31991	13.02668
C	3.28665	12.95639	13.50306
H	2.46911	12.39643	13.96444
H	3.11709	12.90192	12.42586

C	3.26893	14.39688	13.98683
H	3.38568	14.43645	15.07239
H	2.32535	14.88071	13.72839
H	4.08247	14.97142	13.53942
C	4.52426	11.53448	15.09319
H	3.81531	12.03392	15.75864
H	5.50006	11.62741	15.57372
C	4.13592	10.07560	14.92166
H	3.13537	9.99471	14.49064
H	4.13449	9.55858	15.88304
H	4.83082	9.56080	14.25494
C	6.77653	11.54957	13.30774
H	6.79830	10.89358	14.16631
C	7.87711	11.60169	12.49005
H	8.74778	11.00131	12.72178
C	7.89529	12.41224	11.34629
C	8.99676	12.52666	10.44194
C	11.21324	11.89683	10.00486
C	12.29576	11.17260	10.47872
H	12.14613	10.60035	11.38342
C	13.52131	11.19949	9.79846
C	13.59288	12.01661	8.64398
H	14.51231	12.09491	8.08178
C	12.49380	12.72082	8.20639
H	12.57976	13.32546	7.30830
C	11.26535	12.68403	8.86961
C	14.52642	9.70729	11.46258
H	15.31952	8.95763	11.43750
H	13.58837	9.14672	11.49158
C	14.66720	10.56538	12.71295
H	15.67017	10.98757	12.78961
H	14.48573	9.96690	13.60822
H	13.95382	11.39228	12.70752
C	15.90090	10.63233	9.60446
H	15.80171	10.56860	8.51774
H	16.51362	9.77794	9.89717
C	16.60130	11.92680	9.99406
H	15.97251	12.79512	9.78700
H	17.53015	12.04023	9.43110
H	16.84803	11.93691	11.05660
N	14.59410	10.44945	10.21548
N	4.52217	12.26732	13.83760
O	9.61503	14.47773	4.66933
O	7.57545	14.85286	8.16194
O	6.70552	13.97744	9.98444
O	10.06681	11.78707	10.76372
S	9.56221	12.81491	6.71162

Molecule 48_1544743_doublet.xyz
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

61
c48_1544743_doublet.out Energy: -1020434.2200562

Au	9.09817	20.87333	5.81214
C	8.68475	19.77118	7.51786
N	10.08844	22.00975	7.15297
N	3.39535	14.32837	-0.98040
C	9.28277	20.36939	8.66228
O	5.42025	16.05073	2.98291
C	4.71630	16.37461	-1.07448
H	4.55328	16.46489	-2.14800
C	3.00668	14.44972	-2.37789
H	2.80155	15.50500	-2.61524
H	2.04069	13.93253	-2.49518
C	10.06113	21.60708	8.44141
C	2.90879	13.14954	-0.27919
H	3.67865	12.79461	0.42327
H	2.80004	12.34587	-1.02524
C	4.15835	15.27438	-0.35295
C	10.58625	23.30051	5.22961
C	4.02813	13.86488	-3.34195
H	3.68308	13.95866	-4.38268
H	4.19418	12.79617	-3.13425
H	4.99848	14.37761	-3.25426
C	9.81830	22.33217	4.52474
C	11.42047	23.51952	8.94961
H	11.95969	24.13068	9.67692
C	5.48384	17.32867	-0.43958
H	5.90177	18.15758	-1.01700
C	8.12753	19.74192	4.54627
C	6.73856	18.07406	3.02416
C	6.53140	18.20814	1.67599
H	6.96733	19.06061	1.14799
C	5.75420	17.26213	0.94332
C	6.15160	16.92845	3.73479
C	11.00010	24.50898	3.17482
H	11.45598	25.34975	2.64705
C	4.42811	15.20035	1.03352
H	4.03083	14.40879	1.66773
C	11.17126	24.37878	4.55279
H	11.76202	25.12115	5.09593
C	10.72633	23.10495	6.68812
C	10.74659	22.37632	9.38448
H	10.75538	22.08967	10.43620
C	9.66158	22.48406	3.14634
H	9.07485	21.75007	2.58616
C	5.20420	16.17362	1.64434
C	9.12620	19.79245	9.93816
H	9.57708	20.24091	10.82867
C	7.49626	18.99012	3.81376
C	7.93816	18.59904	7.66621
H	7.47333	18.12892	6.79315

C	7.77448	18.00967	8.93389
H	7.19011	17.09189	9.04791
C	10.24677	23.56384	2.47434
H	10.11380	23.66829	1.39417
C	1.58554	13.37689	0.43669
H	0.80270	13.68049	-0.27607
H	1.67347	14.16861	1.19659
H	1.24936	12.45728	0.93873
C	8.37808	18.64098	9.99867
C	11.41984	23.89825	7.60589
H	11.94956	24.79299	7.27834
O	6.25969	16.69795	4.91859

Molecule 48_1544743
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

61
c48_1544743.xyz.out

Au	9.00034	20.84890	5.86773
C	8.09001	20.20340	7.61468
N	9.92588	22.07010	7.16215
N	3.56248	14.34890	-1.10811
C	8.59022	20.91810	8.73647
O	6.80576	15.70010	2.12313
C	3.87202	16.69780	-0.60396
H	3.21651	16.92740	-1.25271
C	2.26002	14.62330	-1.72834
H	1.81123	15.34780	-1.22399
H	1.69448	13.81320	-1.65880
C	9.62061	21.93810	8.47740
C	3.91273	12.93420	-0.95583
H	4.89814	12.84750	-0.94426
H	3.57533	12.43410	-1.74109
C	4.22763	15.32840	-0.43040
C	10.98630	22.84430	5.20240
C	2.36070	15.03070	-3.19127
H	1.46526	15.22300	-3.53983
H	2.76022	14.30020	-3.70700
H	2.92089	15.83070	-3.27042
C	10.22690	21.84990	4.53646
C	11.21660	23.68420	8.90056
H	11.67610	24.24630	9.51273
C	4.44720	17.68710	0.13642
H	4.18157	18.58880	-0.00526
C	8.08144	19.66450	4.59106
C	6.94501	18.00610	2.89948
C	6.00672	18.35780	1.97558
H	5.73359	19.26610	1.91267
C	5.43047	17.40150	1.10954
C	7.38630	16.61190	2.97235
C	12.00170	23.49270	3.12689

H	12.58110	24.06420	2.63641
C	5.27838	15.04010	0.46420
H	5.60399	14.15080	0.55010
C	11.85920	23.66230	4.49734
H	12.35620	24.33430	4.95032
C	10.82240	22.94600	6.66165
C	10.28150	22.75450	9.38090
H	10.10370	22.68510	10.31200
C	10.41540	21.67370	3.17629
H	9.93766	20.99090	2.71939
C	5.82892	16.05470	1.21057
C	8.10822	20.63860	10.01000
H	8.44990	21.10960	10.76100
C	7.55339	18.92380	3.81385
C	7.12281	19.23250	7.81439
H	6.78541	18.74430	7.07348
C	6.64189	18.96820	9.09456
H	5.97673	18.30240	9.22114
C	11.30120	22.49070	2.46862
H	11.42330	22.35980	1.53675
C	3.34826	12.30220	0.30982
H	2.38105	12.45460	0.34727
H	3.77348	12.70630	1.09511
H	3.52606	11.33740	0.30088
C	7.13031	19.67530	10.18470
C	11.47680	23.79160	7.55244
H	12.09590	24.43660	7.23348
O	8.25817	16.19020	3.70003

Molecule 49_7229754
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

69
c49_7229754.xyz.out Energy: -1067797.2877394

O	10.27680	10.93587	11.02651
O	11.27242	9.80162	9.41100
N	10.80518	11.80643	7.50792
N	10.80789	11.70693	5.30745
O	8.59893	12.71592	4.14770
H	9.55068	12.47077	4.23021
C	10.36849	11.91953	8.85112
C	10.68711	10.81073	9.73250
C	9.21722	13.04884	10.63821
C	12.13504	11.81141	7.11032
C	10.03890	11.71826	6.37718
C	12.11179	11.76183	5.73851
C	9.66199	12.98518	9.29127
H	9.42383	13.79372	8.60721
C	9.55367	11.99488	11.49478
C	13.24531	11.82259	8.07275
C	8.57775	11.66403	6.32277

C	13.22858	11.77100	4.78554
C	8.47593	14.10524	11.19174
H	8.19994	14.93791	10.55472
C	9.19157	11.96341	12.82400
H	9.51209	11.11381	13.40939
N	8.02531	12.99985	14.67015
C	7.80198	11.07328	7.32613
H	8.29404	10.58914	8.16052
C	13.08821	11.12998	3.55273
H	12.15621	10.62737	3.32387
C	13.36815	12.82949	9.03054
H	12.64505	13.63696	9.05634
C	7.92329	12.19508	5.19576
C	8.10002	14.10289	12.50995
H	7.53091	14.93952	12.88813
C	8.43811	13.02020	13.37035
C	14.19503	10.80070	8.03151
H	14.08823	10.01175	7.29599
C	14.43099	12.42313	5.07117
H	14.54554	12.95304	6.00947
C	15.47133	12.41723	4.15294
H	16.39577	12.93111	4.38800
C	15.32626	11.76748	2.93239
H	16.13910	11.76510	2.21627
C	6.41967	11.06296	7.25607
H	5.84159	10.59359	8.04153
C	14.12876	11.12797	2.63448
H	14.00479	10.62227	1.68431
C	6.53187	12.20221	5.13767
H	6.06070	12.63540	4.26377
C	5.78564	11.64768	6.16271
H	4.70417	11.65174	6.09904
C	15.36676	11.79382	9.88471
H	16.18960	11.78107	10.58915
C	15.25202	10.78986	8.92846
H	15.98165	9.99029	8.88976
C	14.42351	12.81200	9.93464
H	14.51206	13.59976	10.67296
C	8.41323	11.90848	15.55198
H	7.70182	11.89177	16.37911
H	8.27862	10.96235	15.02330
C	9.83211	12.02326	16.08943
H	9.93002	12.87897	16.75902
H	10.09882	11.12557	16.65049
H	10.55368	12.14347	15.27872
C	7.42279	14.17783	15.28044
H	6.96922	13.85292	16.21760
H	6.59809	14.52960	14.65545
C	8.40684	15.30723	15.54847
H	8.92872	15.60539	14.63707
H	7.88138	16.18110	15.93858

H 9.15727 15.00854 16.28145

Molecule 50_7229755
Cartesian Coordinates (in Angstroms) and Total Electronic Potential Energy (in kcal/mol)

68
c50_7229755.xyz.out Energy: -1020608.9465664
O 5.77570 3.68964 4.65991
N 4.67343 4.38574 8.07366
N 2.70263 4.33026 9.08526
O 3.78366 4.21520 5.46374
N 9.92856 2.61064 2.61271
C 7.70248 3.49343 6.06982
C 6.87832 3.80374 7.18537
H 7.31370 3.83290 8.17875
C 3.59626 3.61822 8.44734
C 5.56033 4.04805 7.01851
C 5.24081 6.82786 8.10391
C 3.17566 5.62334 9.10960
C 7.11019 3.44235 4.80355
C 9.19470 2.87349 3.73256
C 9.80458 2.91156 5.01782
H 10.85924 2.70431 5.12512
C 2.42471 6.69466 9.77605
C 4.38369 5.69100 8.46088
C 7.81391 3.13888 3.65813
H 7.26470 3.10880 2.72820
C 9.07672 3.21701 6.13906
H 9.56672 3.24501 7.10574
C 3.06595 7.79528 10.35084
H 4.14781 7.85770 10.33066
C 3.47607 2.19136 8.13190
C 6.58446 6.87319 8.47977
H 7.00014 6.06094 9.06522
C 1.03248 6.61465 9.85337
H 0.53188 5.75833 9.41818
C 11.30946 2.15797 2.71397
H 11.75019 2.25784 1.72123
H 11.86908 2.84041 3.35873
C 4.95183 4.00217 5.69884
C 2.33129 8.79772 10.96840
H 2.84497 9.64199 11.41277
C 0.29953 7.61658 10.47346
H -0.78033 7.54034 10.52073
C 9.28266 2.51795 1.31135
H 8.59001 3.35496 1.20004
H 10.05547 2.66682 0.55566
C 0.94488 8.71515 11.02943
H 0.37269 9.49761 11.51319
C 4.70033 7.89652 7.38624
H 3.65791 7.85818 7.09097

C	7.37432	7.96321	8.13938
H	8.41462	7.98972	8.44047
C	2.23472	1.69349	7.73440
H	1.39776	2.37594	7.65299
C	6.82783	9.02346	7.42590
H	7.44316	9.87521	7.16266
C	4.56269	1.32087	8.22975
H	5.52204	1.69192	8.57011
C	11.45735	0.72402	3.20177
H	11.02063	0.02090	2.49143
H	12.51309	0.47280	3.32134
H	10.96347	0.57808	4.16443
C	5.48869	8.98882	7.05311
H	5.05839	9.81170	6.49547
C	8.56693	1.19714	1.06891
H	7.85543	0.98008	1.86826
H	8.01774	1.23104	0.12606
H	9.27708	0.37064	1.01501
C	2.08414	0.34744	7.43698
H	1.11772	-0.02904	7.12465
C	3.17131	-0.51463	7.52958
H	3.05314	-1.56538	7.29412
C	4.40930	-0.02557	7.92860
H	5.25587	-0.69578	8.01554

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