

Quantum-chemically-calculated mechanistically interpretable molecular descriptors for drug-action mechanism study – a case study of anthracycline anticancer antibiotics

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Supplementary Information

1. Log GI₅₀ (60 cell lines) for anthracyclines

Name	NSC No. / CAS No.	average Log (GI ₅₀)	Experiment 1			Experiment 2			Experiment 3			Experiment 4			Experiment 5			span of log (GI ₅₀)
			GI ₅₀ (M)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	GI ₅₀ (M)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	GI ₅₀ (M)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	GI ₅₀ (M)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	GI ₅₀ (M)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5	-6.419	3.81E-07	-6.419	-4.0													
Aclacinomycin X	NSC 670120	-7.796	1.60E-08	-7.796	-5.0													
Aclarubicin	57576-44-0	-8.233	5.85E-09	-8.233	-5.0													
Adriamycin 14-octanoate	51898-39-6	-7.119	7.60E-08	-7.119	-4.0													
Aklavin	60504-57-6	-6.701	1.99E-07	-6.701	-4.0													
2'-Bromo-4'-epi-daunorubicin	NSC 650931	-7.330	4.02E-08	-7.396	-4.0	5.43E-08	-7.265	-5.0										0.131
Cinerubin A	NSC 243022 / 34044-10-5	-9.827	1.49E-10	-9.827	-7.0													
N-(1-Cyano-2-methoxyethyl)doxorubicin	NSC 639659	-7.138	7.27E-08	-7.138	-4.0													
Cyanomorpholino doxorubicin	88254-07-3	-10.198	3.38E-11	-10.471	-7.7	1.19E-10	-9.924	-8.0										0.547
Daunomycin 3,4-dichlorobenzoylhydrazone	66996-54-1	-6.824	1.50E-07	-6.824	-4.0													
Daunomycin 4-nitrobenzoylhydrazone	66996-56-3	-6.500	3.16E-07	-6.500	-4.0													
Daunomycin 3-oxime	34610-60-1	-5.951	1.12E-06	-5.951	-4.0													

Daunorubicin / Daunomycin	20830-81-3 / 23541-50-6	-7.220	3.86E- 08	-7.413	-4.0	1.29E- 07	-6.889	-3.3	4.43E- 08	-7.354	-4.0	5.96E- 08	-7.225	-4.3	8.43E- 08	-7.074	-5.0	0.524
4-Demethoxy adriamycin / Medorubicin	64363-63-9	-7.706	1.97E- 08	-7.706	-4.0													
N,N-dibenzyl daunorubicin	70878-51-2	-5.446	1.55E- 05	-4.810	-4.3	8.28E- 07	-6.082	-5.0										1.272
N,N-diethyl adriamycin	70844-09-6	-7.260	5.49E- 08	-7.260	-4.0													
N,N-dimethyl adriamycin	67106-76-7	-7.742	1.81E- 08	-7.742	-4.0													
N,N-dimethyl daunomycin	70095-84-0	-8.030	2.48E- 08	-7.606	-5.0	3.51E- 09	-8.455	-8.0										0.849
Doxorubicin / Adriamycin	25316-40-9 / 23214-92-8	-7.065	1.41E- 07	-6.851	-4.0	9.38E- 08	-7.028	-4.6	6.63E- 08	-7.178	-6.6	6.27E- 08	-7.203	-4.3				0.352
Duborimycin	NSC 180510	-5.941	1.18E- 06	-5.928	-4.0	1.11E- 06	-5.955	-5.0										0.027
Epirubicin	56390-09-1	-6.691	2.00E- 07	-6.699	-4.0	2.07E- 07	-6.684	-4.3										0.035
Esorubicin	63950-06-1	-7.356	4.23E- 08	-7.374	-3.7	4.58E- 08	-7.339	-5.0										0.350
11-Hydroxy aclacinomycin A	NSC 670121	-8.338	4.59E- 09	-8.338	-6.0													
11-Hydroxy aclacinomycin X	NSC 670122	-8.152	7.04E- 09	-8.152	-6.0													
3'-Hydroxy daunorubicin	64842-75-7	-5.867	1.06E- 06	-5.975	-4.0	1.74E- 06	-5.759	-5.0										0.215
Idarubicin	57852-57-0	-7.594	1.70E- 08	-7.770	-4.0	3.81E- 08	-7.419	-6.0										
5-Imino daunorubicin	67324-99-6	-6.500	3.16E- 07	-6.500	-5.0													
Marcellomycin	63710-10-1	-7.517	3.04E- 08	-7.517	-4.6													

Menogaril	71628-96-1	-6.091	7.78E-07	-6.109	-4.0	8.44E-07	-6.074	-5.0										0.035	
4'-O-methyl doxorubicin	77121-90-5	-7.130	7.42E-08	-7.130	-4.0														
Morpholino adriamycin	89196-04-3	-8.929	1.34E-08	-7.873	-5.0	5.77E-09	-8.239	-5.7	2.11E-11	-10.676	-9.6							2.803	
MX2	NCI 619003	-7.192	4.74E-08	-7.324	-4.0	8.70E-08	-7.060	-4.6										0.264	
NSC 286628	NSC 286628 / 67903-59-7	-5.854	1.40E-06	-5.854	-4.0														
Nogalamycin	1404-15-5	-7.963	1.09E-08	-7.963	-6.0														
Pirarubicin	72496-41-4	-6.962	5.34E-07	-6.272	-4.3	2.23E-08	-7.652	-5.0										1.379	
Pyromycin	668-17-7	-7.240	5.76E-08	-7.240	-3.8														
Rhodomyconone	21288-60-8	-5.539	2.89E-06	-5.539	-4.0														
Steffimycin	11033-34-4	-5.672	2.06E-06	-5.686	-3.7	2.20E-06	-5.658	-4.0										0.029	
Steffimycin B	NCI 204856	-5.407	3.92E-06	-5.407	-4.0														
Theprubicin	95343-20-7	-6.109	1.68E-07	-6.109	-4.0														
Valrubicin	56124-62-0	-6.310	4.90E-07	-6.310	-4.0														
Zorubicin / Rubidazone	36508-71-1	-6.500	3.16E-07	-6.500	-3.9														
																		average of the span	0.587
																		standard deviation of the span	0.750

2. Log GI₅₀ (leukemia K-562) for anthracyclines

Name	NSC No. / CAS No.	average Log (GI ₅₀)	Experiment 1		Experiment 2		Experiment 3		Experiment 4		Experiment 5		span of log (GI ₅₀)
			Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	Log (GI ₅₀)	Log (Highest concentration of drugs for experiments)	Log (GI ₅₀)	Log(Highest concentration of drugs for experiments)	Log (GI ₅₀)	Log(Highest concentration of drugs for experiments)	Log (GI ₅₀)	Log(Highest concentration of drugs for experiments)	
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5	-6.062	-6.062	-4.0									
Aclacinomycin X	NSC 670120	-9.000	-9.000	-5.0									
Aclarubicin	57576-44-0	-8.772	-8.772	-5.0									
Adriamycin 14-octanoate	51898-39-6	-7.254	-7.254	-4.0									
Aklavin	60504-57-6	-7.135	-7.135	-4.0									
2'-Bromo-4'-epi-daunorubicin	NSC 650931	-7.499	-7.692	-4.0	-7.305	-5.0							0.387
Cinerubin A	NSC 243022 / 34044-10-5	-10.054	-10.054	-7.0									
N-(1-Cyano-2-methoxyethyl)doxorubicin	NSC 639659	-7.382	-7.382	-4.0									
Cyanomorpholino doxorubicin	88254-07-3	-10.288	-10.697	-7.7	-9.878	-8.0							0.819
Daunomycin 3,4-dichlorobenzoylhydrazone	66996-54-1	-6.705	-6.705	-4.0									
Daunomycin 4-nitrobenzoylhydrazone	66996-56-3	-6.449	-6.449	-4.0									
Daunomycin 3-oxime	34610-60-1	-6.257	-6.257	-4.0									
Daunorubicin	20830-81-3 / 23541-50-6	-7.531	-7.827	-4.0	-6.990	-3.3	-8.000	-4.0	-7.307	-4.3	-7.207	-5.0	0.837

4-demethoxydaunorubicin / Medorubicin	64363-63-9	-7.929	-7.929	-4.0									
N,N-dibenzyl daunorubicin	70878-51-2	-5.107	-5.213	-4.3	-6.430	-5.0							0.213
N,N-diethyl daunorubicin	70844-09-6	-7.579	-7.579	-4.0									
N,N-dimethyl daunorubicin	67106-76-7	-7.851	-7.851	-4.0									
N,N-dimethyl daunomycin	70095-84-0	-8.419	-8.341	-5.0	-8.497	-8.0							0.156
Doxorubicin	25316-40-9 / 23214-92-8	-6.948	-6.711	-4.0	-6.996	-4.6	-7.033	-6.6	-7.051	-4.3			0.340
Duborimycin	NSC 180510	-5.804	-5.656	-4.0	-5.952	-5.0							0.296
Epirubicin	56390-09-1	-6.747	-6.662	-4.0	-6.832	-4.3							0.100
Esorubicin	63950-06-1	-7.470	-7.420	-3.7	-7.520	-5.0							0.882
11-Hydroxy aclacinomycin A	NSC 670121	-9.562	-9.562	-6.0									
11-Hydroxy aclacinomycin X	NSC 670122	-9.708	-9.708	-6.0									
3'-Hydroxydaunorubicin	64842-75-7	-5.940	-6.034	-4.0	-5.845	-5.0							0.189
Idarubicin	57852-57-0	-7.522	-7.963	-4.0	-7.081	-6.0							
5-Imino daunorubicin	67324-99-6	-6.484	-6.484	-5.0									
Marcellomycin	63710-10-1	-7.961	-7.961	-4.6									
Menogaril	71628-96-1	-5.892	-5.874	-4.0	-5.909	-5.0							0.035

4'-O-methylodoxorubicin	77121-90-5	-7.546	-7.546	-4.0									
Morpholino adriamycin	89196-04-3	-10.037	-8.112	-5.0	-8.397	-5.7	-13.6020	-9.6					5.490
MX2	NCI 619003	-7.150	-7.371	-4.0	-6.929	-4.6							0.442
NSC 286628	NSC 286628 / 67903-59-7	-6.132	-6.132	-4.0									
Nogalamycin	1404-15-5	-7.810	-7.810	-6.0									
Pirarubicin	72496-41-4	-6.899	-6.190	-4.3	-7.607	-5.0							1.417
Pyrrromycin	668-17-7	-7.535	-7.535	-3.8									
Rhodomyconone	21288-60-8	-5.707	-5.707	-4.0									
Steffimycin	11033-34-4	-5.325	-4.999	-3.7	-5.650	-4.0							0.651
Steffimycin B	NCI 204856	-5.446	-5.446	-4.0									
Theprubicin	95343-20-7	-6.725	-6.725	-4.0									
Valrubicin	56124-62-0	-6.472	-6.472	-4.0									
Zorubicin / Rubidazone	36508-71-1	-6.405	-6.405	-3.9									
												average of the span	0.817
												standard deviation of the span	1.346

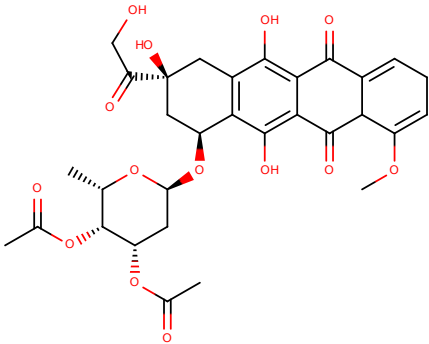
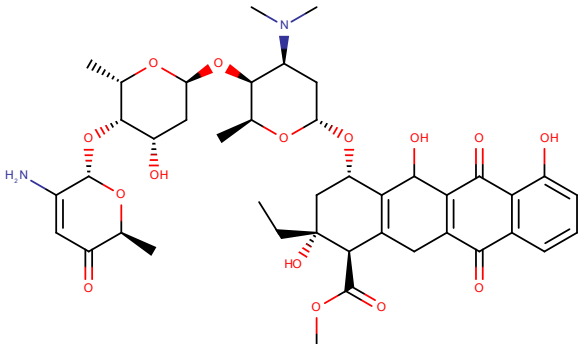
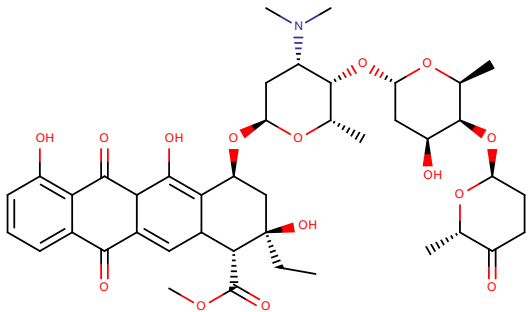
3. Polarizability, dipole moment, HOMO energies, vdW molecular volumes and radii, values of the functions for the dipole-dipole, dipole-induced dipole and dispersion interactions, electronic energies of neutral state and free radical, and one-electron reduction energies of anthracyclines.

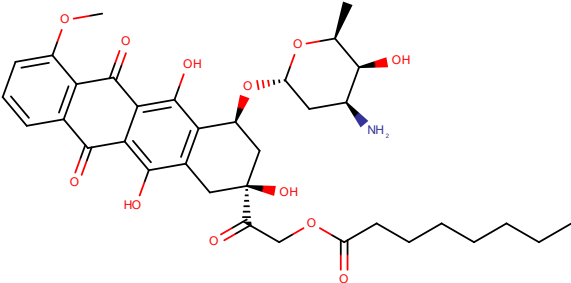
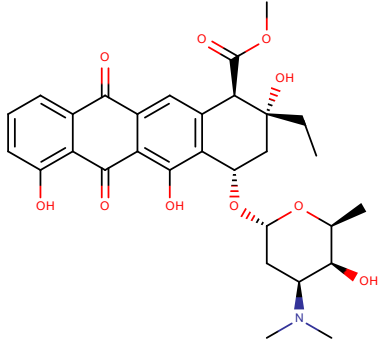
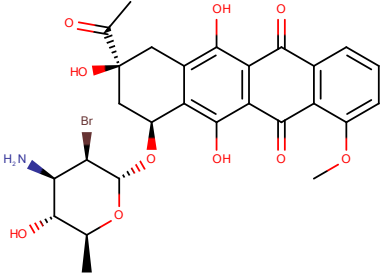
Name	NSC No. / CAS No.	polarizability (au ³)	dipole moment (debye)	electronic energy (kcal/mol)	HOMO (hartree)	vdW molecular volume (Å ³)	vdW radius (Å)	$-\frac{\mu_1\mu_2}{d^3}$	$-\frac{\mu_1^2\alpha_2 + \mu_2^2\alpha_1}{d^6}$	$-\frac{\alpha_1\alpha_2}{d^6} \frac{I_1I_2}{I_1 + I_2}$	semi-quinone free radicals of anthracyclines	one-electron reduction
Name	NSC No. / CAS No.	polarizability (au ³)	dipole moment (debye)	electronic energy (kcal/mol)	HOMO (hartree)	vdW molecular volume (Å ³)	vdW radius (Å)	function for dipole-dipole interaction	function for dipole-induced dipole interaction	function for dispersion interaction	electronic energy (kcal/mol) (radical)	energy of reaction (radical - neutral) (kcal/mol)
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5	520.0164	3.6706	-1414291.54	-0.3045	706.1354179	5.5251	-0.04808	-0.09270	-0.01950	-1414369.39	-77.85
Aclacinomycin X	NSC 670120	691.5540	10.1622	-1800812.72	-0.3301	990.2484339	6.1843	-0.11330	-0.10526	-0.01951	-1800895.60	-82.88
Aclarubicin	57576-44-0	668.5867	5.8670	-1766835.88	-0.3288	981.0424	6.1651	-0.06571	-0.09036	-0.01900	-1766917.76	-81.88
Adriamycin 14-octanoate	51898-39-6	582.1358	13.1595	-1454056.90	-0.3089	787.9678	5.7308	-0.16376	-0.13047	-0.01984	-1454133.81	-76.91
Aklavin	60504-57-6	494.3718	4.6581	-1237058.44	-0.3290	675.3166	5.4435	-0.06228	-0.09421	-0.02003	-1237139.54	-81.10
2'-Bromo-4'-epi-daunorubicin	NSC 650931	488.0688	7.7512	-2776447.91	-0.3047	639.8651206	5.3465	-0.10622	-0.10862	-0.02004	-2776528.67	-80.76
Cinerubin A	NSC 243022 / 34044-10-5	691.6419	7.0341	-1814023.65	-0.3087	990.0320833	6.1839	-0.07843	-0.09523	-0.01892	-1814105.67	-82.02
N-(1-Cyano-2-methoxyethyl) doxorubicin	NSC 639659	529.1029	14.9515	-1389310.93	-0.3090	729.1326852	5.5844	-0.19295	-0.14409	-0.01940	-1389390.88	-79.95
Cyanomorpholino doxorubicin	88254-07-3	543.6735	5.8983	-1413224.41	-0.3069	713.6916	5.5447	-0.07688	-0.10125	-0.02027	-1413302.18	-77.77
Daunomycin 3,4-dichlorobenzoyl hydrazone	66996-54-1	614.5053	2.5992	-1978195.77	-0.3015	795.8841592	5.7499	-0.03219	-0.09583	-0.02051	-1978274.23	-78.46
Daunomycin 4-nitrobenzoylhydrazone	66996-56-3	607.4330	5.4857	-1529730.29	-0.3031	805.8943454	5.7739	-0.06755	-0.09895	-0.02009	-1529804.23	-73.94
Daunomycin 3-oxime	34610-60-1	478.3110	13.8858	-1197739.38	-0.3083	617.7005	5.2841	-0.19335	-0.14894	-0.02039	-1197818.35	-78.97
Daunorubicin / Daunomycin	20830-81-3 / 23541-50-6	465.2971	5.8725	-1163027.93	-0.3066	607.7865	5.2557	-0.08237	-0.10174	-0.02008	-1163112.60	-84.67

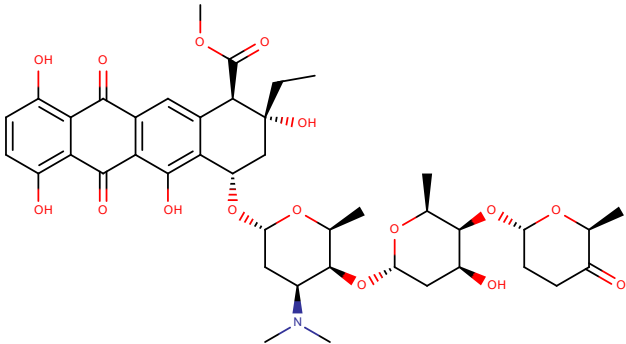
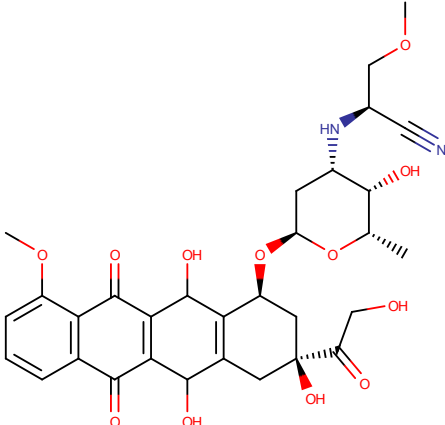
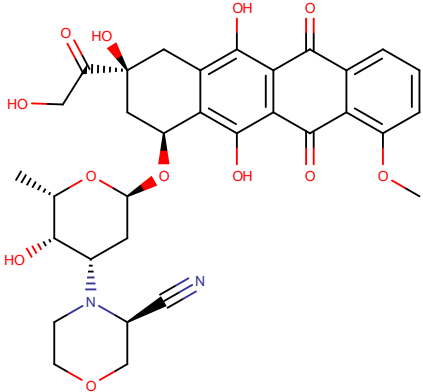
4-Demethoxyadriamycin / Medorubicin	64363-63-9	442.5370	6.7760	-1138372.19	-0.3095	591.2679	5.2076	-0.09623	-0.10317	-0.01966	-1138452.09	-79.90
N,N-dibenzyl-daunorubicin	70878-51-2	651.3391	5.0847	-1502343.67	-0.3095	898.1425	5.9863	-0.05945	-0.09434	-0.01961	-1502421.04	-77.37
N,N-diethyladriamycin	70844-09-6	526.8030	3.3488	-1308898.51	-0.3058	713.2771222	5.5437	-0.04366	-0.09241	-0.01961	-1308978.73	-80.22
N,N-dimethyladriamycin	67106-76-7	501.5233	11.1572	-1259562.34	-0.3072	673.5098	5.4387	-0.14936	-0.12342	-0.01973	-1259641.93	-79.59
N,N-dimethyl-daunomycin	70095-84-0	495.4331	8.0812	-1212368.14	-0.3075	650.4180	5.3758	-0.10992	-0.10983	-0.02013	-1212446.69	-78.55
Doxorubicin / Adriamycin	25316-40-9 / 23214-92-8	468.2626	8.9525	-1210223.31	-0.3066	612.2277	5.2684	-0.12516	-0.11507	-0.02007	-1210301.62	-78.31
Duborimycin	NSC 180510	470.2137	7.7633	-1163785.42	-0.3048	613.6512	5.2725	-0.10842	-0.10939	-0.02006	-1163868.32	-82.90
Epirubicin	56390-09-1	470.8064	9.0254	-1210233.22	-0.3051	614.1359	5.2739	-0.12600	-0.11563	-0.02008	-1210309.15	-75.93
Esorubicin	63950-06-1	467.2721	3.9429	-1163029.04	-0.3064	606.9269	5.2532	-0.05534	-0.09665	-0.02018	-1163106.41	-77.37
11-Hydroxy aclacinomycin A	NSC 670121	691.7573	5.7777	-1814045.88	-0.3136	976.3583332	6.1553	-0.06486	-0.09351	-0.01933	-1814129.40	-83.52
11-Hydroxy aclacinomycin X	NSC 670122	719.3567	8.7084	-1848023.87	-0.3184	993.199931	6.1905	-0.09695	-0.10328	-0.01990	-1848106.91	-83.04
3'-Hydroxy daunorubicin	64842-75-7	463.0718	5.5233	-1175503.34	-0.3066	602.3300	5.2399	-0.07779	-0.10094	-0.02014	-1175582.36	-79.02
Idarubicin	57852-57-0	437.3788	2.5473	-1091165.56	-0.3080	572.1987	5.1510	-0.03671	-0.09285	-0.01996	-1091243.63	-78.07
5-Imino daunorubicin	67324-99-6	463.2888	9.9261	-1150560.66	-0.2941	605.6616	5.2495	-0.13945	-0.12067	-0.01966	-1150631.46	-70.80
Marcellomycin	63710-10-1	700.6283	2.3262	-1861999.59	-0.3100	1020.7432	6.2472	-0.02555	-0.08551	-0.01863	-1862085.71	-86.12
Menogaril	71628-96-1	487.9738	3.8940	-1187689.34	-0.3186	609.7507	5.2613	-0.05454	-0.10020	-0.02138	-1187770.72	-81.38

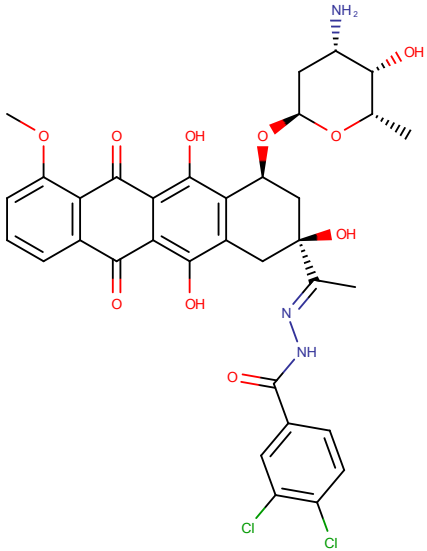
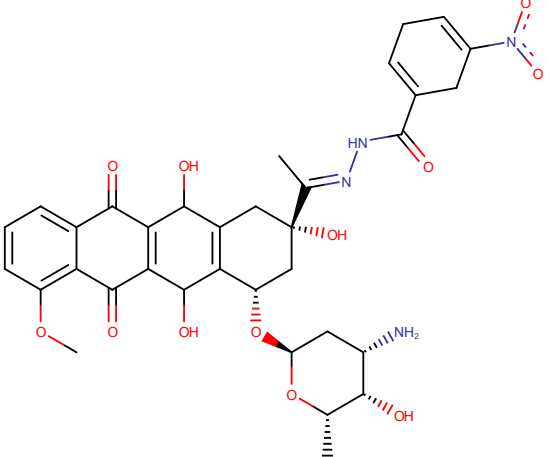
4'-O-methylodoxorubicin	77121-90-5	483.6345	6.4192	-1234889.50	-0.3060	636.143927	5.3362	-0.08820	-0.10300	-0.02001	-1234967.10	-77.60
Morpholino adriamycin	89196-04-3	528.9651	9.3615	-1355339.29	-0.3072	721.9789	5.5661	-0.12137	-0.11105	-0.01952	-1355419.75	-80.46
MX2	NCI 619003	518.3925	6.7066	-1284240.02	-0.3159	681.2624	5.4594	-0.08931	-0.10392	-0.02045	-1284325.37	-85.35
NSC 286628	NSC 286628 / 67903-59-7	541.8562	7.0350	-1308023.15	-0.3074	702.3169576	5.5151	-0.09238	-0.10626	-0.02052	-1308099.54	-76.39
Nogalamycin	1404-15-5	658.0645	4.2489	-1740748.35	-0.3187	928.2166	6.0524	-0.04889	-0.09072	-0.01946	-1740829.65	-81.30
Pirarubicin	72496-41-4	553.4498	8.1748	-1380021.85	-0.3039	771.5144	5.6906	-0.10275	-0.10330	-0.01909	-1380104.84	-82.99
Pyromycin	668-17-7	519.1163	4.1183	-1284259.84	-0.3146	685.7169	5.4713	-0.05468	-0.09600	-0.02031	-1284344.51	-84.67
Rhodomyconone	21288-60-8	389.9991	2.8675	-958532.96	-0.3151	471.7197	4.8299	-0.04496	-0.09893	-0.02130	-958615.24	-82.28
Steffimycin	11033-34-4	493.5643	6.3736	-1294557.12	-0.3268	658.8005	5.3988	-0.08619	-0.10143	-0.02039	-1294639.29	-82.17
Steffimycin B	NCI 204856	504.0612	6.2970	-1319219.10	-0.3285	673.4409	5.4385	-0.08430	-0.10103	-0.02046	-1319301.66	-82.56
Theprubicin	95343-20-7	540.8079	11.1695	-1380017.23	-0.3063	720.3297	5.5619	-0.14496	-0.12268	-0.01997	-1380095.42	-78.19
Valrubicin	56124-62-0	572.5026	6.7839	-1662658.47	-0.3008	815.9468	5.7978	-0.08304	-0.09615	-0.01864	-1662737.14	-78.67
Zorubicin / Rubidazone	36508-71-1	590.5316	4.8960	-1401403.87	-0.3093	753.2377	5.6453	-0.06223	-0.10123	-0.02101	-1401483.79	-79.92
Dummy for complete calculation of van der Waals forces: AG-TC base pairs		749.0275	22.321374		-0.2783	1107.495038	6.4194					

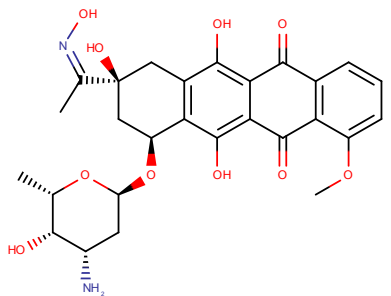
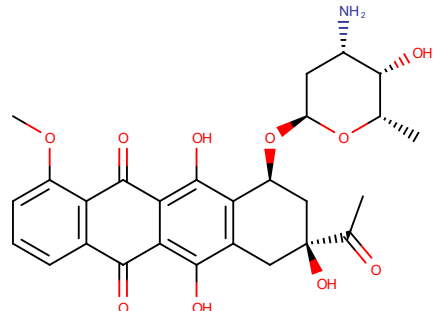
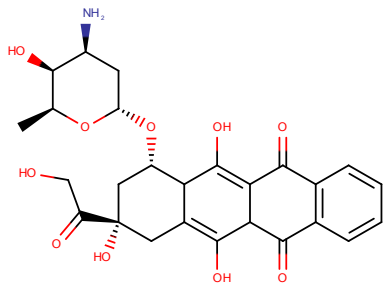
4. Chemical structures of anthracyclines

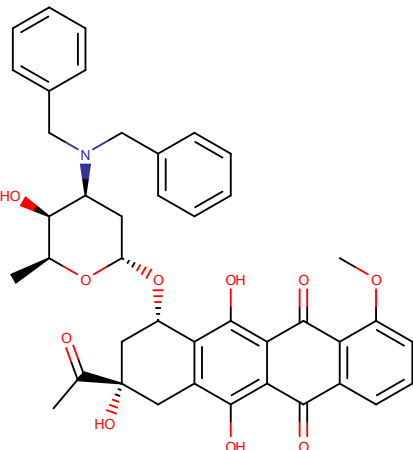
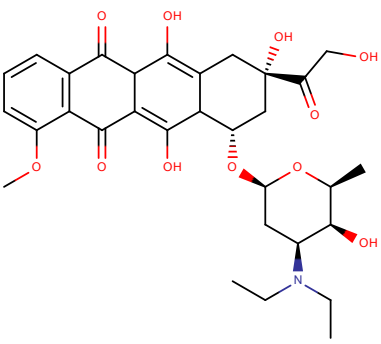
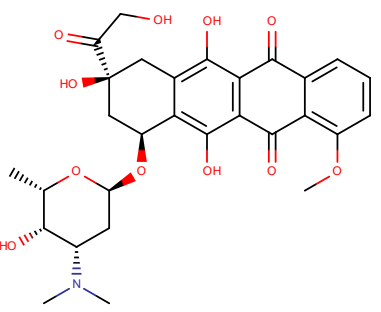
Name	NSC No. / CAS No.	Chemical structures
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5	 <p>The structure shows a tetracyclic anthracycline core with a methoxy group at C-10, hydroxyl groups at C-1, C-5, and C-7, and a carbonyl group at C-9. It is linked at C-13 to a 2,6-dideoxy-3'-O-acetyl-4'-O-acetyl-β-D-glucopyranoside sugar moiety.</p>
Aclacinomycin X	NSC 670120	 <p>The structure features a tetracyclic anthracycline core with a methoxy group at C-10, hydroxyl groups at C-1, C-5, and C-7, and a carbonyl group at C-9. It is linked at C-13 to a complex sugar moiety consisting of a 2,6-dideoxy-3'-O-(2-amino-6-methyl-4-hydroxy-2-pyridinyl)-β-D-glucopyranoside unit connected to a 2,6-dideoxy-3'-O-(2-dimethylamino)-β-D-glucopyranoside unit.</p>
Aclarubicin	57576-44-0	 <p>The structure shows a tetracyclic anthracycline core with a methoxy group at C-10, hydroxyl groups at C-1, C-5, and C-7, and a carbonyl group at C-9. It is linked at C-13 to a complex sugar moiety consisting of a 2,6-dideoxy-3'-O-(2-dimethylamino)-β-D-glucopyranoside unit connected to a 2,6-dideoxy-3'-O-(2-amino-6-methyl-4-hydroxy-2-pyridinyl)-β-D-glucopyranoside unit.</p>

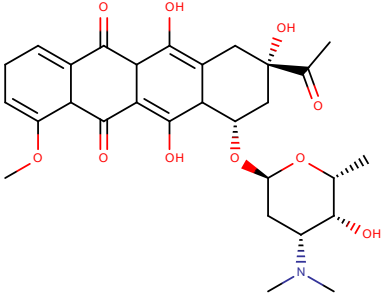
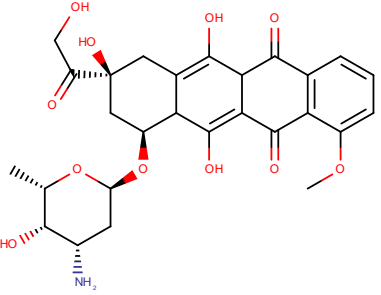
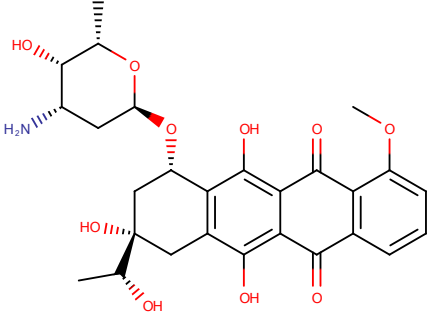
<p>Adriamycin 14-octanoate</p>	<p>51898-39-6</p>	 <p>The structure shows the anthracycline core of Adriamycin with an octanoate ester group attached to the 14-position of the D-glucosamine moiety. The anthracycline core consists of a tetracyclic system with a phenanthrene-like core fused to a six-membered ring containing a ketone and a hydroxyl group. The D-glucosamine moiety is attached to the 14-position of the anthracycline core and has a primary amine group and a hydroxyl group. The octanoate ester group is attached to the 14-position of the D-glucosamine moiety.</p>
<p>Aklavin</p>	<p>60504-57-6</p>	 <p>The structure shows the anthracycline core of Aklavin with a methyl ester group attached to the 14-position of the D-glucosamine moiety. The anthracycline core consists of a tetracyclic system with a phenanthrene-like core fused to a six-membered ring containing a ketone and a hydroxyl group. The D-glucosamine moiety is attached to the 14-position of the anthracycline core and has a primary amine group and a hydroxyl group. The methyl ester group is attached to the 14-position of the D-glucosamine moiety.</p>
<p>2'-Bromo-4'-epi-daunorubicin</p>	<p>NSC 650931</p>	 <p>The structure shows the anthracycline core of 2'-Bromo-4'-epi-daunorubicin with a bromine atom at the 2' position and a methyl group at the 4' position of the D-glucosamine moiety. The anthracycline core consists of a tetracyclic system with a phenanthrene-like core fused to a six-membered ring containing a ketone and a hydroxyl group. The D-glucosamine moiety is attached to the 14-position of the anthracycline core and has a primary amine group and a hydroxyl group. The bromine atom is attached to the 2' position and the methyl group is attached to the 4' position of the D-glucosamine moiety.</p>

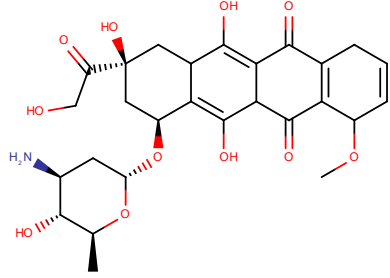
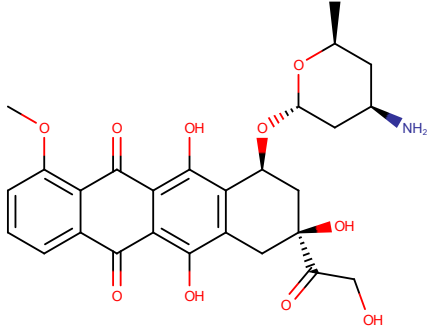
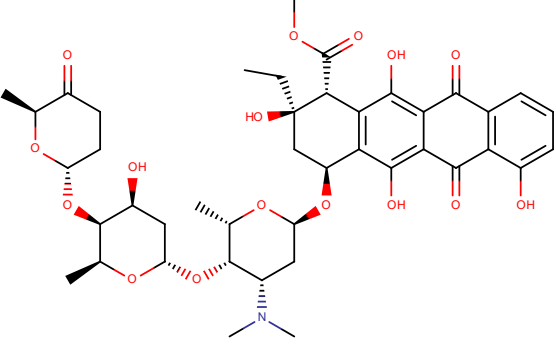
<p>Cinerubin A</p>	<p>NSC 243022 / 34044-10-5</p>	 <p>The structure of Cinerubin A features a tetracycline core with a 4-hydroxyphenyl group at C4, a methyl group at C5, and a 2-methoxyethyl group at C6. It is linked via a glycosidic bond to a disaccharide chain consisting of a 2-deoxy-2-(dimethylamino)ribose unit and a 2-deoxyribose unit.</p>
<p>N-(1-Cyano-2-methoxyethyl)doxorubicin</p>	<p>NSC 639659</p>	 <p>This structure is a doxorubicin derivative with a methoxy group at C7 and a 1-cyano-2-methoxyethyl group attached to the C12 hydroxyl group. The tetracycline core has hydroxyl groups at C11 and C13, and a methyl group at C14.</p>
<p>Cyanomorpholino doxorubicin</p>	<p>88254-07-3</p>	 <p>The structure shows a doxorubicin core with a methoxy group at C7 and a 1-cyano-2-morpholinoethyl group attached to the C12 hydroxyl group. The tetracycline core has hydroxyl groups at C11 and C13, and a methyl group at C14.</p>

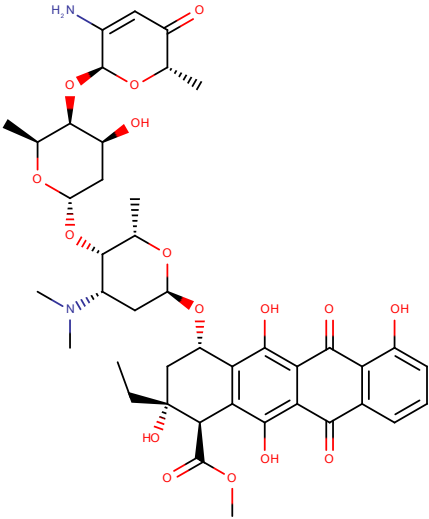
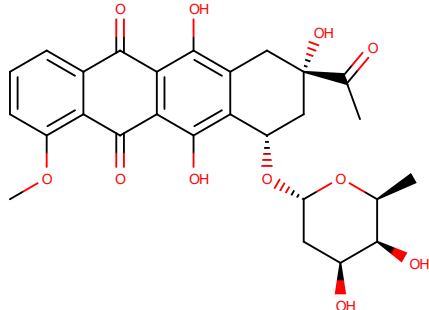
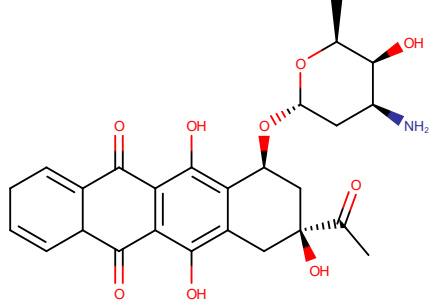
<p>Daunomycin 3,4-dichlorobenzoyl hydrazone</p>	<p>66996-54-1</p>	
<p>Daunomycin 4-nitrobenzoylhydrazone</p>	<p>66996-56-3</p>	

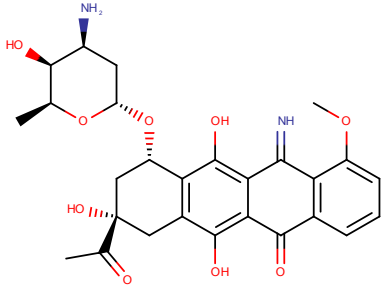
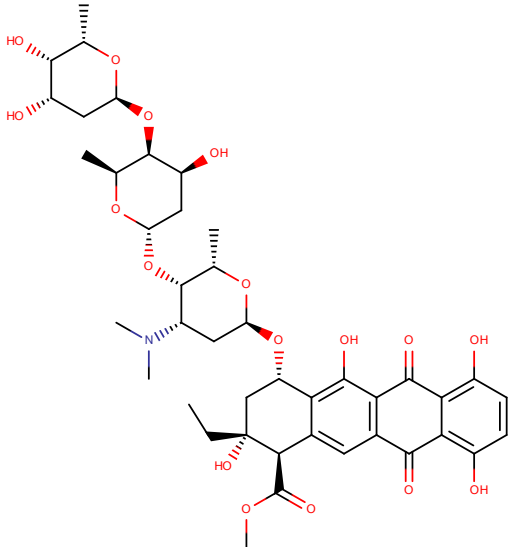
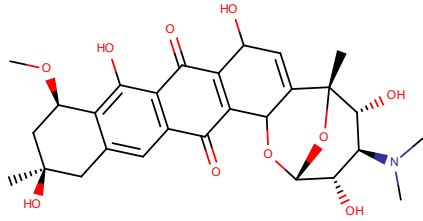
<p>Daunomycin 3-oxime</p>	<p>34610-60-1</p>	 <p>The structure shows a tetracyclic anthracycline core with a 3-oxime group at C-13, a 4-O-methyl group at C-10, and a 2-deoxy-3-amino-4-hydroxy sugar moiety at C-14. Stereochemistry is indicated with wedges and dashes.</p>
<p>Daunorubicin / Daunomycin</p>	<p>20830-81-3 / 23541-50-6</p>	 <p>The structure shows a tetracyclic anthracycline core with a 4-O-methyl group at C-10, a 2-deoxy-3-amino-4-hydroxy sugar moiety at C-14, and a 2-acetyl-3-hydroxy sugar moiety at C-13. Stereochemistry is indicated with wedges and dashes.</p>
<p>4-Demethoxyadriamycin / Medorubicin</p>	<p>64363-63-9</p>	 <p>The structure shows a tetracyclic anthracycline core with a 4-O-methyl group at C-10, a 2-deoxy-3-amino-4-hydroxy sugar moiety at C-14, and a 2-hydroxy-3-acetyl sugar moiety at C-13. Stereochemistry is indicated with wedges and dashes.</p>

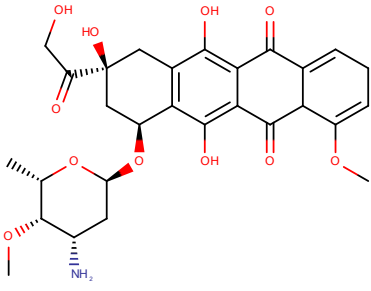
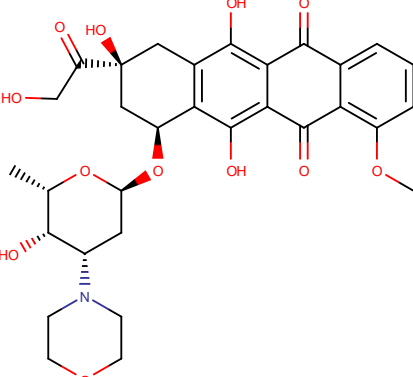
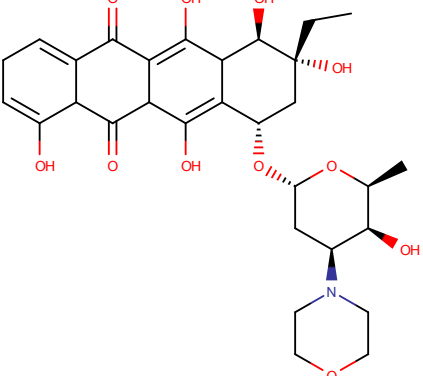
<p>N,N-dibenzyl-daunorubicin</p>	<p>70878-51-2</p>	 <p>The structure shows a daunosamine sugar moiety (a six-membered ring with a methyl group at C2, a hydroxyl group at C3, and a glycosidic bond at C4) linked to the C7 position of a tetracyclic anthracycline core. The core consists of a phenanthrene ring system with a methyl ketone at C13, a hydroxyl group at C14, and a methoxy group at C10. The nitrogen atom of the daunosamine is substituted with two benzyl groups.</p>
<p>N,N-diethyl-adriamycin</p>	<p>70844-09-6</p>	 <p>The structure shows an adriamycin sugar moiety (a six-membered ring with a methyl group at C2, a hydroxyl group at C3, and a glycosidic bond at C4) linked to the C7 position of a tetracyclic anthracycline core. The core features a phenanthrene ring system with a methyl ketone at C13, a hydroxyl group at C14, and a methoxy group at C10. The nitrogen atom of the adriamycin is substituted with two ethyl groups.</p>
<p>N,N-dimethyl-adriamycin</p>	<p>67106-76-7</p>	 <p>The structure shows an adriamycin sugar moiety (a six-membered ring with a methyl group at C2, a hydroxyl group at C3, and a glycosidic bond at C4) linked to the C7 position of a tetracyclic anthracycline core. The core features a phenanthrene ring system with a methyl ketone at C13, a hydroxyl group at C14, and a methoxy group at C10. The nitrogen atom of the adriamycin is substituted with two methyl groups.</p>

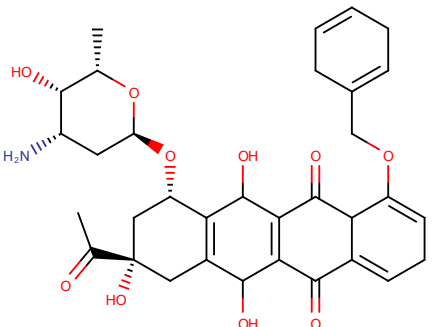
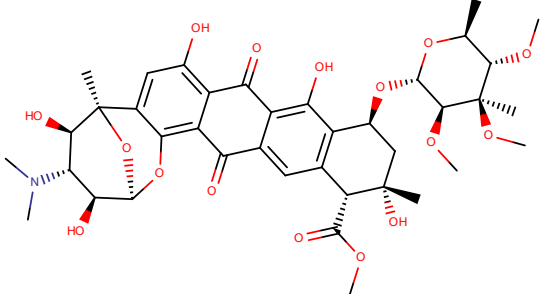
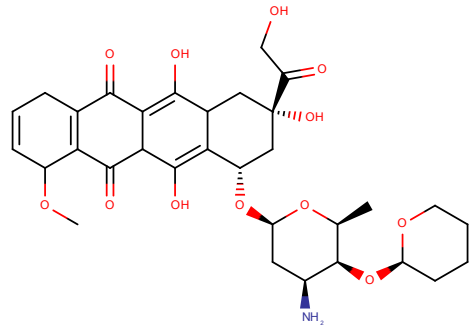
<p>N,N-dimethyl-daunomycin</p>	<p>70095-84-0</p>	 <p>The structure shows a tetracyclic anthracycline core with a dimethylamino group on the aglycone chain and a 2,6-dideoxy-3,4-dihydroxy-5-(dimethylamino)ribose sugar attached to the C-13 position.</p>
<p>Doxorubicin / Adriamycin</p>	<p>25316-40-9 / 23214-92-8</p>	 <p>The structure shows a tetracyclic anthracycline core with a 2,6-dideoxy-3,4-dihydroxyribose sugar attached to the C-13 position and a primary amino group at the C-2 position of the sugar.</p>
<p>Duborimycin</p>	<p>NSC 180510</p>	 <p>The structure shows a tetracyclic anthracycline core with a 2,6-dideoxy-3,4-dihydroxy-5-amino-ribose sugar attached to the C-13 position and a methyl group at the C-14 position of the aglycone chain.</p>

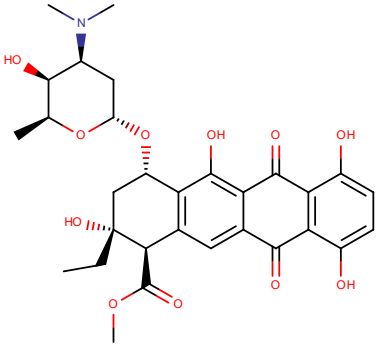
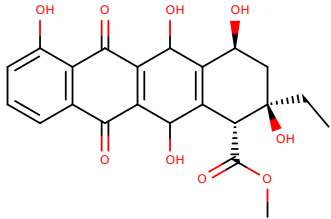
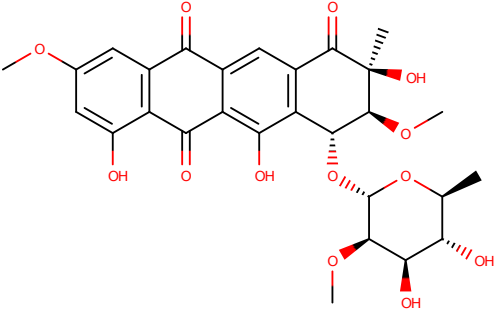
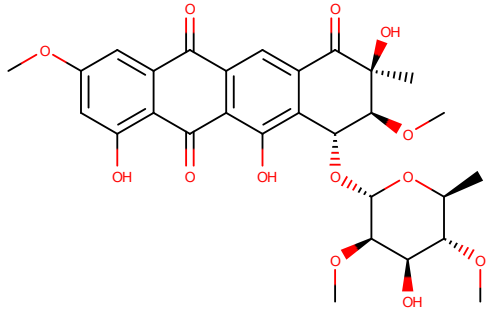
<p>Epirubicin</p>	<p>56390-09-1</p>	 <p>The chemical structure of Epirubicin is a tetracyclic anthracycline derivative. It features a central anthraquinone core with a 14a-hydroxy group and a 10-methoxy group. Attached to the 7-position of the anthraquinone is a 4,5-dihydro-2H-pyridin-2-ylidene group. At the 12-position, there is a 2,3,4-trihydroxybutyl side chain. At the 13-position, there is a 2-amino-2-deoxy-3,4,5-trihydroxyhexyl side chain.</p>
<p>Esorubicin</p>	<p>63950-06-1</p>	 <p>The chemical structure of Esorubicin is a tetracyclic anthracycline derivative. It features a central anthraquinone core with a 14a-hydroxy group and a 10-methoxy group. Attached to the 7-position of the anthraquinone is a 2-amino-2-deoxy-3,4,5-trihydroxyhexyl side chain. At the 12-position, there is a 2,3,4-trihydroxybutyl side chain. At the 13-position, there is a 2,3,4-trihydroxybutyl side chain.</p>
<p>11-Hydroxy aclacinomycin A</p>	<p>NSC 670121</p>	 <p>The chemical structure of 11-Hydroxy aclacinomycin A is a complex tetracyclic anthracycline derivative. It features a central anthraquinone core with a 14a-hydroxy group and a 10-methoxy group. Attached to the 7-position of the anthraquinone is a 2,3,4-trihydroxybutyl side chain. At the 12-position, there is a 2,3,4-trihydroxybutyl side chain. At the 13-position, there is a 2,3,4-trihydroxybutyl side chain. The structure is highly substituted with various hydroxyl and methoxy groups.</p>

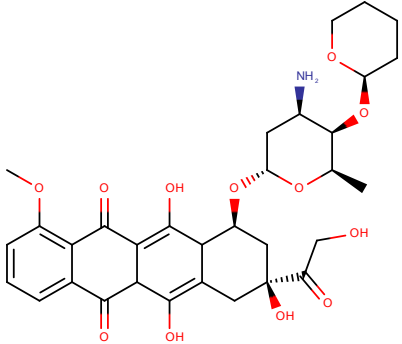
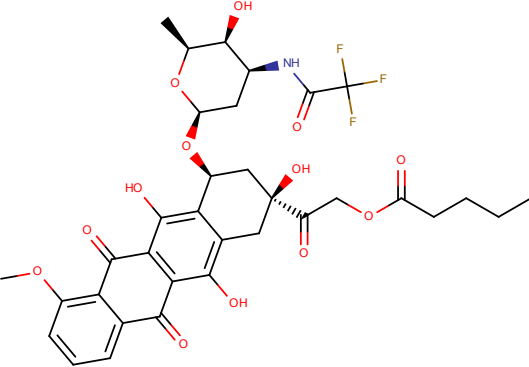
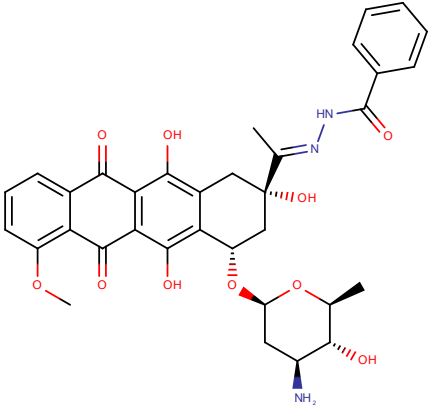
<p>11-Hydroxy aclacinomycin X</p>	<p>NSC 670122</p>	 <p>The structure shows a complex polycyclic molecule. It features a central tetracyclic core with a phenanthrene-like system. Attached to this core are two sugar rings. The upper sugar ring is a pyranose with a methyl group at C2, a hydroxyl group at C3, and a glycosidic linkage at C4 to a pyrimidine-2,4,6-trione ring. The lower sugar ring is also a pyranose with a methyl group at C2, a hydroxyl group at C3, and a glycosidic linkage at C4 to the C10 position of the tetracyclic core. A dimethylamino group is attached to the C12 position of the core.</p>
<p>3'-Hydroxy daunorubicin</p>	<p>64842-75-7</p>	 <p>The structure shows a tetracyclic core with a phenanthrene-like system. It has a methyl group at C12 and a hydroxyl group at C13. A glycosidic linkage at C10 connects to a pyranose sugar ring. This sugar ring has a methyl group at C2, a hydroxyl group at C3, and another hydroxyl group at C4. The C1 position of the sugar is linked to the C10 of the tetracyclic core.</p>
<p>Idarubicin</p>	<p>57852-57-0</p>	 <p>The structure shows a tetracyclic core with a phenanthrene-like system. It has a methyl group at C12 and a hydroxyl group at C13. A glycosidic linkage at C10 connects to a pyranose sugar ring. This sugar ring has a methyl group at C2, a hydroxyl group at C3, and an amino group at C4. The C1 position of the sugar is linked to the C10 of the tetracyclic core.</p>

<p>5-Imino daunorubicin</p>	<p>67324-99-6</p>	 <p>The structure shows a tetracyclic anthracycline core. It features a 5-imino group (NH) at the C11 position, a methoxy group at C12, and a 2-deoxy-3-amino-4-hydroxy sugar moiety attached to the C13 position. The C7 position has a methyl group, and the C14 position has a methyl ester group. Hydroxyl groups are present at C4 and C10.</p>
<p>Marcellomycin</p>	<p>63710-10-1</p>	 <p>The structure shows a tetracyclic anthracycline core with a 11-deoxy-5-imino group (NH) at the C11 position. It has a methoxy group at C12 and a 2-deoxy-3,4,6-trihydroxy sugar moiety at C13. The C7 position has an ethyl group, and the C14 position has a methyl ester group. Hydroxyl groups are present at C4, C10, and C11.</p>
<p>Menogaril</p>	<p>71628-96-1</p>	 <p>The structure shows a tetracyclic anthracycline core with a 11-deoxy-5-imino group (NH) at the C11 position. It has a methoxy group at C12 and a 2-deoxy-3,4,6-trihydroxy sugar moiety at C13. The C7 position has a methyl group, and the C14 position has a methyl ester group. Hydroxyl groups are present at C4, C10, and C11.</p>

<p>4'-O-methyladriamycin</p>	<p>77121-90-5</p>	 <p>The structure shows the adriamycin core with a methyl group at the 4' position of the aglycone ring. It is linked to a glucose molecule at the C-13 position. The glucose is further linked to a morpholine ring at the C-2 position. The morpholine ring has a methyl group at the 4-position and an amino group at the 3-position.</p>
<p>Morpholino adriamycin</p>	<p>89196-04-3</p>	 <p>The structure shows the adriamycin core with a hydroxyl group at the 4' position of the aglycone ring. It is linked to a glucose molecule at the C-13 position. The glucose is further linked to a morpholine ring at the C-2 position. The morpholine ring has a methyl group at the 4-position and a hydroxyl group at the 3-position.</p>
<p>MX2</p>	<p>NCI 619003</p>	 <p>The structure shows the adriamycin core with a hydroxyl group at the 4' position of the aglycone ring. It is linked to a glucose molecule at the C-13 position. The glucose is further linked to a morpholine ring at the C-2 position. The morpholine ring has a methyl group at the 4-position and a hydroxyl group at the 3-position. Additionally, there is a methyl group at the C-14 position of the aglycone ring.</p>

<p>NSC 286628</p>	<p>NSC 286628 / 67903-59-7</p>	 <p>The structure of NSC 286628 is a complex polycyclic molecule. It features a central tetracyclic core consisting of a benzene ring fused to a six-membered ring, which is further fused to two five-membered rings. This core is substituted with several hydroxyl groups (OH) and a carbonyl group (C=O). A side chain includes a six-membered ring with a hydroxyl group and an amino group (NH₂). Another side chain consists of a benzyl group attached to an oxygen atom, which is linked to the main structure.</p>
<p>Nogalamycin</p>	<p>1404-15-5</p>	 <p>The structure of Nogalamycin is a highly complex polycyclic molecule. It features a central tetracyclic core with multiple hydroxyl groups (OH) and carbonyl groups (C=O). The molecule is heavily substituted with various side chains, including a six-membered ring with a hydroxyl group and a methyl group, and a complex side chain with multiple oxygen atoms and methyl groups.</p>
<p>Pirarubicin</p>	<p>72496-41-4</p>	 <p>The structure of Pirarubicin is a complex polycyclic molecule. It features a central tetracyclic core with multiple hydroxyl groups (OH) and carbonyl groups (C=O). The molecule is substituted with a side chain containing a six-membered ring with a hydroxyl group and a methyl group, and another side chain containing a six-membered ring with a hydroxyl group and a methyl group. A side chain also includes a six-membered ring with a hydroxyl group and a methyl group.</p>

<p>Pyrrromycin</p>	<p>668-17-7</p>	 <p>The structure of Pyrrromycin features a central naphthoquinone core. The left ring is substituted with a 2-hydroxy-2-(dimethylamino)ethyl group and a methyl group. The right ring is substituted with two hydroxyl groups and a methyl group. A side chain is attached to the central ring, containing a methyl group, a hydroxyl group, and a methyl ester group.</p>
<p>Rhodomycinone</p>	<p>21288-60-8</p>	 <p>Rhodomycinone consists of a naphthoquinone core. The left ring has a hydroxyl group. The right ring has two hydroxyl groups and a methyl group. A side chain is attached to the central ring, featuring a methyl group, a hydroxyl group, and a methyl ester group.</p>
<p>Steffimycin</p>	<p>11033-34-4</p>	 <p>Steffimycin has a naphthoquinone core. The left ring is substituted with a methoxy group and a hydroxyl group. The right ring has a hydroxyl group and a methyl group. A side chain is attached to the central ring, containing a methyl group, a hydroxyl group, and a methyl ester group. A second side chain is attached to the right ring, consisting of a methyl group, a hydroxyl group, and a methyl ester group.</p>
<p>Steffimycin B</p>	<p>NCI 204856</p>	 <p>Steffimycin B is structurally similar to Steffimycin, featuring a naphthoquinone core with a methoxy group and a hydroxyl group on the left ring, and a hydroxyl group and a methyl group on the right ring. It has two side chains, each containing a methyl group, a hydroxyl group, and a methyl ester group.</p>

<p>Theprubicin</p>	<p>95343-20-7</p>	 <p>The chemical structure of Theprubicin is a complex polycyclic molecule. It features a central tetracyclic core with a methoxy group on the leftmost ring and two hydroxyl groups on the rightmost ring. Attached to the core are a 2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene group and a 2-amino-2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene group. The stereochemistry is indicated with wedges and dashes.</p>
<p>Valrubicin</p>	<p>56124-62-0</p>	 <p>The chemical structure of Valrubicin is a complex polycyclic molecule. It features a central tetracyclic core with a methoxy group on the leftmost ring and two hydroxyl groups on the rightmost ring. Attached to the core are a 2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene group and a 2-(2,2,2-trifluoroethylamino)-2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene group. The stereochemistry is indicated with wedges and dashes.</p>
<p>Zorubicin / Rubidazone</p>	<p>36508-71-1</p>	 <p>The chemical structure of Zorubicin / Rubidazone is a complex polycyclic molecule. It features a central tetracyclic core with a methoxy group on the leftmost ring and two hydroxyl groups on the rightmost ring. Attached to the core are a 2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene group and a 2-(2-amino-2,6-dihydroxy-4-methyl-3,4-dihydro-2H-pyridin-2-ylidene)phenylamino group. The stereochemistry is indicated with wedges and dashes.</p>

5. Cartesian coordinates of the optimized chemical structures of anthracyclines and the structure of AG-TC base pairs

Name	NSC No. / CAS No.	Cartesian coordinates				
3'-Acetoxy-4'-O-acetyl-doxorubicin	73113-92-5	H	1.0	-2.6798993224	-1.5955487037	-6.7702171546
		H	1.0	-0.9381479833	-1.9767177027	-6.8230672273
		H	1.0	-2.1308666448	-3.2995678371	-6.7355112319
		C	6.0	-1.9007862047	-2.2780012176	-6.4099268698
		H	1.0	-4.1739141992	-3.0031275529	-5.7777895662
		O	8.0	-1.7465141383	-2.1989152218	-4.9980378715
		C	6.0	-4.0283569223	-2.9247452992	-4.7082150061
		H	1.0	-6.0315442907	-3.5536282759	-4.2733328612
		C	6.0	-2.7863492911	-2.5115134075	-4.1983955424
		C	6.0	-5.0817784519	-3.2362936709	-3.8535324721
		C	6.0	-2.6010544414	-2.4107494485	-2.7894218080
		O	8.0	-0.3139238470	-1.7222412406	-2.8914113515
		H	1.0	2.0013149165	6.6187307810	-2.9093277557
		C	6.0	-4.9237297525	-3.1428766319	-2.4762845658
		H	1.0	0.8994520101	2.3216774067	-3.0982283371
		C	6.0	-1.3126182273	-1.9902424146	-2.1864895483
		H	1.0	-5.7278136934	-3.3784549176	-1.7900854712
		C	6.0	-3.6965445711	-2.7335618506	-1.9506289634
		H	1.0	3.1027845475	5.5098830528	-2.0552506674
		C	6.0	2.0888143666	5.6380664794	-2.4436726353
		H	1.0	0.7923258696	-1.3719722903	-1.8204701933
		O	8.0	4.8404783918	4.2610062471	-0.4120577301
		H	1.0	2.5976643268	3.4905424844	-1.4774349220
		H	1.0	1.9282268692	4.8658214721	-3.2029326653
		C	6.0	0.2811786481	2.0461223143	-2.2373516611
		H	1.0	-0.1460217789	1.0604189211	-2.4322608700
		C	6.0	1.0319331224	5.5594370436	-1.3564847550
		H	1.0	5.6775682017	6.5116458091	0.5333201727
		H	1.0	-0.5280923141	2.7726648026	-2.1342057900
		O	8.0	0.2631102757	6.4601047069	-1.1234045600
C	6.0	-1.2234169976	-1.8814495079	-0.7271788884		
O	8.0	1.0702000936	-1.2039393434	-0.8696439639		
C	6.0	-3.5847330255	-2.6488886661	-0.4709089843		
H	1.0	1.8836761631	1.2216933380	-1.0556767250		
C	6.0	4.3064246627	4.8746383849	0.4892069149		
C	6.0	1.8597061254	3.3285037605	-0.6914153824		
C	6.0	1.1218505945	2.0065323645	-0.9708883193		
O	8.0	0.9139646878	4.4090792473	-0.6333696927		

		C	6.0	4.8284482116	6.1471834271	1.1103193917
		C	6.0	-0.0177940025	-1.4564074881	-0.1391739164
		O	8.0	-4.5617768737	-2.9561177180	0.2467578224
		C	6.0	-2.3279092331	-2.2058185299	0.1077563748
		H	1.0	3.3775248819	2.4969524312	0.5720098985
		H	1.0	4.0394473926	6.9026182870	1.1490264103
		O	8.0	3.1470628021	4.4955833098	1.0742772689
		C	6.0	2.5724901464	3.2308906579	0.6657141815
		H	1.0	5.1428414968	5.9505334784	2.1400971951
		O	8.0	0.2343499664	1.6692752842	0.1068385969
		C	6.0	0.0805227836	-1.3017042872	1.2780531742
		C	6.0	-2.2022985739	-2.1191079488	1.5030411509
		O	8.0	1.8151793685	0.4850222999	1.3727684012
		H	1.0	2.1769847426	-1.4803731771	1.4895268596
		H	1.0	-3.9646367466	-2.7179928860	1.7417115180
		C	6.0	1.5871023193	2.8290112775	1.7557531926
		C	6.0	0.8642300208	1.5364225695	1.3633332406
		C	6.0	1.3991242389	-0.8082995761	1.8559519154
		C	6.0	-0.9811181409	-1.6765696399	2.0879023797
		H	1.0	0.8454147915	3.6240985259	1.8727520906
		O	8.0	-3.2061550716	-2.4388905862	2.3299006188
		H	1.0	2.1078252667	2.6914691856	2.7071628847
		H	1.0	1.5986281246	-5.4292964906	3.7242127188
		H	1.0	0.0433913960	1.3296035729	2.0596455265
		O	8.0	1.1743798957	-5.5502107748	4.5922514412
		C	6.0	1.4324793243	-0.7710498837	3.3989348341
		C	6.0	-0.8909182218	-1.6642897133	3.5945586468
		H	1.0	1.0726985441	0.2060127279	3.7380836964
		O	8.0	1.6288692837	-3.5915239358	2.8920558074
		H	1.0	-1.2767058621	-0.7221901704	4.0059695393
		H	1.0	2.4756284828	-0.8584639020	3.7243998239
		C	6.0	1.0463705375	-3.2419760817	3.9067003836
		H	1.0	-1.5301845712	-2.4489644093	4.0068063301
		C	6.0	0.7930371625	-4.2684117422	5.0034710336
		C	6.0	0.5523687187	-1.8021601991	4.1138135092
		H	1.0	-0.2688841283	-4.2389118832	5.2888696615
		H	1.0	1.3476680966	-3.9468617374	5.9006231377
		O	8.0	0.4735682967	-1.5241562230	5.5147439823
		H	1.0	1.3727579621	-1.4038905405	5.8512239243
Aclacinomycin X	NSC 670120	H	1.0	-0.2713988734	10.3179677365	3.5902798120
		H	1.0	1.2734978703	11.4349715173	1.9880488749
		C	6.0	0.4026226600	9.7425675644	2.9650594822
		C	6.0	1.2668625354	10.3521786095	2.0699424625
		O	8.0	-0.4756906174	7.8055098426	3.9660035666

C	6.0	0.3787562633	8.3402418392	3.0862299501
C	6.0	2.1306700016	9.5902127058	1.2707014124
H	1.0	2.8118845884	10.0528474312	0.5662796456
H	1.0	-0.3579878502	6.8244345184	3.9201478057
C	6.0	1.2475871145	7.5546565963	2.2837626109
C	6.0	2.1221814230	8.2055454995	1.3754220009
O	8.0	0.4491180475	5.5283646951	3.2109811618
C	6.0	1.2353691653	6.0985531292	2.3964592205
C	6.0	3.0505808501	7.4148458328	0.5141201691
O	8.0	3.8124236724	7.9658530727	-0.2727554919
C	6.0	2.1337369123	5.3057945612	1.5650747076
H	1.0	0.7929915166	3.9259548271	2.9754975014
C	6.0	3.0165519232	5.9291587015	0.6476161088
O	8.0	1.3167178256	3.2365782385	2.4896589166
C	6.0	2.1318378567	3.8928531872	1.6537445826
C	6.0	3.8620805202	5.1646631553	-0.1374791541
H	1.0	4.5261151602	5.6718802672	-0.8291708599
H	1.0	-2.7199902468	1.6084534089	-0.4663208355
H	1.0	-3.5294296923	1.4392457104	-2.0192104706
H	1.0	-1.9246736453	2.1981467920	-1.9471762943
H	1.0	-0.8000548652	1.4571888650	0.4047535486
C	6.0	-2.5557817973	1.3936081171	-1.5236559959
C	6.0	3.0092062292	3.1197391215	0.8545151013
C	6.0	3.8646587164	3.7594784336	-0.0401598418
H	1.0	8.2476269759	4.8374102464	0.2987574691
H	1.0	-1.2121834400	-0.1882619439	0.9238514831
C	6.0	-0.5344362509	0.4041890969	0.3024765116
H	1.0	0.8908179835	0.4043845427	1.9367426856
H	1.0	2.8038291470	1.3192946621	1.9961641307
C	6.0	2.9160136798	1.6124402430	0.9468023722
O	8.0	1.6875894423	1.2654233643	0.2508043873
N	7.0	-1.9954399529	0.0544737208	-1.7101474095
H	1.0	4.8345465904	3.3965317147	-1.9096240002
C	6.0	4.8494867218	2.9756715731	-0.9011019446
C	6.0	0.8843595545	0.2498455679	0.8523071947
O	8.0	6.9772224344	4.0035390480	-1.1365884253
H	1.0	8.7342291542	4.9697959555	-1.4236273345
C	6.0	6.2454966396	3.2151512254	-0.3221959674
C	6.0	8.3000182235	4.3223048693	-0.6629096626
H	1.0	-3.0129994693	-0.0801887746	-3.5359635329
O	8.0	6.6554740725	2.7839239019	0.7356700480
C	6.0	-0.6398433345	-0.0819237977	-1.1509068902
H	1.0	0.0676140303	0.5140874566	-1.7624333066
H	1.0	2.5669937728	1.4130447617	-1.4318704318

H	1.0	-5.7265849356	-2.5307930155	-1.8306842921
H	1.0	-3.5001807177	-1.9295989705	-0.7123656505
C	6.0	-2.0190960082	-0.2933611324	-3.1329355829
H	1.0	-1.2859145036	0.2824093069	-3.7295829140
H	1.0	-4.9899862504	-3.3929291695	0.5295119568
C	6.0	4.1270519390	0.9002691137	0.3400311469
H	1.0	4.9830264423	1.0383246286	1.0079044654
O	8.0	3.3881840627	1.3623779031	-1.9494762494
H	1.0	-2.7483729919	-3.0184636430	1.3874841454
C	6.0	4.4926282913	1.4585319564	-1.0443458022
H	1.0	8.8931067904	3.4124027911	-0.5461823194
H	1.0	-4.4585968467	-1.9921218604	-2.9452804796
O	8.0	1.4212399567	-1.0371290040	0.6655388684
C	6.0	-4.7457560314	-2.7815280022	-2.2480497926
H	1.0	-6.6174902979	-6.7188283108	2.7441117213
C	6.0	-3.7047926643	-2.9172348981	-1.1449443438
H	1.0	-1.8353914209	-1.3593018814	-3.2728171381
C	6.0	-4.1355801657	-3.8448934794	0.0044430622
C	6.0	-0.1145111058	-1.5357942503	-1.1871588107
H	1.0	3.9016119599	-0.1664685346	0.2863022991
H	1.0	-5.9313657816	-5.3539890090	0.9292810084
O	8.0	-0.9241686233	-2.3756201705	-0.3605090401
H	1.0	-5.0295842850	-6.9647305222	3.4993955248
C	6.0	-2.9682070285	-4.0166019485	0.9921038122
O	8.0	-3.2943461655	-4.8083225835	2.1158860750
H	1.0	1.9305067278	-0.9026998706	-1.3435539889
C	6.0	-5.8064622459	-7.4388031744	2.8935865117
C	6.0	1.3409472748	-1.5490401098	-0.6771431859
H	1.0	-4.8159079864	-3.7156557957	-2.8120467345
H	1.0	-6.2148935549	-8.2943523477	3.4368383147
H	1.0	5.9326851954	1.2558807430	-2.6184520780
C	6.0	5.6648662349	0.7066995809	-1.7067471434
H	1.0	-0.1105111035	-1.9134063322	-2.2161654783
H	1.0	6.5329585511	0.7506463326	-1.0405089123
O	8.0	-2.5054848596	-3.3898796192	-1.7846672303
H	1.0	-3.4930541155	-5.7059704675	1.7927189788
O	8.0	-4.5656746964	-5.0963112384	-0.5809648622
C	6.0	-5.3724258925	-5.9417950876	0.1817043449
C	6.0	-1.3954111157	-3.5843112175	-0.9243789455
C	6.0	-1.7367004147	-4.5227123296	0.2336679007
H	1.0	-0.8859129041	-4.5971129689	0.9153791216
N	7.0	-6.8433772018	-5.8717886092	-1.7462001300
O	8.0	-4.5436598822	-6.8951021855	0.8291173060
C	6.0	-5.2301086093	-7.9339699852	1.5634688681

		C	6.0	-6.3634515959	-6.6473918891	-0.7388517287
		H	1.0	4.4965365387	-0.8088837478	-2.7309839452
		C	6.0	1.9649849428	-2.9350012614	-0.6360081751
		C	6.0	-6.7872765929	-7.9089394213	-0.4491029830
		C	6.0	5.3678238892	-0.7490778795	-2.0751453024
		H	1.0	1.4076175428	-3.5816527604	0.0456274746
		H	1.0	-0.6310515590	-4.0215971250	-1.5779885537
		H	1.0	5.1748487333	-1.3658460829	-1.1914259756
		H	1.0	-6.2522279722	-5.1111994245	-2.0491995262
		H	1.0	2.9962642665	-2.8713220091	-0.2795264709
		H	1.0	-1.9476029200	-5.5170866073	-0.1734462412
		C	6.0	-6.3062225374	-8.6240640953	0.7135363088
		H	1.0	-7.4305650140	-6.3008067299	-2.4457609386
		H	1.0	-4.4544842950	-8.6788918179	1.7601072858
		H	1.0	-7.5300939458	-8.4086044236	-1.0648351035
		H	1.0	1.9749114211	-3.3862517630	-1.6332238569
		H	1.0	6.2230004413	-1.1891831271	-2.5975672651
		O	8.0	-6.7240971481	-9.7222091248	1.0701937954
		H	1.0	6.1955225443	-2.7142906328	1.0984376253
		H	1.0	5.8712986380	-2.6996655267	-1.3431434774
		H	1.0	4.4620575664	-2.8111795504	0.7387311147
		C	6.0	5.3445389721	-2.1708231435	0.6759850280
		H	1.0	-1.8379507899	-3.2231655764	1.4289739625
		C	6.0	5.6294212953	-1.7898183867	-0.7789946509
		H	1.0	-1.3232228397	-3.7084213893	-0.2162927273
		H	1.0	-6.6176302270	-1.7307806341	6.1614273520
		H	1.0	8.6463998664	-1.5588871912	-5.0615263196
		H	1.0	-3.0410027067	-3.4812755919	0.1740133011
		H	1.0	6.5102929814	-1.1407105439	-0.8268049899
		H	1.0	5.1756050220	-1.2915088203	1.3059984352
		C	6.0	-2.0367746787	-3.0929320765	0.3646269640
		H	1.0	-0.5524007770	-1.5222696772	4.0678566591
		O	8.0	3.3386270459	-1.9774273809	-1.4023465676
		H	1.0	2.0158926997	-1.6151263311	3.3947876468
		H	1.0	-0.0915987405	-2.1920285767	1.9459189104
		H	1.0	-5.3947723969	-1.5193072489	7.4211218563
		H	1.0	-4.8567497201	-2.6951603753	3.9206870937
		H	1.0	-7.6061466053	-1.0038957190	8.4700968727
		O	8.0	-2.4343409802	-1.7598851106	3.4753630911
		O	8.0	6.9060229905	-1.2283467463	-4.0793707403
		H	1.0	2.5272676424	-1.4421300842	-1.4240728703
		H	1.0	4.7479599384	-1.9450433770	-3.4587294782
		C	6.0	-6.1461961717	-0.9958645430	6.8211332287
Aclarubicin	57576-44-0	H	1.0	6.1955225443	-2.7142906328	1.0984376253
		H	1.0	5.8712986380	-2.6996655267	-1.3431434774
		H	1.0	4.4620575664	-2.8111795504	0.7387311147
		C	6.0	5.3445389721	-2.1708231435	0.6759850280
		H	1.0	-1.8379507899	-3.2231655764	1.4289739625
		C	6.0	5.6294212953	-1.7898183867	-0.7789946509
		H	1.0	-1.3232228397	-3.7084213893	-0.2162927273
		H	1.0	-6.6176302270	-1.7307806341	6.1614273520
		H	1.0	8.6463998664	-1.5588871912	-5.0615263196
		H	1.0	-3.0410027067	-3.4812755919	0.1740133011
		H	1.0	6.5102929814	-1.1407105439	-0.8268049899
		H	1.0	5.1756050220	-1.2915088203	1.3059984352
		C	6.0	-2.0367746787	-3.0929320765	0.3646269640
		H	1.0	-0.5524007770	-1.5222696772	4.0678566591
		O	8.0	3.3386270459	-1.9774273809	-1.4023465676
		H	1.0	2.0158926997	-1.6151263311	3.3947876468
		H	1.0	-0.0915987405	-2.1920285767	1.9459189104
		H	1.0	-5.3947723969	-1.5193072489	7.4211218563
		H	1.0	-4.8567497201	-2.6951603753	3.9206870937
		H	1.0	-7.6061466053	-1.0038957190	8.4700968727
		O	8.0	-2.4343409802	-1.7598851106	3.4753630911
		O	8.0	6.9060229905	-1.2283467463	-4.0793707403
		H	1.0	2.5272676424	-1.4421300842	-1.4240728703
		H	1.0	4.7479599384	-1.9450433770	-3.4587294782
		C	6.0	-6.1461961717	-0.9958645430	6.8211332287

C	6.0	8.2378104649	-0.7886808698	-4.4085662622
H	1.0	-1.8445668809	-0.1119520327	5.5719704042
C	6.0	4.4601231239	-1.0947232092	-1.5055192002
H	1.0	-4.3675153530	-3.0226720216	2.2452925725
C	6.0	-1.3336788219	-0.8839857239	3.6375599334
H	1.0	8.8416784037	-0.6899055517	-3.5036134413
H	1.0	0.0602492204	-1.7499098066	-0.4832815712
C	6.0	-7.1944623085	-0.3222070896	7.7215304543
H	1.0	-8.0437565426	0.0139307590	7.1070300560
H	1.0	1.9429034950	-1.3355860288	0.9102977167
C	6.0	2.0075753781	-0.6201252138	2.9387802080
C	6.0	-4.6973320152	-2.2461562710	2.9383030304
C	6.0	-0.0937288971	-1.1635920049	1.5667316386
O	8.0	-4.4265037091	-0.5677023180	5.2341471070
H	1.0	3.0405461744	-0.2712948231	2.8600222175
C	6.0	4.7963443891	-0.9421563281	-3.0270518168
H	1.0	8.2064685046	0.1753279814	-4.9210299426
N	7.0	-1.9967016925	-1.6753137951	-0.0009282559
C	6.0	-1.6657710254	0.2847053577	4.5671738471
C	6.0	6.2032242216	-0.3977409376	-3.2813469659
C	6.0	-3.6550490899	-1.1411356483	3.0250940374
H	1.0	3.9232018666	0.2305793710	0.1423482029
C	6.0	1.3652117845	-0.6629314096	1.5610766294
C	6.0	-0.6347827435	-1.1291923489	0.1181584276
H	1.0	-1.9498811405	-1.9373419733	-2.1421121654
C	6.0	-5.4128853113	0.0464962803	5.9885984127
H	1.0	1.4636291415	0.0688107171	3.5891414237
H	1.0	-0.8221647415	0.9779589257	4.6099359970
O	8.0	-0.8905420490	-0.3305963182	2.4109438214
H	1.0	-3.5477957249	-1.9799814571	-1.3664331950
C	6.0	4.1329353085	0.2911798106	-0.9273063872
H	1.0	-6.1102215990	0.6011323105	5.3383849351
H	1.0	-5.6490301471	-1.8433021684	2.5756312427
C	6.0	-2.5674690669	-1.4965519467	-1.3360243523
C	6.0	-4.0717568890	0.0084467183	3.9582051971
H	1.0	-3.4787962396	-0.7178235985	2.0278541189
H	1.0	4.4401192671	-0.8255738950	-5.7175826591
H	1.0	5.0011083528	0.9419902245	-1.0710934802
C	6.0	-6.6826793666	0.9208126453	8.4387274657
O	8.0	1.6890273311	0.2520264231	-1.2600776293
O	8.0	6.6444163361	0.6483328253	-2.8523135786
C	6.0	3.8223237438	-0.0471640131	-3.7859634469
C	6.0	-2.9223235078	1.0208191120	4.0882426274
O	8.0	-7.1166070792	1.2794029869	9.5153186619

O	8.0	-4.7695021184	0.9707283200	6.8891615351
H	1.0	-7.0578893473	2.5430818025	6.2030799689
C	6.0	3.7991646070	-0.1257026757	-5.1921847088
O	8.0	1.4491350399	0.6774521224	1.0433614222
H	1.0	-3.5410200486	1.8034138597	5.7561872042
C	6.0	2.9245650613	0.9310053993	-1.6137627513
H	1.0	-4.9548691778	0.5096671337	3.5355550483
C	6.0	-0.5232867375	0.3208879411	-0.3766150752
H	1.0	-2.7207786183	-0.4398036991	-1.5617207337
C	6.0	0.8998434956	0.8629880072	-0.2377710262
O	8.0	-3.2480007148	2.1388412139	4.8895447987
H	1.0	-0.7969281176	0.4189575878	-1.4280209932
C	6.0	2.9959110762	0.8580730341	-3.1233819365
C	6.0	-5.6409795135	1.7736871842	7.7016686415
H	1.0	-2.7341909060	1.4177191696	3.0842593589
H	1.0	-1.1927548685	0.9493341516	0.2178165204
C	6.0	-6.3085611410	2.9100389773	6.9112993966
H	1.0	2.8361581080	1.9776337038	-1.3033785022
O	8.0	3.7076471797	-0.2240601235	-7.9942170653
C	6.0	2.9618022920	0.6883415441	-5.9351954658
H	1.0	-4.9905186250	2.2085243631	8.4654419217
H	1.0	-5.5465395278	3.4546944517	6.3475822784
H	1.0	-6.8050012518	3.5957050413	7.6028755511
H	1.0	0.9120717799	1.9465591504	-0.3975682845
C	6.0	2.9715957675	0.5724823509	-7.4225111011
C	6.0	2.1265447548	1.6865424220	-3.8741300454
C	6.0	2.1075237981	1.6162668575	-5.2880182168
O	8.0	1.3386010309	2.5312402493	-3.1963712086
H	1.0	2.6931241794	0.6589391535	-10.0555489669
C	6.0	2.0514529076	1.4638718326	-8.1893651024
C	6.0	2.0361283260	1.3743309810	-9.5750845510
H	1.0	0.8172388652	3.0378447416	-3.8725208745
C	6.0	1.2185889859	2.4787321701	-6.0575544212
C	6.0	1.2077352807	2.3842151257	-7.5151017229
C	6.0	1.1791262546	2.2012486268	-10.3147331382
O	8.0	0.4597305685	3.3041115463	-5.4664153388
H	1.0	1.1667211397	2.1310221495	-11.3982991016
C	6.0	0.3458847130	3.2153328598	-8.2782581662
C	6.0	0.3450850587	3.1089279542	-9.6819478320
O	8.0	-0.4800382534	4.1082941111	-7.7208745397
H	1.0	-0.3229552168	3.7560112975	-10.2399122612
H	1.0	-0.3505910002	4.0470012913	-6.7421601284

Adriamycin 14-octanoate	51898-39-6	H	1.0	5.8918845272	1.1063231062	-1.7508609126
		O	8.0	6.4309807628	-1.3853261070	-1.5039537114
		H	1.0	4.2130010362	0.8719841807	-1.2214052890
		C	6.0	5.2597672369	0.6736829267	-0.9707811073
		H	1.0	4.8698083862	-3.3225565572	-1.2049849733
		H	1.0	6.1874391070	3.2424070332	-0.3294295358
		H	1.0	0.1780434896	-2.0529232557	-4.5761091420
		C	6.0	5.4939557562	-0.8195980935	-0.9888819198
		H	1.0	4.7333682992	5.3634511830	-0.3911708940
		H	1.0	5.5623544199	-3.1379864143	0.4069774273
		H	1.0	3.2476054882	7.4995062603	-0.4958935126
		H	1.0	3.7151665632	3.0945053715	-0.7595047854
		O	8.0	0.6834507945	-2.2675874132	-3.7424585881
		H	1.0	-2.8290641618	-0.3897601520	-6.6334961967
		O	8.0	-1.0930872165	-1.3196806360	-5.2977296089
		H	1.0	2.2688296505	5.1960681827	-0.8584937198
		C	6.0	4.6887106813	-2.9067044733	-0.2062296462
		C	6.0	5.5124374435	2.8237859934	0.4301971562
		O	8.0	4.5150547241	-1.4806075057	-0.3055295875
		C	6.0	4.0440753842	4.9186643335	0.3408439590
		C	6.0	5.6077870480	1.2907089272	0.4012555774
		H	1.0	1.7168095121	-3.5694178376	-1.8735673731
		H	1.0	2.6111620835	-2.0763367051	-1.6414882642
		H	1.0	6.6293063202	0.9929124593	0.6669609898
		C	6.0	4.1008690058	3.3902340450	0.2253558891
		C	6.0	2.5942787125	7.0258139537	0.2456536121
		C	6.0	2.6404131962	5.4993995612	0.1297966600
		H	1.0	-4.9272193958	0.8986605895	-7.1121219998
		H	1.0	1.5808406005	7.4087194512	0.0881811984
		C	6.0	-3.3953788148	0.0841378939	-5.8412175432
		C	6.0	-1.6828489063	-0.8143408521	-4.3174493616
		H	1.0	5.8958100426	3.1712401972	1.3986819767
		C	6.0	-0.0020211671	-1.7025597141	-2.7415277567
		C	6.0	1.7784062701	-2.6717450655	-1.2512494065
		H	1.0	4.4173048705	5.2220551507	1.3294311108
		C	6.0	3.4793094313	-3.6136547591	0.4148632723
		H	1.0	2.9250082543	7.3586498452	1.2359977734
		C	6.0	-4.5584437060	0.7998726688	-6.0955966518
		H	1.0	4.9479004262	0.8625313468	1.1654567032
		H	1.0	3.4206937700	2.9439786999	0.9651619131
C	6.0	-2.9332937669	-0.0357728750	-4.5286255177		
H	1.0	1.9513795910	5.0554959033	0.8610344008		
C	6.0	-1.1782176829	-0.9665164353	-2.9644813338		
O	8.0	3.7026840139	-4.6244006644	1.0449254015		

C	6.0	0.5074797488	-1.8712270132	-1.4197537386
C	6.0	2.0287707120	-3.1033107058	0.2086818345
O	8.0	1.1606120415	-4.1795317527	0.5044622551
H	1.0	2.4501395151	-1.0843340512	0.8794443415
C	6.0	-5.2629197950	1.3966679505	-5.0536707595
C	6.0	-3.6238210544	0.5582548343	-3.4433147381
C	6.0	-1.8690240079	-0.3727448323	-1.8699521457
H	1.0	-6.1667998567	1.9492174079	-5.2748551823
H	1.0	0.5032056218	-3.8776593515	1.1507460945
C	6.0	1.7824536254	-1.9060423358	1.1526226516
C	6.0	-0.1599977539	-1.2841545842	-0.3574841927
C	6.0	-4.8137112909	1.2880427346	-3.7275248483
C	6.0	-3.0959914442	0.4046861980	-2.0643752557
H	1.0	1.9899943601	-2.1872669447	2.1878440706
C	6.0	-1.3556881663	-0.5366371716	-0.5723432770
C	6.0	0.3301975131	-1.4293387428	1.0682902758
H	1.0	0.2320294164	-0.4655988358	1.5782743768
O	8.0	-5.4718725575	1.8535517731	-2.6942510206
H	1.0	-6.4793804902	3.4520705632	-3.5925450946
O	8.0	-3.6692310682	0.9177828405	-1.0788003456
O	8.0	-0.5525174855	-2.3767080909	1.7252652199
O	8.0	-1.9462172409	0.0045500847	0.4995915389
H	1.0	-3.1000783277	-3.6213797623	5.2161332545
C	6.0	-6.6639304647	2.5876093736	-2.9432699489
H	1.0	-7.4424022592	1.9567144825	-3.3891532815
H	1.0	-2.7506481801	0.4870411565	0.1392806058
H	1.0	0.8026668902	-2.0889775492	5.7730080842
H	1.0	-2.9372125466	-2.9004003338	2.7576343992
C	6.0	-2.4929053427	-2.7552802170	4.8872437336
C	6.0	-0.9897814488	-2.0154483258	3.0101003642
H	1.0	-4.1484086985	-1.5716579099	4.6182857227
H	1.0	-6.9984675289	2.9361639130	-1.9661077430
N	7.0	-3.2139720860	-1.4864418579	5.0090551013
C	6.0	-2.0762581533	-2.9972656169	3.4275952230
H	1.0	-0.8110891525	-3.7495454001	5.7537017107
C	6.0	-0.1206681286	-1.7943233893	5.2628611499
H	1.0	-1.3719350246	-0.9874788265	2.9915286523
O	8.0	0.1356936123	-2.1081396605	3.8837963307
C	6.0	-1.2328973173	-2.7338067415	5.7768962788
H	1.0	0.5227298749	0.2543714132	5.1168279145
H	1.0	-1.2514839405	0.0652334998	5.0435242561
C	6.0	-0.3354747817	-0.2999628138	5.5092701547
H	1.0	-3.3097815283	-1.2596314216	5.9960485310
H	1.0	-1.6773260549	-4.0118056930	3.3144414166

		O	8.0	-1.5402016256	-2.3554387798	7.1200356330
		H	1.0	-0.4044675769	-0.1152365246	6.5845697965
		H	1.0	-2.0109505093	-3.0909901932	7.5337786150
		H	1.0	4.9786410930	-0.5111178516	-5.0094058534
		H	1.0	2.3995311219	-3.3392588447	-2.1565787019
		C	6.0	4.9740848183	-0.3687210602	-3.9295050616
		H	1.0	2.9381181943	-5.1435695844	-0.5583688619
		O	8.0	3.6192865064	-0.6258422300	-3.5125207378
		H	1.0	5.2658291838	0.6521751174	-3.6732793427
		H	1.0	5.6615377845	-1.0660112070	-3.4452676574
		H	1.0	3.6339039083	-2.7893381855	-1.0252526463
		C	6.0	2.5800436596	-3.0768542054	-1.1061915076
		H	1.0	1.4324532667	-1.1106045074	-2.7769451772
		C	6.0	2.3101946095	-4.3070340953	-0.2359042115
		H	1.0	1.2644304843	-4.6117256444	-0.3145827974
		C	6.0	3.3845024783	-0.4862745315	-2.1910510240
		C	6.0	1.9121625900	-0.7438033627	-1.8660530076
		H	1.0	2.5330051054	-4.1212760653	0.8196589644
		C	6.0	1.7045925238	-1.8499674085	-0.7784163843
		H	1.0	1.3515583739	1.3076610591	-3.5552354965
		O	8.0	0.3444552432	-2.2849697016	-0.8695790173
		O	8.0	4.2413129202	-0.1757164616	-1.3895386341
		H	1.0	-0.1882258212	-1.7428115558	-0.2636129176
		O	8.0	0.6858897769	3.4759750143	-4.5216812212
		C	6.0	1.0931714672	1.5445349338	-2.5286634166
		C	6.0	1.2890350866	0.5994847268	-1.5025437118
		H	1.0	-4.8058284311	-2.9589688156	0.5042228127
		H	1.0	-0.1906638668	-5.1367267409	3.1833401830
		C	6.0	2.0060781153	-1.2510775932	0.6046313128
		H	1.0	3.0381688429	-0.8869287869	0.6087395146
		H	1.0	1.9052207450	-2.0032806444	1.3893959862
		H	1.0	-0.3190624781	-3.1769990320	1.6457993802
		H	1.0	-2.3928725887	-4.0800482176	2.2629910576
		H	1.0	-4.4355915294	-4.0671697286	1.8453561596
		C	6.0	-4.8833364359	-3.1029681435	1.5968698341
		H	1.0	-2.5917828381	-1.9964548737	1.0092568315
		C	6.0	0.3894088743	3.7682648090	-3.3685206197
		H	1.0	-5.9438867778	-3.1547809026	1.8585075497
		C	6.0	0.5730628980	2.7967047941	-2.2513374347
		H	1.0	1.1883435102	-4.0481472007	3.4397560743
		H	1.0	-0.0770908668	5.7538245532	-5.0593321662
		C	6.0	0.1027759162	-4.1414756322	3.5311324867
		C	6.0	0.9537271777	0.9168818731	-0.1876804467
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		C	6.0	-0.5888759333	-3.0664420816	2.7060292009
		C	6.0	1.0766450260	-0.0830068874	0.9415033441
		H	1.0	-4.9231640811	-0.3985825705	1.1092603055
		O	8.0	-0.2800231341	-0.5369851221	1.2010572435
		C	6.0	-2.1169217804	-3.1513916558	2.7911866704
		C	6.0	-2.7942647720	-1.9441388698	2.0942621958
		H	1.0	-0.1764219976	-4.0417440828	4.5816630831
		C	6.0	-0.3474158399	6.0367543255	-4.0488070507
		N	7.0	-4.2504286895	-2.0215824369	2.3563234380
		C	6.0	-0.1676602303	5.1112954107	-3.0292014469
		C	6.0	0.2232902603	3.1477967345	-0.9230245138
		C	6.0	-4.9853839006	-0.7739203897	2.1467389534
		H	1.0	1.4392241931	0.4284259678	1.8395132595
		C	6.0	0.4084470051	2.1911350532	0.1041225629
		H	1.0	-6.0409213420	-0.9483716926	2.3745569152
		O	8.0	-0.0804913142	-1.8042989191	3.1802360920
		O	8.0	-2.5338830126	-3.2079053687	4.1428576272
		C	6.0	-0.6458783052	-0.6718403723	2.5762924204
		C	6.0	-2.1721475462	-0.6560228308	2.6519919260
		H	1.0	-2.5224980897	0.2301348877	2.1190609017
		H	1.0	-1.0090241329	8.0278077542	-4.5493550889
		H	1.0	-4.6303968674	0.0076391966	2.8196177255
		C	6.0	-0.8683672555	7.3040033841	-3.7521540144
		H	1.0	-3.4531605437	-2.8844262034	4.1210839137
		C	6.0	-0.5058688953	5.4365928612	-1.6900331346
		C	6.0	-0.3204670645	4.4651325057	-0.6153532541
		H	1.0	-0.2322362170	0.1826348800	3.1232294872
		O	8.0	0.0879690006	2.4496886783	1.3786859087
		H	1.0	-2.4432889470	-0.5594521673	3.7079911425
		H	1.0	-0.2534073953	3.3816344292	1.4026164096
		C	6.0	-1.2072206853	7.6479231340	-2.4533205829
		O	8.0	-0.6298588833	4.7660742959	0.5766128881
		C	6.0	-1.0327083143	6.7240831536	-1.4055680024
		H	1.0	-1.6109192227	8.6241710535	-2.2078154284
		H	1.0	-1.1903938336	6.3447836930	0.4291294528
		O	8.0	-1.3764549325	7.1089380405	-0.1711831007
		H	1.0	7.3542139530	-1.4272334406	2.4109184099
		H	1.0	7.3802480993	-1.9998916822	0.0260258414
		H	1.0	7.3912019085	-1.5333340267	-2.2033840326
		H	1.0	6.7345104169	-3.1555906218	-1.8258993713
		C	6.0	6.4803902773	-1.2146974106	1.8023445818
		C	6.0	6.4965904275	-1.5399870402	0.4489444744
		C	6.0	6.5092658459	-2.1811451300	-2.2760037229
2'-Bromo-4'-epi-daunorubicin	NSC 650931	H	1.0	7.3542139530	-1.4272334406	2.4109184099
		H	1.0	7.3802480993	-1.9998916822	0.0260258414
		H	1.0	7.3912019085	-1.5333340267	-2.2033840326
		H	1.0	6.7345104169	-3.1555906218	-1.8258993713
		C	6.0	6.4803902773	-1.2146974106	1.8023445818
		C	6.0	6.4965904275	-1.5399870402	0.4489444744
		C	6.0	6.5092658459	-2.1811451300	-2.2760037229

H	1.0	6.2498957047	-2.3202935392	-3.3255498607
H	1.0	5.3215916285	-0.3605656141	3.4218924139
C	6.0	5.3595296739	-0.6239632744	2.3720817402
C	6.0	5.3836310613	-1.2780166822	-0.3667976495
O	8.0	5.3658249709	-1.5799425834	-1.6814408046
C	6.0	4.2429380136	-0.3565982194	1.5769353545
C	6.0	4.2235017656	-0.6732934399	0.1966667816
O	8.0	3.1213914336	0.5446948993	3.4608832658
C	6.0	3.0719227991	0.2766190097	2.2403991574
C	6.0	3.0149504035	-0.3688709382	-0.6093894910
O	8.0	2.9580612912	-0.6290060383	-1.8301755300
C	6.0	1.8913535275	0.5692653598	1.4453509984
H	1.0	1.6553678539	1.2117224887	3.7179999507
C	6.0	1.8655523006	0.2543447478	0.0573291579
H	1.0	1.5119282786	-0.1263298526	-2.2464019544
O	8.0	0.7625530739	1.4831080116	3.3633382127
C	6.0	0.7767498959	1.1715137720	2.0613185383
C	6.0	0.7107925336	0.5485304316	-0.6959227724
O	8.0	0.6265763053	0.2811917920	-2.0060082187
C	6.0	-0.3760021370	1.4633424004	1.2881565060
C	6.0	-0.4079297449	1.1494331575	-0.0609949468
H	1.0	-1.2576673881	-2.9110028985	-1.8972884387
H	1.0	-0.8303127862	-1.8088198340	-3.2342759143
H	1.0	-2.8774086924	-3.6145801344	0.7577452300
H	1.0	-1.5397709260	-3.4007676261	-3.5719793276
H	1.0	-1.7840236508	-1.0740499007	-0.6284373335
C	6.0	-1.5529569529	-2.5495909242	-2.8823458818
H	1.0	-3.0695054083	-4.5856192460	-0.5470600021
N	7.0	-2.9174346302	-3.6222635331	-0.2589507888
H	1.0	-1.3699719136	2.4485998070	2.9114450071
O	8.0	-0.2717561310	4.7634804550	0.8747243475
C	6.0	-1.5907850857	2.1063077888	1.8968244286
H	1.0	-1.4947428496	1.4242212464	-1.9019836443
C	6.0	-1.6582596218	1.5353513546	-0.8282900388
H	1.0	-2.3834291358	1.3512519200	1.9525449244
C	6.0	-1.3495890959	4.5415604091	1.3929441799
C	6.0	-2.7485948969	-0.6022031317	-0.8541400045
H	1.0	-1.2521097639	3.6238830607	-0.9141196491
BR	35.0	-3.6801063560	-1.3408485448	1.7917969971
H	1.0	-1.2295620080	6.2555335568	2.6665783033
O	8.0	-2.7899012052	0.7225868621	-0.4404058201
C	6.0	-2.9481546254	-1.9256061685	-2.8768080374
C	6.0	-2.1571171329	3.2699455038	1.0223202977
C	6.0	-2.0294863279	2.9816311506	-0.4935561036

		C	6.0	-4.0389945029	-2.7936205904	-0.7037712340
		H	1.0	-2.1844784727	4.9157958914	3.3601103884
		O	8.0	-2.9933189581	-0.6181348392	-2.2630472097
		C	6.0	-1.9423762150	5.4620002721	2.4410791447
		C	6.0	-3.8965582109	-1.3552433364	-0.1837812577
		H	1.0	-4.0571351926	-3.7821393190	-2.6345471497
		C	6.0	-4.0913971195	-2.7518242034	-2.2588929441
		H	1.0	-3.2403209950	-1.7231171942	-3.9130877492
		H	1.0	-5.0213308458	-3.1657270692	-0.3737517639
		H	1.0	-2.9850472977	3.2267654029	-0.9634454710
		H	1.0	-3.7138103533	3.1886278925	2.2212843624
		H	1.0	-4.8175926740	-0.7968540241	-0.3501237585
		O	8.0	-3.5430981279	3.4648077655	1.3114387526
		H	1.0	-2.8803582829	5.8863559674	2.0709422428
		O	8.0	-5.3427737291	-2.2154061682	-2.6763190454
		H	1.0	-5.2364538704	-1.2522040834	-2.6813715934
Cinerubin A	NSC 243022 / 34044-10-5	H	1.0	8.6792426136	0.5238216094	-5.7700783716
		H	1.0	6.9848068025	0.4708190807	-5.2358525703
		C	6.0	7.9881339309	0.8182054948	-4.9756683856
		H	1.0	7.9734730476	1.9115418069	-4.9257189422
		H	1.0	8.4513692298	-0.9058864366	-3.7709004217
		O	8.0	10.8077693454	0.0401431481	-3.7814015170
		C	6.0	8.4275459797	0.1803388943	-3.6490555149
		C	6.0	9.8566642809	0.6121992156	-3.2877713084
		H	1.0	-9.1225014984	-1.5063059926	-2.5595543475
		O	8.0	7.4932942479	0.4131751687	-2.5834389841
		H	1.0	9.9705195066	2.7038323603	-3.0264791499
		H	1.0	7.3102178164	2.4851764697	-2.6946447748
		C	6.0	10.0064293358	1.8181838344	-2.3736221148
		H	1.0	5.2107913303	3.0408579516	-1.7477793160
		H	1.0	-8.3088110604	-3.0389729197	-2.1009906453
		C	6.0	-8.6666810642	-2.0705142656	-1.7468808384
		H	1.0	-1.1234306254	1.8574386607	-2.6658007005
		H	1.0	11.0069275017	1.7955649945	-1.9345966820
		H	1.0	2.9477003574	2.3274077628	-2.9488948317
		C	6.0	7.5316684188	1.7028552864	-1.9471824485
		H	1.0	-9.3835087028	-2.2293040431	-0.9381760171
		H	1.0	4.7714208628	3.0075235462	0.5570890158
		H	1.0	-2.6836398601	1.2170442114	-2.1151756301
		O	8.0	-7.5583418289	-1.2668036850	-1.2929225536
		C	6.0	8.8992349938	1.9160314458	-1.3139539008
		C	6.0	5.2216986052	2.0348331078	-1.2992511682
		C	6.0	-1.7944262333	1.7755848747	-1.8063724866

H	1.0	0.6930363233	3.9407639927	-1.6885260207
O	8.0	3.0584766583	2.3792596795	-0.2689471652
H	1.0	5.0730754704	1.2415452087	-3.3011757848
C	6.0	4.4358610796	2.1085294608	0.0291126374
C	6.0	3.0971470462	1.3569559493	-2.4633530431
O	8.0	6.5709791152	1.6934106606	-0.9442895244
H	1.0	9.0242173723	1.1445552875	-0.5469622057
H	1.0	-2.0770420224	2.7837985731	-1.5015693119
O	8.0	1.0929539363	1.8123041617	-1.2907562030
H	1.0	-0.8225704014	0.0255034061	-1.0520235420
C	6.0	4.5935417352	1.0663013785	-2.3258873248
H	1.0	-5.3048517500	-0.4315925252	-0.8185970506
H	1.0	8.9235026818	2.8885692812	-0.8129008810
H	1.0	-0.0980921884	5.5134019879	-1.4609335474
C	6.0	2.4165603186	1.4109239078	-1.1031404699
H	1.0	-7.5962495883	0.6271135741	-0.5750313240
H	1.0	2.6366369690	0.5858647527	-3.0873172628
O	8.0	-3.3738628754	-5.4018327992	-0.2291039883
H	1.0	-4.7061964556	-3.3645149142	-0.2790356482
C	6.0	0.3886964901	4.6767971548	-0.9497510732
H	1.0	-2.6350484143	-6.8651640384	-0.2984192079
C	6.0	-1.0880087876	1.0212032268	-0.6792281141
C	6.0	-6.8135640749	-1.8109287706	-0.2870577717
O	8.0	-1.9579082440	-7.4989037097	0.0702392203
O	8.0	-7.0461637990	1.2138792569	-0.0351730474
H	1.0	1.3020377315	5.0586807308	-0.4567512026
C	6.0	-5.7047780251	-0.8426050570	0.1173333492
C	6.0	0.2219316941	1.6571352200	-0.1636793262
C	6.0	4.6234402630	0.9114657145	0.9659291946
H	1.0	5.6654270384	0.8608270761	1.2904065620
H	1.0	3.9898059454	1.0462135953	1.8475731514
H	1.0	2.4459466716	0.4269414989	-0.6106623226
C	6.0	-4.1987557796	-2.8371511325	0.5168890759
H	1.0	-4.5644511471	1.5090898029	0.3106571889
N	7.0	-0.5590278605	4.0888767985	0.0031885195
O	8.0	-7.0654046156	-2.8910804893	0.1935491411
O	8.0	4.7540682371	-0.2906606231	-1.9479663584
C	6.0	-2.8097689825	-4.8669162513	0.7496636686
H	1.0	0.6733135183	0.9191588008	0.5137470510
H	1.0	5.7125332742	-0.4473098776	-1.9419791066
O	8.0	-1.9511450599	0.7454966914	0.4368390874
C	6.0	-4.5689065392	-1.5255660781	0.8750837243
C	6.0	-6.2939873598	0.4099507438	0.8687010471
C	6.0	-1.3949617537	-6.8668119113	1.1046465464

		H	1.0	-8.6988007179	-1.3060599725	1.4063180467
		H	1.0	4.3801686875	-0.0352002733	0.4820093012
		H	1.0	-1.3357590567	6.0015536518	0.3074271005
		C	6.0	0.0051657106	2.9196541820	0.7158819076
		C	6.0	-3.1823653615	-3.5008517814	1.1803524579
		H	1.0	-2.7907868109	2.6056953052	0.7631559392
		H	1.0	-0.1152233049	-8.5471676841	1.5087256630
		C	6.0	-5.0891436812	1.2786118090	1.2410506344
		C	6.0	-1.7661082995	-5.5668169634	1.4961380100
		H	1.0	-9.1086114401	0.4229662870	1.2941678088
		C	6.0	-1.0261745699	5.1407831432	0.9067744978
		C	6.0	-0.3840120198	-7.5462414087	1.8292206802
		H	1.0	0.9855961501	3.1808334961	1.1533390855
		C	6.0	-2.2163032548	1.8417756075	1.3085038368
		C	6.0	-8.5961347410	-0.3339433542	1.8944271752
		H	1.0	-5.4505913394	2.2239980679	1.6571137308
		C	6.0	-3.8616406917	-0.8506970956	1.8753872846
		C	6.0	-7.1331064921	0.0615007864	2.1303334936
		H	1.0	-1.8954389238	4.8211920753	1.4851484473
		H	1.0	-0.2487694057	5.4891318203	1.6138791703
		C	6.0	-0.9176285818	2.4304217922	1.8524925390
		C	6.0	-2.5236779515	-2.8843956324	2.2735367093
		C	6.0	-4.1339946303	0.6095240455	2.2281496446
		C	6.0	-1.1251368620	-4.9470990348	2.6129566140
		H	1.0	-6.6247477088	-0.7254816194	2.6994501204
		H	1.0	-9.1170578752	-0.4052026969	2.8540841062
		C	6.0	-2.8844283673	-1.5609862990	2.6266105057
		H	1.0	-0.4162499922	1.6317808099	2.4082293812
		C	6.0	0.2323541745	-6.9509291033	2.9042528938
		O	8.0	-2.9312478501	1.3711113443	2.4173663767
		H	1.0	-7.1275420761	0.9567775544	2.7639508764
		C	6.0	-1.4997844244	-3.5986262475	3.0229778745
		H	1.0	-1.1410699455	3.2181529809	2.5732420985
		C	6.0	-0.1244400552	-5.6437030685	3.3185053433
		H	1.0	1.0064304441	-7.4641024746	3.4648709507
		H	1.0	-4.5747628023	0.6267517287	3.2319247642
		O	8.0	-0.9335377545	-3.0568732982	4.0230222693
		O	8.0	-2.3355427241	-0.9519823063	3.6800396622
		H	1.0	-1.6869895442	-1.5918966901	4.0731596979
		O	8.0	0.5210492877	-5.1337470194	4.3752974680
		H	1.0	0.1442360850	-4.2281915552	4.5211614663

N-(1-Cyano-2-methoxyethyl) doxorubicin	NSC 639659	H	1.0	1.8992085013	-3.4299937713	-7.0592418538
		O	8.0	1.7242968667	-4.3228912438	-6.7128703673
		H	1.0	0.1945471498	-4.4996197113	-5.3099133926
		C	6.0	1.2248424157	-4.1260161431	-5.4184704050
		O	8.0	1.5898292705	-1.8266903381	-5.8695597145
		C	6.0	1.2222935221	-2.6549160945	-5.0503569173
		H	1.0	1.8136531585	-4.6731819570	-4.6669892860
		H	1.0	0.0026083473	-0.4748577378	-4.6152334559
		H	1.0	2.5002407344	-0.9428051637	-3.4573756633
		C	6.0	0.7824196068	-2.2426686391	-3.6385668145
		H	1.0	-1.2274733476	-1.5312701433	-3.9508117992
		C	6.0	-0.2450283613	-1.0959452638	-3.7451498492
		H	1.0	2.7630985833	-2.5654340852	-2.7901596165
		C	6.0	2.0378726064	-1.7512049646	-2.8818237675
		O	8.0	-2.2846620537	0.7091648966	-3.5262410462
		H	1.0	-2.9654781054	1.4119694387	-3.3313680809
		O	8.0	0.2177898562	-3.3958788939	-3.0312484769
		C	6.0	-0.3378725785	-0.1904940551	-2.5403886902
		C	6.0	-1.4137779501	0.7457646937	-2.5128497085
		C	6.0	1.6932736894	-1.2455409617	-1.4830125219
		H	1.0	0.3669655520	-3.3334140770	-2.0728995833
		H	1.0	2.5885103646	-0.8315148712	-1.0097628190
		C	6.0	0.5867915366	-0.1991544470	-1.5060448988
		O	8.0	-3.5043729770	2.6075101151	-2.3469723116
		C	6.0	-1.5338389898	1.6628021235	-1.4561091787
		O	8.0	1.2524611000	-2.3975439345	-0.7188068007
		C	6.0	-2.6456210890	2.5986485312	-1.4402117338
		C	6.0	0.4831920335	0.7470511813	-0.4438506483
		C	6.0	-0.5706854038	1.6764612694	-0.4111258627
		H	1.0	-4.5216380474	4.4005667746	-1.1601376350
		H	1.0	-0.5689118790	-2.1807428496	1.1863859972
		O	8.0	1.4245286359	0.7375009401	0.5191756431
		H	1.0	0.0284251610	-3.8472578152	1.1269989013
		C	6.0	-2.7401539760	3.5731734280	-0.3203441332
		C	6.0	1.5199151333	-2.3960741035	0.6634428004
		C	6.0	-3.8098270823	4.4690320357	-0.3467871271
C	6.0	0.2784275407	-2.8251288078	1.4334908788		
H	1.0	1.8269144543	-1.3872156935	0.9513525729		
H	1.0	1.1643990002	1.5004993235	1.1321879063		
C	6.0	-0.6591939755	2.6280047926	0.7013990954		
C	6.0	-1.7724656403	3.6036729063	0.7152677776		
O	8.0	2.5849066664	-3.3037545773	0.8963907282		
N	7.0	-2.3601373018	-0.3664784646	2.2754845067		
O	8.0	0.2077810729	2.6040866831	1.6079746125		

		C	6.0	-3.9324058792	5.4200668657	0.6585671689
		H	1.0	-4.7624268295	6.1198862782	0.6499653027
		H	1.0	1.1050385957	-0.7862858428	2.8147900639
		C	6.0	-1.5644243266	-0.5675839216	3.0974399945
		C	6.0	0.5831527640	-2.7902346084	2.9404590086
		C	6.0	-1.9104862614	4.5957969338	1.7279201152
		H	1.0	-0.2271527562	-3.2724435926	3.4977694139
		C	6.0	-2.9928929891	5.4891514117	1.6828583895
		N	7.0	0.7170868437	-1.4245263006	3.5058354385
		C	6.0	3.0489430546	-3.3029629873	2.2608033724
		H	1.0	3.3187103941	-1.1279735943	2.5676309064
		H	1.0	1.6127519496	-4.6575994950	3.0966016256
		H	1.0	4.7109739574	-1.9798178687	1.8887504166
		O	8.0	-0.9784204736	4.6463330938	2.7063444136
		C	6.0	1.8718838558	-3.6010774520	3.2365996842
		H	1.0	3.7223729037	-4.1647139195	2.3068373634
		C	6.0	-0.4828483279	-0.8238563606	4.0849332746
		C	6.0	3.8838170317	-2.0634194814	2.5989632094
		H	1.0	-3.1070634078	6.2404501934	2.4533533827
		H	1.0	0.2137211762	1.2311553985	4.0414991910
		H	1.0	-0.9690554974	6.6912156536	3.1439668050
		H	1.0	-0.8823555304	-1.5075280984	4.8422549433
		C	6.0	-1.0171673370	5.7170207893	3.6442098328
		C	6.0	-0.1175688717	0.4931468616	4.7890749346
		O	8.0	2.2587712348	-3.4408848859	4.5867451120
		H	1.0	4.2968784550	-2.1690500035	3.6048379823
		H	1.0	-0.1324860050	5.5881752960	4.2681416195
		H	1.0	2.0609673877	-2.5075412179	4.7813368500
		H	1.0	-1.9137534741	5.6735532859	4.2740022934
		O	8.0	-1.2658692533	0.9417226465	5.4699077270
		H	1.0	0.7185447646	0.2960572471	5.4773671885
		H	1.0	-0.9947951281	2.9692774546	5.0848159221
		C	6.0	-1.1512059823	2.2773401837	5.9247725339
		H	1.0	-2.0886622895	2.5239751685	6.4276497693
		H	1.0	-0.3229919579	2.3950942304	6.6403893236
Cyanomorpholino doxorubicin	88254-07-3	H	1.0	-3.8281566150	4.2835384587	4.8247096228
		H	1.0	-5.3426700467	4.3295688437	3.8676906509
		C	6.0	-4.2506037533	4.2490935991	3.8140808784
		H	1.0	-3.8544532917	5.0788607328	3.2293917257
		H	1.0	-5.2777775670	2.5809230063	5.3254844946
		O	8.0	-3.8465973379	3.0719863182	3.1197750254
		C	6.0	-4.9156446884	1.7081898643	4.7978937448
		C	6.0	-4.1569241853	1.8636880492	3.6249788901

H	1.0	-5.7983970599	0.3489371694	6.1999459181
C	6.0	-5.2091539067	0.4416707350	5.2927292333
O	8.0	-2.6398582732	1.9027070366	1.1437001142
C	6.0	-3.6857859128	0.7098242631	2.9344984724
C	6.0	-2.8946017057	0.8029422443	1.6890613530
H	1.0	-1.8197510566	1.4950289029	-0.1013633695
C	6.0	-4.7508751251	-0.6974452979	4.6394533068
C	6.0	-3.9941144068	-0.5650586980	3.4747180458
O	8.0	-1.3103706302	0.8159729208	-0.6508440133
H	1.0	-4.9606882306	-1.6930240792	5.0106329193
H	1.0	5.8924515014	-0.3274572045	-0.9842794943
C	6.0	-2.3905073065	-0.4348420197	1.0846568998
C	6.0	-1.5888913102	-0.3596722999	-0.0655775142
C	6.0	-3.5105333216	-1.8162805081	2.8313574203
H	1.0	5.5363061212	-0.6597801520	0.7184002667
O	8.0	4.5985454231	1.9087158582	-1.2675071566
H	1.0	4.5401340906	1.3773367166	-2.0760347989
H	1.0	-0.4772020351	-0.5825342135	-2.4687235305
C	6.0	5.1866341058	-0.8133760848	-0.3067918999
C	6.0	-2.6835520295	-1.7109409923	1.6387754283
H	1.0	1.8721321403	-0.4916535390	-3.1532619406
H	1.0	5.1753903003	-1.8859672685	-0.5151439758
O	8.0	-3.8046384019	-2.9261046537	3.3227417876
C	6.0	-1.0498953277	-1.5412847757	-0.6477139456
C	6.0	-0.1141823508	-1.3932340710	-1.8276760050
C	6.0	-2.1756065237	-2.8752228972	1.0384162934
H	1.0	-0.9118141181	-2.8733447831	-3.1839969475
C	6.0	3.7204034445	1.2952194484	-0.3217976965
C	6.0	2.0253474732	-0.2113128433	-2.1035826745
C	6.0	3.7917081562	-0.2335864457	-0.4685592355
H	1.0	2.2805746515	1.8454588101	-2.6661999880
H	1.0	4.0706695568	1.5994943931	0.6698145563
C	6.0	-1.3361066251	-2.7870428754	-0.1119197253
H	1.0	2.0360022592	5.8335035370	-2.2365200462
H	1.0	-3.0244519155	-3.9610070143	2.3119193889
O	8.0	1.1687124009	-1.0075310282	-1.2664602484
O	8.0	3.3524939650	-0.5722479725	-1.8138463500
C	6.0	0.0193251659	-2.6842210701	-2.6398078054
O	8.0	-2.4417439438	-4.0964247709	1.5135311841
O	8.0	0.4550862175	5.3485278137	-1.0645580209
C	6.0	1.7558706805	1.2840632963	-1.8846635833
N	7.0	2.0153645217	3.1277462769	-0.1256024906
H	1.0	0.8158813502	-2.5700763474	-3.3834515561
H	1.0	-1.6623176177	-4.5863870685	-1.2072764782

		H	1.0	3.1097792442	-0.7002404788	0.2522014679
		C	6.0	2.2445886632	1.7335623282	-0.4876122458
		C	6.0	0.7396672506	3.4774133810	0.4919074892
		C	6.0	1.6043457140	4.9277574224	-1.8002083189
		H	1.0	-1.0672600894	4.6378446613	0.0697231081
		C	6.0	-0.8273027165	-4.0736180042	-0.7134093866
		C	6.0	-0.1992815462	4.2472485497	-0.4680087502
		H	1.0	2.9896001184	4.9793596705	-0.1686274349
		C	6.0	2.6115848796	4.2342836341	-0.8829458477
		H	1.0	0.6865676798	1.4762574115	-1.9945058644
		C	6.0	0.3202048519	-3.8945395748	-1.7281387051
		H	1.0	1.2936812939	4.2593200220	-2.6206843686
		H	1.0	0.2225776502	2.5606160064	0.7926227722
		H	1.0	1.6824877764	1.1465475118	0.2475712626
		O	8.0	-0.5842273018	-5.5912071184	-3.1756806862
		H	1.0	-0.4881431077	-4.7394991215	0.0855114147
		H	1.0	1.7500440748	-2.8020819745	-0.9700291968
		H	1.0	-0.5489426067	3.5396343582	-1.2376513165
		C	6.0	0.4042461316	-5.1441174514	-2.6144369925
		O	8.0	1.5741798046	-3.7527135491	-1.0754336868
		H	1.0	3.4677200538	3.8570942268	-1.4426204467
		C	6.0	1.7497892937	-5.8140405530	-2.8139703402
		H	1.0	0.7083450359	-6.9542274502	-3.9318857086
		H	1.0	2.4674283385	-5.0568432234	-3.1644834961
		O	8.0	1.6532267008	-6.8890988197	-3.7067007505
		H	1.0	2.1186639548	-6.1276378440	-1.8245616383
		C	6.0	0.9724745760	4.2673905407	1.7285636031
		N	7.0	1.1495487552	4.8747741606	2.7018653047
		H	1.0	5.8146283887	2.2219171277	-0.2328913815
		H	1.0	4.9089211062	3.0294388671	1.0426054788
		H	1.0	4.3686097310	3.1542974577	-0.6452952071
		C	6.0	4.8046056857	2.4833349680	0.1062882112
		H	1.0	4.9307269146	1.3477508706	-1.9769413531
		O	8.0	4.9126450275	0.1021559015	-3.9063001400
		N	7.0	4.4361874521	0.4839868226	-1.7700525325
		C	6.0	3.9600522021	1.2453748012	0.3086319894
		C	6.0	4.3607323350	-0.3243241854	-2.8962858774
		H	1.0	4.9082062713	0.5139503402	2.6019170382
		O	8.0	4.2870413703	1.2521948006	2.6840561382
		H	1.0	2.7357495978	3.1921084021	1.8516891517
		N	7.0	3.8069767477	0.3178600419	-0.5723155856
		C	6.0	3.2797960402	1.0865603295	1.6711737607
		H	1.0	3.2516161599	-1.9076861550	-0.7956704631
Daunomycin 3,4-dichlorobenzoyl hydrazone	66996-54-1	H	1.0	5.8146283887	2.2219171277	-0.2328913815
		H	1.0	4.9089211062	3.0294388671	1.0426054788
		H	1.0	4.3686097310	3.1542974577	-0.6452952071
		C	6.0	4.8046056857	2.4833349680	0.1062882112
		H	1.0	4.9307269146	1.3477508706	-1.9769413531
		O	8.0	4.9126450275	0.1021559015	-3.9063001400
		N	7.0	4.4361874521	0.4839868226	-1.7700525325
		C	6.0	3.9600522021	1.2453748012	0.3086319894
		C	6.0	4.3607323350	-0.3243241854	-2.8962858774
		H	1.0	4.9082062713	0.5139503402	2.6019170382
		O	8.0	4.2870413703	1.2521948006	2.6840561382
		H	1.0	2.7357495978	3.1921084021	1.8516891517
		N	7.0	3.8069767477	0.3178600419	-0.5723155856
		C	6.0	3.2797960402	1.0865603295	1.6711737607
		H	1.0	3.2516161599	-1.9076861550	-0.7956704631

C	6.0	2.2682780976	2.2079809613	1.9401978034
C	6.0	3.6602952027	-1.6498484563	-2.8997182959
H	1.0	1.2071749848	2.6778269454	0.1042810196
C	6.0	3.1675498413	-2.3371962265	-1.7822361613
H	1.0	1.9764078187	2.0996041262	2.9898302257
H	1.0	3.9292065796	-1.7077174817	-5.0271622380
C	6.0	1.0109913266	2.1679321528	1.0540847322
C	6.0	3.5352712695	-2.2357385311	-4.1677753669
H	1.0	3.2018923878	-1.0892258598	1.5811807584
C	6.0	2.5618645977	-0.2537052904	1.8765325705
H	1.0	0.1312351625	4.0659713757	4.0062095325
O	8.0	0.0080557617	3.0013570614	1.6625128793
H	1.0	-1.3242814772	6.0844301179	4.7653494718
H	1.0	2.3999098021	-0.3590831338	2.9568055680
C	6.0	2.5553500242	-3.5773932576	-1.9392510467
H	1.0	-1.4477229794	5.2032995105	2.4728061652
H	1.0	2.1602038540	-4.1024485217	-1.0780760726
C	6.0	0.5416175009	0.7585966778	0.7191144433
C	6.0	2.9225070462	-3.4729711314	-4.3268583279
C	6.0	1.2471305266	-0.3588426518	1.1406881629
C	6.0	-0.8492538420	3.6192230500	3.8098313688
N	7.0	-2.1770882443	5.7080866339	4.3574974341
C	6.0	2.4253702542	-4.1516765032	-3.2043002656
C	6.0	-1.8595442036	4.6950563388	3.3540065359
O	8.0	-1.1617523876	1.7035880088	-0.6249214387
C	6.0	-0.6965366744	2.4918765458	2.7821687616
H	1.0	-0.1666569469	1.6362643860	3.2170928824
CL	17.0	2.7906163727	-4.1483452520	-5.9342528650
C	6.0	-0.6084276925	0.6024891891	-0.1146627959
H	1.0	-2.3528699664	3.4326114151	0.9967458866
H	1.0	-1.2040653258	3.1799794019	4.7504114356
C	6.0	0.7468517693	-1.6596787330	0.8549666065
H	1.0	-1.9370109602	1.3774983961	-1.1744075531
H	1.0	-2.6968432046	5.2566198321	5.1081969830
CL	17.0	1.6425914174	-5.7043132080	-3.3508674142
O	8.0	1.4438294389	-2.7097596342	1.3194560330
O	8.0	-1.9613532836	1.9644801485	2.4101147689
C	6.0	-3.1622452485	3.9993883986	2.9194736122
C	6.0	-1.1101138390	-0.6810453162	-0.4007107369
C	6.0	-2.8593241435	2.9516364976	1.8403553452
H	1.0	-3.8566878461	4.7540762859	2.5352823183
C	6.0	-0.4273293790	-1.8212096166	0.1046150217
H	1.0	0.9183637540	-3.5180835685	1.0499587427
O	8.0	-2.8636548238	0.2050577246	-1.6937439277

		C 6.0 -2.3086855122 -0.8172679373 -1.2331049319 O 8.0 -3.8099189595 3.3954609338 4.0443114190 H 1.0 -3.3941020248 2.5264443740 4.1510947695 C 6.0 -0.9178768225 -3.1590348566 -0.1770412467 H 1.0 -3.8104130712 1.4659754018 0.5938782224 C 6.0 -4.0883315987 2.2049593943 1.3479543215 H 1.0 -4.7927971292 2.9099064670 0.8952729058 O 8.0 -0.3198513567 -4.1745958871 0.2477254570 C 6.0 -2.8341959648 -2.1783365058 -1.5017952919 C 6.0 -2.1502361886 -3.3098311458 -0.9906415285 H 1.0 -4.5976634967 1.7023183034 2.1740095484 O 8.0 -4.6653111985 -1.3269368363 -2.7556722248 C 6.0 -4.0109517750 -2.4019087832 -2.2724017082 C 6.0 -2.6028216537 -4.6087057142 -1.2318018357 H 1.0 -6.1762137214 -0.5118939078 -3.7981113911 H 1.0 -2.0396920293 -5.4379654356 -0.8219960885 H 1.0 -5.6385854230 -2.0848686854 -4.4450276399 C 6.0 -5.8434250758 -1.5148260275 -3.5310060053 C 6.0 -4.4516460855 -3.7160787998 -2.5025358936 C 6.0 -3.7523175041 -4.8035351420 -1.9876741674 H 1.0 -5.3449816549 -3.8909275131 -3.0879293116 H 1.0 -6.6303200074 -2.0169546509 -2.9555321989 H 1.0 -4.1132434914 -5.8088204480 -2.1824724819
Daunomycin 4-nitrobenzoylhydrazone	66996-56-3	H 1.0 5.4908286068 2.2622406386 -0.6868782380 H 1.0 3.9813489074 3.1806136401 -0.7923204181 H 1.0 4.7636028729 2.9221820912 0.7800266940 C 6.0 4.5387574635 2.4591671108 -0.1804213267 H 1.0 4.4088978016 1.4043847682 -2.4177132744 O 8.0 4.1253905193 -0.0098413429 -4.3157981476 H 1.0 2.6488307502 3.0012929988 1.8091875565 N 7.0 4.1229575932 0.4757272670 -2.1168219687 H 1.0 -4.9036458963 2.7785607982 1.0535205130 H 1.0 -2.4648579651 3.2995933220 1.1523968717 C 6.0 3.9306866569 -0.4027431643 -3.1733183509 H 1.0 1.0519133120 2.6533221419 0.0849054221 H 1.0 -3.9266642643 1.3738335413 0.5916926071 C 6.0 3.7641761670 1.1786514243 0.0245285419 H 1.0 -3.9362810897 4.4515734988 2.8526320268 N 7.0 3.6000849214 0.2705789381 -0.8696118311 H 1.0 -1.5326251888 4.9216042977 2.7674309730 C 6.0 -4.1888675679 2.0349744334 1.4200374655 C 6.0 2.1796617710 2.0139948581 1.8260768060 C 6.0 -2.9502343377 2.7345359403 1.9552518457

H	1.0	2.5444986218	-1.9629940894	-4.7786563316
O	8.0	-0.0934882309	2.8194316931	1.7060087076
C	6.0	0.8900357489	2.0532840383	0.9875429038
O	8.0	4.2385724120	1.0066883699	2.3698169077
C	6.0	3.5215588863	-1.8129944013	-2.8773565757
C	6.0	3.1705883500	0.9193660624	1.4137862908
C	6.0	-3.2279318119	3.6673989896	3.1404854602
H	1.0	1.9283542559	1.8100116467	2.8718240254
C	6.0	2.7900308325	-2.4906574487	-3.8635133744
H	1.0	4.8274280490	0.2529008316	2.2188284753
N	7.0	-2.2120244260	5.2351755318	4.7108041375
C	6.0	-1.9169908481	4.3261012207	3.6054602015
H	1.0	-4.6792894927	1.4526527254	2.2041878657
O	8.0	-1.3124888732	1.7564752112	-0.6797855817
H	1.0	4.4798374856	-2.0143528037	-0.9410359993
H	1.0	-1.3498389557	5.5789816371	5.1278177328
H	1.0	-2.7045992291	4.7082109697	5.4299614427
H	1.0	-2.0957607123	1.4874000571	-1.2488267343
O	8.0	-2.0352799339	1.7004868624	2.4030680883
C	6.0	3.8906321923	-2.4869559892	-1.7109140067
C	6.0	-0.7617222404	2.1975667733	2.7903020867
C	6.0	0.4124094867	0.6803124257	0.5318560973
O	8.0	-3.8403484489	2.9501282116	4.2173773138
C	6.0	2.3843774476	-3.8100088916	-3.6650371005
C	6.0	-0.7506494089	0.6087987548	-0.2954590972
C	6.0	-0.8898283007	3.2189908313	3.9268722782
H	1.0	0.0939300194	3.6520364245	4.1368412071
H	1.0	1.8038823686	-4.3195278727	-4.4269776278
C	6.0	2.4525068266	-0.4322663099	1.5485084817
H	1.0	-3.4204783866	2.0764609532	4.2229211255
O	8.0	3.4154375038	-5.6279351188	-0.1155975180
C	6.0	3.4798118567	-3.8028931173	-1.5380858899
H	1.0	-0.2153528085	1.3068483393	3.1217935319
H	1.0	3.0767528044	-1.2532693194	1.1877016172
C	6.0	1.1246165353	-0.4723627081	0.8285191556
O	8.0	-3.0257008008	0.3763826735	-1.8781403250
C	6.0	2.7192473740	-4.4797621906	-2.4890936251
H	1.0	2.3082632549	-0.6042818720	2.6228820898
H	1.0	-1.2146830623	2.6883033346	4.8303046505
N	7.0	3.8546706367	-4.4928316625	-0.2928991429
C	6.0	-1.2526934416	-0.6384074531	-0.7110476464
C	6.0	-2.4625913102	-0.6874140237	-1.5347633291
H	1.0	2.4081123922	-5.4987359323	-2.2976638605
H	1.0	-6.3854750621	-0.1231680249	-3.9722588851

		C 6.0 0.6214615495 -1.7401291305 0.4156432358 O 8.0 4.5860496532 -3.8949191514 0.4965968375 C 6.0 -0.5621976581 -1.8240823850 -0.3342002288 O 8.0 -4.8470239441 -1.0384314464 -3.0620359197 H 1.0 -5.8698726175 -1.6214026261 -4.7912682070 C 6.0 -6.0468887901 -1.1477033885 -3.8181810764 O 8.0 1.3145124202 -2.8299090088 0.7718212900 C 6.0 -2.9934306170 -2.0137660261 -1.9367145213 C 6.0 -4.1856491557 -2.1576337973 -2.7032958513 C 6.0 -1.0520630512 -3.1251542840 -0.7541497802 H 1.0 0.8076652373 -3.6091322807 0.4031801263 H 1.0 -6.8179880420 -1.7068256235 -3.2747405705 C 6.0 -2.3017617602 -3.1904745612 -1.5568467702 O 8.0 -0.4476056563 -4.1794946445 -0.4566917316 C 6.0 -4.6337637906 -3.4410016898 -3.0572405007 H 1.0 -5.5391446909 -3.5556397278 -3.6391277417 C 6.0 -2.7628236344 -4.4582410366 -1.9189321221 C 6.0 -3.9272579147 -4.5754360620 -2.6674312937 H 1.0 -2.1958419244 -5.3247420842 -1.6014732725 H 1.0 -4.2960386362 -5.5559151892 -2.9533569756
Daunomycin 3-oxime	34610-60-1	H 1.0 -7.5411482061 2.1703858771 -3.6790894865 H 1.0 -6.7927443540 3.5463663287 -2.8254463611 C 6.0 -7.1169085661 2.5104413258 -2.7268283743 H 1.0 -8.1456486318 0.2703356866 -2.5743821244 O 8.0 -5.9452002998 1.7794446571 -2.3844213313 C 6.0 -7.2362726599 -0.2574158683 -2.3180471139 C 6.0 -6.0272307543 0.4470249049 -2.1945074307 H 1.0 -8.2300782399 -2.1542650912 -2.2150861193 C 6.0 -7.2827172199 -1.6334098648 -2.1142999509 O 8.0 -3.4040335573 1.6628374613 -1.8712805027 H 1.0 -7.8798942041 2.4419310708 -1.9422027207 C 6.0 -4.8341533300 -0.2545797116 -1.8576307034 H 1.0 2.6827539568 -1.0160524961 -1.8511841879 H 1.0 -1.8626184754 1.9163847423 -1.6137381464 C 6.0 -3.5268104244 0.4296031342 -1.7098881053 C 6.0 -6.1306571153 -2.3377056986 -1.7856147465 H 1.0 1.4401479257 1.0095573101 -1.4748106053 C 6.0 -4.9190719776 -1.6553467938 -1.6592855618 O 8.0 -0.9463450204 1.5729610317 -1.3819104113 H 1.0 -6.1409785616 -3.4083973585 -1.6229919129 C 6.0 -2.3508010076 -0.3770274328 -1.3626634742 C 6.0 -1.1040811858 0.2532033250 -1.2167592444 H 1.0 1.4186613900 -3.3389364986 -1.2319814331

C	6.0	-3.7187765014	-2.4619844603	-1.3095026810
C	6.0	-2.4400607956	-1.7842143521	-1.1686170148
O	8.0	-3.8248137515	-3.6959381639	-1.1441701550
C	6.0	0.0527332689	-0.5124556001	-0.8910941708
C	6.0	1.3616139727	0.2260437815	-0.7148815927
C	6.0	-1.2943154202	-2.5283273273	-0.8382202882
C	6.0	2.5790984314	-0.6991385781	-0.8079236035
C	6.0	-0.0329198944	-1.8800352093	-0.6910026131
H	1.0	-2.2821381864	-4.1228298249	-0.7860439859
O	8.0	-1.3311385442	-3.8522494684	-0.6522308049
H	1.0	3.4754753571	-0.1340109465	-0.5428923556
C	6.0	1.1689194493	-2.7306933665	-0.3517460479
H	1.0	3.9018923884	-3.1127514158	-2.0918651550
H	1.0	1.2949819865	2.7464347712	-0.2344984952
C	6.0	3.6249601516	-2.8890921885	0.0481494093
H	1.0	5.5454476698	1.4892533024	0.3642540645
C	6.0	2.4204984339	-1.9358217213	0.0938126705
H	1.0	5.2301217089	-3.7126680222	-1.0776477719
H	1.0	0.9114971659	-3.4499867950	0.4304679520
C	6.0	4.4914302182	-2.9176564877	-1.1866166228
O	8.0	1.2826342271	0.8679438187	0.5866994213
O	8.0	3.1027350926	2.3670905623	0.5345738056
C	6.0	1.6962077387	2.2295636041	0.6436297523
N	7.0	3.9291799602	-3.7664594004	0.9386033267
H	1.0	5.6080875229	3.0449499775	1.2202796667
C	6.0	5.3288553952	1.9924631452	1.3102772236
H	1.0	5.0180572578	-1.9692273233	-1.3426787876
H	1.0	1.7478934661	-0.6843186572	1.4837251524
C	6.0	3.8573261606	1.8508969288	1.6647305396
H	1.0	3.6098463857	0.7911169964	1.8039139392
O	8.0	2.2810555647	-1.4997846682	1.4618743433
H	1.0	5.9454421354	1.5404066109	2.0927382815
C	6.0	1.1475483598	2.8370690449	1.9364353410
H	1.0	1.2005186775	3.9279262318	1.8379229245
H	1.0	3.5625533116	4.2446346551	1.8582542124
H	1.0	0.0903303319	2.5710455595	2.0311969137
O	8.0	3.1725003153	-3.8576282503	2.0949170603
H	1.0	2.6480420273	-3.0336624487	2.1859919272
C	6.0	3.4446988215	2.6274153693	2.9206945479
O	8.0	3.7467512619	4.0181221140	2.7823237717
C	6.0	1.9439639529	2.4208510142	3.1922286531
H	1.0	1.7874563927	1.3488245698	3.3726217244
H	1.0	4.0134829396	2.2747474386	3.7873405344
H	1.0	1.8642199553	4.1082955612	4.3082558775

		N	7.0	1.5830078005	3.1351463838	4.4129205445
		H	1.0	0.5752029255	3.1229232028	4.5504577328
Daunorubicin / Daunomycin	20830-81-3 / 23541-50-6	H	1.0	-0.9428939383	6.5012132365	2.3004151205
		O	8.0	-0.1569866796	4.8214284458	0.5952610197
		H	1.0	-2.6426611920	6.1179461781	1.8793821135
		C	6.0	-1.6844629576	5.7070506936	2.2113024881
		H	1.0	-1.3499749952	3.5839659295	-1.0115572443
		C	6.0	-1.1948801366	4.6764075451	1.2121102538
		H	1.0	-1.8538619870	5.2577731654	3.1972041399
		H	1.0	-3.0585077224	3.1180265680	-0.8556407486
		C	6.0	-2.0538688767	2.9585878840	-0.4572730316
		C	6.0	-2.0546478169	3.3985273561	1.0267985435
		O	8.0	2.9265282829	-0.7313891178	-1.7378416030
		H	1.0	-1.5366962029	1.3232688075	-1.7674363754
		H	1.0	1.4539497611	-0.2663608955	-2.1268736819
		O	8.0	-3.4121341594	3.6521929157	1.3967334502
		C	6.0	3.0389115401	-0.3704647131	-0.5472637682
		C	6.0	-1.6534627186	1.4992241575	-0.6969222479
		O	8.0	0.5853498919	0.1689042718	-1.8787812323
		C	6.0	0.7320700653	0.5431018034	-0.6017945903
		C	6.0	1.9217930411	0.3096985457	0.1179192812
		C	6.0	-0.3577976361	1.1961767979	0.0332414217
		H	1.0	7.3337348546	-1.6953317404	-2.2393643320
		O	8.0	3.3359581177	0.8796622085	3.4237399784
		C	6.0	2.0123650536	0.7370178711	1.4732458562
		H	1.0	-3.4817055048	3.6155780232	2.3601326723
		C	6.0	-0.2631306207	1.6146013074	1.3502647707
		C	6.0	3.2292841806	0.5110600128	2.2328506655
		C	6.0	0.9256179518	1.3880300676	2.0892083207
		C	6.0	4.2845414854	-0.6104214882	0.2246772041
		H	1.0	-1.1893182230	2.7206435670	2.9380887365
		C	6.0	-1.4514380555	2.3043212240	1.9613936924
		H	1.0	1.8825962314	1.5630869549	3.6928562962
		C	6.0	4.3694450654	-0.1768645365	1.5701545735
		O	8.0	0.9718472159	1.8045318550	3.3617822615
O	8.0	5.3354694104	-1.6823161066	-1.6196976213		
C	6.0	5.4164843309	-1.2662134732	-0.3387702689		
H	1.0	6.1383011435	-2.5721063500	-3.2309565305		
C	6.0	6.4477390656	-2.3411699224	-2.2115670487		
C	6.0	5.5230564647	-0.3786152867	2.3313739094		
H	1.0	5.5344074936	-0.0265435183	3.3554852054		
C	6.0	6.5675718351	-1.4602820387	0.4421908021		
O	8.0	-2.7245189029	0.6669660535	-0.2020483377		

		C 6.0 6.6160892357 -1.0191315972 1.7617212862 H 1.0 7.4305753651 -1.9573202656 0.0185905190 H 1.0 -2.2512744978 1.5694997997 2.1038811205 H 1.0 7.5187025341 -1.1804166782 2.3434797279 O 8.0 -3.1400942953 -0.4992771678 -2.1113627051 H 1.0 6.6925875627 -3.2728288712 -1.6870992598 H 1.0 -3.6520970328 -1.4378116493 -3.7970475721 C 6.0 -2.7569555585 -0.6255060481 -0.7411388519 H 1.0 -1.1949791072 -1.6122480372 -3.5569964932 H 1.0 -1.7700335543 -1.1032033133 -0.6767740303 C 6.0 -3.2184998668 -1.7356195813 -2.8319820225 H 1.0 -4.7345960795 -0.8613374405 0.0087324197 C 6.0 -1.8509307710 -2.3648416286 -3.1114133210 C 6.0 -3.7992518063 -1.4315568069 0.0227472304 H 1.0 -5.2276438606 -2.1387298845 -2.2205630286 H 1.0 -3.4922098392 -1.5406005623 1.0692718167 H 1.0 -1.3900212679 -2.7584380043 -2.2053629462 C 6.0 -4.2543647812 -2.6451531955 -2.1250228038 H 1.0 -1.9601842139 -3.1953000428 -3.8157764813 C 6.0 -4.0053890870 -2.8144722218 -0.6167516169 H 1.0 -4.5056203629 -3.8671870301 -3.6343753302 O 8.0 -4.3207758789 -3.9537072160 -2.6902646572 H 1.0 -4.9259424569 -3.2587432608 -0.1997720886 N 7.0 -2.8260442148 -3.6584052807 -0.3850942741 H 1.0 -2.7904193222 -3.9307192289 0.5943332553 H 1.0 -2.9287040707 -4.5117190620 -0.9293632225
4-Demethoxyadriamycin / Medorubicin	64363-63-9	H 1.0 2.3679665419 4.1239917310 -7.3585782794 H 1.0 0.8830197837 2.1746833423 -6.8678341138 C 6.0 2.3519709802 3.6849771179 -6.3657238228 C 6.0 1.5216697972 2.5995617858 -6.1014642279 O 8.0 -0.1090304691 0.4079846825 -5.4683611314 H 1.0 3.8128922790 5.0569430343 -5.5655379389 C 6.0 3.1659996258 4.2106759198 -5.3554445670 H 1.0 -0.8682524114 -0.8259705162 -4.6991467710 C 6.0 1.4974633245 2.0295022332 -4.8231024347 C 6.0 0.6100429997 0.8712480400 -4.5581559214 O 8.0 -1.0104287374 -1.3547971829 -3.8649239952 C 6.0 3.1488516267 3.6513658007 -4.0809426875 C 6.0 2.3170339651 2.5598305304 -3.8049793370 C 6.0 0.6058809602 0.2970587868 -3.2148657970 H 1.0 3.7700601857 4.0410274136 -3.2822106701 C 6.0 -0.2195008359 -0.8037095695 -2.9380271399 C 6.0 2.3085756633 1.9750383646 -2.4425753468

H	1.0	-2.1107142977	-2.3915927760	-1.8681130071
C	6.0	1.4342449989	0.8369660949	-2.1858430857
H	1.0	-0.7077150386	-3.4389815759	-1.9530238056
C	6.0	-0.2414097171	-1.3841154057	-1.6323796222
C	6.0	-1.1329071034	-2.5819707869	-1.4156884148
O	8.0	3.0370882168	2.4547610341	-1.5467118019
C	6.0	1.4071478912	0.2619951322	-0.9051426382
O	8.0	-1.1922075731	-5.3168614830	-0.4392495048
C	6.0	0.5644147948	-0.8553992611	-0.6374350082
C	6.0	-1.3387150600	-2.9677139811	0.0632825727
C	6.0	-1.7994122991	-4.4288605521	0.1394261883
O	8.0	-2.3466807726	-2.1742023622	0.6733851080
O	8.0	2.1682592489	0.7237724517	0.0942814136
H	1.0	2.6853189451	1.4928123761	-0.2828533864
H	1.0	-1.9128216065	-1.4120683882	1.0954884776
H	1.0	0.7277793176	-3.5333895090	0.3577076152
C	6.0	0.5469723800	-1.4183819006	0.7671429344
C	6.0	0.0049469754	-2.8503217186	0.8157278523
H	1.0	-3.8725664662	-4.2101321315	0.5707990592
H	1.0	1.5657215078	-1.3904815460	1.1691002593
C	6.0	-3.0166890516	-4.7726771883	0.9757424675
O	8.0	-0.2886751687	-0.5259882809	1.5455953350
H	1.0	-2.5686180798	-6.5349014683	0.4044921656
H	1.0	-2.8641857142	-4.3772763562	1.9915028578
H	1.0	-0.1234437788	-3.1624871177	1.8577806163
H	1.0	-1.8865101774	1.2258573424	2.2412075381
O	8.0	-3.2507666388	-6.1539143911	0.9853707946
H	1.0	0.4327043600	2.1921433236	2.0748050313
H	1.0	-3.7807891386	0.3364128040	3.6174879940
C	6.0	-0.0230317293	-0.4822024649	2.9603922983
C	6.0	-1.7863247757	1.1063045114	3.3273271980
H	1.0	0.2677143257	-1.4827610684	3.3039775380
H	1.0	1.9426231855	0.3899429073	2.6687631761
O	8.0	-1.2424071912	-0.2120284745	3.6031912525
H	1.0	-3.6506247187	2.1034736199	3.7434122866
C	6.0	0.5734968971	1.9923792651	3.1438617141
C	6.0	-3.1569572125	1.1564350875	3.9817053021
H	1.0	-1.1892708432	3.1578381930	3.6566934786
C	6.0	1.0620616501	0.5433764549	3.2961657872
C	6.0	-0.7940247397	2.1522436171	3.8493952943
H	1.0	1.3820507901	3.8545453976	3.3682848521
N	7.0	1.6071757807	2.8999116772	3.6427663598
H	1.0	-3.0715779987	1.0809429523	5.0682581201
H	1.0	1.3727332020	0.3739159663	4.3351552862

		H	1.0	1.5588008470	2.8883158536	4.6616681479
		O	8.0	-0.6432836505	2.0540748617	5.2669312249
		H	1.0	-0.6372974996	1.1078878801	5.4757079530
N,N-dibenzyldaunorubicin	70878-51-2	H	1.0	6.0613902494	-0.3502483281	-7.3524045694
		H	1.0	5.2509529449	2.2494894797	-1.2064298550
		C	6.0	5.1082321459	-0.4184108915	-6.8359735784
		H	1.0	4.9314161324	1.7115842223	-6.5425344841
		H	1.0	4.9971143134	-2.5657013016	-6.9812175631
		C	6.0	4.4733932393	0.7402613128	-6.3773523466
		C	6.0	4.5961581147	1.4346058863	-0.9093421241
		C	6.0	4.5107454609	-1.6605277290	-6.6286691152
		H	1.0	5.1801839886	1.5143418276	1.1664646950
		H	1.0	3.8067076086	1.1448549271	-2.8962248483
		C	6.0	4.5608392318	1.0187615825	0.4240862855
		C	6.0	3.7889921398	0.8146543298	-1.8626063790
		C	6.0	3.2509862025	0.6536851513	-5.7150032917
		C	6.0	3.2839921823	-1.7442321094	-5.9635073217
		H	1.0	2.7444632730	1.5465229177	-5.3596952099
		C	6.0	3.7184656791	-0.0283720940	0.7988791049
		H	1.0	2.7691385187	-1.5429082152	-3.1604170238
		H	1.0	2.8191633695	-2.7147730517	-5.8059345852
		C	6.0	2.9379545698	-0.2369385643	-1.4987387281
		C	6.0	2.6428490666	-0.5920415011	-5.4997601177
		H	1.0	3.6557292135	-0.3416417572	1.8365989771
		C	6.0	2.9200607382	-0.6529618189	-0.1622442461
		C	6.0	2.0895429824	-0.9480827120	-2.5411587496
		N	7.0	1.3254823401	-0.0774810728	-3.4567958485
		H	1.0	0.7860659354	2.0101128956	-1.8967740140
		H	1.0	5.1480306363	-0.2369908032	4.7975843453
		C	6.0	1.2924651511	-0.6517551427	-4.8124328958
		H	1.0	2.2570600539	-1.4625027592	0.1350838336
		H	1.0	0.6624682547	0.6113404995	-0.8490412689
		H	1.0	1.4248465874	-1.6727003054	-2.0375336241
		H	1.0	-0.2342930206	2.8488893398	-3.7726543151
		C	6.0	0.1577556493	1.1474930476	-1.6497263605
		H	1.0	0.6038681881	-0.0592609279	-5.4149319880
		H	1.0	0.9157389958	-1.6921490243	-4.8221451576
		O	8.0	-0.2765140259	2.1826289792	-4.4736235504
		C	6.0	4.5975611907	-0.9698810804	5.3873051257
C	6.0	-0.0019647155	0.2795950854	-2.9112859821		
H	1.0	4.6426489837	-0.6907041509	6.4467099056		
H	1.0	5.0505229367	-1.9592046546	5.2507034422		
C	6.0	-0.9112971468	1.0406509360	-3.9095007576		

O	8.0	3.2641362280	-0.9300318017	4.8919357398
H	1.0	-0.9935094384	2.4326992002	-0.3464271016
H	1.0	0.5706094903	0.8394962040	2.2677719438
H	1.0	-0.5592500545	-0.6357012098	-2.6298244561
H	1.0	-1.1673867181	0.3960530026	-4.7559800671
C	6.0	-1.1693852683	1.6518270370	-1.0934535863
O	8.0	1.4236764822	0.0938314957	3.3723968276
O	8.0	-1.9703396269	2.2745407517	-2.0905165123
H	1.0	-2.7063994721	3.0676151033	-4.5358710287
O	8.0	-0.2904436021	0.9621969050	1.7646123077
C	6.0	-2.2356181868	1.4190840052	-3.2198928023
H	1.0	3.6369557554	-2.6813495033	6.8764992103
C	6.0	2.3283133441	-1.7306022596	5.4465256396
O	8.0	-1.8355701709	0.5590443371	-0.4918936279
C	6.0	-3.1883176052	2.1736655162	-4.1339816534
C	6.0	0.6082542344	-0.7191745015	3.8604911561
C	6.0	2.6286329843	-2.6234463866	6.4879170854
H	1.0	-2.7149035593	0.4980953050	-2.8617763801
H	1.0	-2.6546550143	1.9275133605	0.8216296884
H	1.0	-3.4905494731	1.5405251687	-4.9740307430
C	6.0	-1.1414314391	0.0771985986	2.2933835327
C	6.0	0.9981514842	-1.6579986505	4.9418375724
C	6.0	-2.7825611492	0.8728344204	0.5372412753
H	1.0	-4.0844770528	2.4705219145	-3.5829245870
H	1.0	-4.9467475308	3.4190129368	0.8065808254
C	6.0	-0.7680245370	-0.7625064770	3.3584707429
H	1.0	-6.2282183675	3.6660458875	2.0097672779
C	6.0	-2.4640437139	0.0149359884	1.7540570689
H	1.0	-4.4706389733	1.4670064348	-0.6740175458
C	6.0	1.6425255680	-3.4421657654	7.0315683655
C	6.0	-5.8294318885	2.9662248619	1.2742026052
C	6.0	-4.1946727309	0.6397386362	-0.0155534826
H	1.0	1.9010682443	-4.1230356073	7.8369291422
C	6.0	0.0232097053	-2.5129670171	5.5126513147
H	1.0	-6.5579988706	2.7751442030	0.4832231635
H	1.0	-4.1737990868	-0.2674514738	-0.6282814816
C	6.0	-1.7393412938	-1.6324062231	3.9293374887
C	6.0	0.34111114814	-3.3943245919	6.5483080327
C	6.0	-5.4372359053	1.6772633068	1.9712986440
C	6.0	-3.4212842835	-0.7883504389	2.3524535598
C	6.0	-1.3825961954	-2.5140137236	5.0261381927
C	6.0	-5.2462009514	0.4231805504	1.0723253140
C	6.0	-3.0568884797	-1.6292394471	3.4438374544
O	8.0	-5.3199887171	1.6086563604	3.1801580400

		H	1.0	-0.4433070080	-4.0238541950	6.9499585074
		C	6.0	-4.8614491762	-0.8064659682	1.8984093768
		O	8.0	-6.4879956134	0.2075098774	0.3852153990
		O	8.0	-2.2239828197	-3.2713440873	5.5582818555
		H	1.0	-5.0478428281	-1.6933874954	1.2794865861
		H	1.0	-5.5005507299	-0.8918949869	2.7816883707
		H	1.0	-7.1394302409	-0.0826438946	1.0401487495
		H	1.0	-3.5693787948	-2.9217334655	4.7025050819
		O	8.0	-4.0089421213	-2.4129267289	3.9639344225
N,N-diethyladriamycin	70844-09-6	H	1.0	-2.2050997465	-6.8519243335	-3.3512364011
		H	1.0	-2.4855731537	-4.6357095907	-4.0708047529
		H	1.0	3.0601055105	2.3162568467	-4.3908436287
		H	1.0	-1.7515154695	-7.7680128435	-1.9122329890
		H	1.0	-4.9353226805	-4.0933535903	-4.0170053582
		H	1.0	-0.6082134282	-6.6291348196	-2.6327594954
		C	6.0	-1.6662774194	-6.7908724893	-2.4001486346
		O	8.0	2.6416415489	3.0346935803	-3.8960642883
		H	1.0	-4.5984911453	-5.4990435288	-3.0087686806
		C	6.0	-4.4166133756	-4.4255409369	-3.1119332003
		C	6.0	-2.9279696654	-4.0884868043	-3.2151182823
		H	1.0	-0.3682500634	-3.8326656525	-2.9836164229
		H	1.0	0.8716029601	1.2973078239	-3.2002157493
		H	1.0	-2.8454293202	-3.0274811006	-3.4676521673
		H	1.0	2.4126588790	0.4596426080	-2.9664288342
		H	1.0	0.6785613794	3.7916969725	-2.6630910869
		H	1.0	0.8432260752	-1.4679499847	-2.7106998646
		H	1.0	-1.6105996686	-1.6797630422	-2.5948679542
		C	6.0	-2.2380990759	-5.6938876091	-1.4828668230
		H	1.0	-3.2893964276	-5.9240738874	-1.2798249569
		C	6.0	2.4254006241	2.5858925464	-2.5543833760
		C	6.0	1.7410057618	1.2142880492	-2.5394003943
		N	7.0	-2.1834456687	-4.3103000113	-1.9716691208
		H	1.0	-4.8641453426	-3.9187854731	-2.2515475008
		C	6.0	-0.8606313937	-3.6620809851	-2.0036947572
		C	6.0	1.4784249044	3.6256472037	-1.9299920713
		H	1.0	1.8246778323	-3.4684865059	-2.1250856475
		H	1.0	1.9793287955	4.5903366636	-1.8146805568
		C	6.0	-1.0175998273	-2.1375396177	-1.7992403499
		H	1.0	-1.7480076769	-5.7168888192	-0.5080330304
		C	6.0	3.7644931655	2.5810791741	-1.8008274292
		O	8.0	3.9790261163	1.8404874041	-0.8541789995
		C	6.0	0.3274172435	-1.4219964104	-1.7301970496
		H	1.0	4.4415226514	4.5598223459	-2.3052070999

H	1.0	5.1440315232	3.2816176981	-3.2776228794
H	1.0	0.3522265174	-5.2454693222	-1.1182141910
C	6.0	4.8593121636	3.5433810354	-2.2458861451
O	8.0	0.0786812816	-0.1007256981	-1.3542004954
C	6.0	0.1465595375	-4.1845861312	-0.9487024534
C	6.0	1.2386454383	0.7352262462	-1.1624296186
C	6.0	1.4660606152	-3.3988395431	-1.0837068715
H	1.0	-1.5484213678	-1.9594520793	-0.8591460583
O	8.0	1.1879295324	-2.0283830051	-0.7681306873
C	6.0	0.9046947933	3.1904072992	-0.6034833753
H	1.0	2.0100791170	0.1559412761	-0.6515767538
O	8.0	0.5525759873	5.4795330285	-0.1278174570
H	1.0	2.8629437631	-4.8933592080	-0.3922278598
C	6.0	0.8095710106	1.8580677116	-0.2364251672
C	6.0	2.5559616662	-3.8745911959	-0.1359656011
H	1.0	3.4273109609	-3.2185114934	-0.2041225281
O	8.0	-0.3373820700	-4.0795044059	0.3838481506
O	8.0	5.9577625579	3.4911132621	-1.3802840550
C	6.0	0.4627829366	4.2091702677	0.2881998516
H	1.0	0.2007125233	6.0362139843	0.6245313200
H	1.0	5.7461937253	2.7913614356	-0.7367907004
H	1.0	-0.2454485282	-3.1466581878	0.6339302618
H	1.0	2.1902929030	-3.8736776566	0.8929422554
C	6.0	0.3344994267	1.5068766613	1.0679057073
C	6.0	-0.0489660175	3.8720676908	1.5511124939
O	8.0	0.3470725520	0.2200502262	1.4137367726
C	6.0	-0.1053532257	2.5089471793	1.9548328153
O	8.0	-0.4419652307	6.1314914081	2.1128612111
C	6.0	-0.4956964512	4.9261241586	2.4445554684
H	1.0	-0.0041175964	0.1963386430	2.3534097482
C	6.0	-0.5961233837	2.1275390656	3.2837932864
C	6.0	-1.0281374538	4.5498159970	3.7801625202
O	8.0	-0.5966643094	0.9262711338	3.6267688106
H	1.0	-1.4024547708	6.6029216132	4.2422339130
C	6.0	-1.0837175849	3.1959747684	4.1929721267
C	6.0	-1.4693913479	5.5854522182	4.6072141627
C	6.0	-1.6101410070	2.9136083082	5.4862704691
C	6.0	-1.9781116663	5.2875434722	5.8649087982
O	8.0	-1.6684493965	1.6246820230	5.8792182764
C	6.0	-2.0501623451	3.9681500353	6.3031335628
H	1.0	-2.3241675213	6.0842200331	6.5165609736
C	6.0	-2.1934449284	1.3075464084	7.1621600092
H	1.0	-3.2390445851	1.6235715283	7.2607191844
H	1.0	-2.1355623747	0.2217504974	7.2381963594

		H	1.0	-2.4510015170	3.7587051176	7.2864483978
		H	1.0	-1.5992553891	1.7599869202	7.9653467510
N,N-dimethyladriamycin	67106-76-7	H	1.0	3.3633584971	0.4360563807	-6.0746623568
		H	1.0	5.6111551685	1.5444561224	-5.9637403273
		C	6.0	3.8459493215	0.6435981389	-5.1275674832
		O	8.0	1.3814717189	-0.5764472639	-5.2274436965
		C	6.0	5.0906879253	1.2569762414	-5.0552154069
		H	1.0	-0.0462665172	-1.2946266556	-4.8684226018
		O	8.0	-0.6831677059	-1.6331038643	-4.1787766006
		C	6.0	1.8588508358	-0.3733042823	-4.0905149489
		C	6.0	3.1882778287	0.2795517078	-3.9508908102
		H	1.0	6.6532422780	1.9889999419	-3.7888875761
		C	6.0	5.6834182764	1.5097397929	-3.8215033035
		C	6.0	-0.1136365481	-1.3797525476	-2.9952965556
		C	6.0	1.1431908749	-0.7612963382	-2.8860207898
		H	1.0	-5.8432029026	-2.4965651989	-1.2252347390
		C	6.0	3.7615579767	0.5201485081	-2.6771656189
		H	1.0	-2.7401402826	-1.9189979515	-2.7813409251
		C	6.0	5.0380041603	1.1505973805	-2.6265738104
		H	1.0	-5.5661899262	-2.9258790736	0.4493494719
		H	1.0	-1.9943735322	-3.4583866839	-2.3976382050
		C	6.0	-5.5207788035	-3.3250811607	-0.5751944147
		C	6.0	-2.1668075205	-2.4454415975	-2.0126889902
		H	1.0	6.8390666273	3.0162013280	-1.7644304703
		O	8.0	-6.3291990428	-4.4595296564	-0.7261811194
		H	1.0	7.6356367568	1.4134297188	-1.8145718917
		C	6.0	-0.8341251234	-1.7626710933	-1.8253526236
		C	6.0	1.7152171145	-0.5223826911	-1.6051590559
		O	8.0	5.5825796954	1.3807861361	-1.4148619027
		C	6.0	3.0285356890	0.1133704756	-1.4541747113
		C	6.0	6.8552971135	2.0104933072	-1.3277041245
		H	1.0	-5.7348666486	-5.1561617302	-1.0570597806
		C	6.0	-4.0739234575	-3.6358154331	-0.9072858696
		C	6.0	-3.0196208470	-2.5358070917	-0.7317329214
		C	6.0	-0.2763857439	-1.5267067503	-0.5791704653
O	8.0	-3.7112390858	-1.3200127672	-0.4828675413		
O	8.0	3.4990909908	0.2976266831	-0.3102214257		
C	6.0	1.0021977784	-0.9084580860	-0.4577385422		
H	1.0	7.0695381385	2.0834069302	-0.2614917793		
H	1.0	-3.1786389169	-0.7966645178	0.1413077125		
O	8.0	-3.7682449545	-4.7556087730	-1.2883693872		
H	1.0	-1.6601738384	-3.8992183154	0.2545717968		
C	6.0	-2.1161720094	-2.9249426596	0.4588831299		

		C	6.0	-1.0212486780	-1.8785314604	0.6902538496
		H	1.0	2.3920571766	-0.2947285692	0.6356459380
		O	8.0	1.4948318250	-0.7307876515	0.7745538772
		H	1.0	-2.5942382771	1.6236935076	1.3730431240
		O	8.0	-1.5964307254	-0.6397416070	1.1764467268
		H	1.0	-2.7205681749	-3.0298585215	1.3665358542
		H	1.0	-0.3007434069	-2.2476098156	1.4284839516
		H	1.0	-5.0128757184	1.5836296889	2.0056735456
		H	1.0	-4.3019396290	3.1933829978	2.2491272766
		H	1.0	-0.2398501401	1.7231309823	1.9712284622
		C	6.0	-2.8984608234	1.5670538906	2.4257911556
		C	6.0	-4.2895990603	2.1546271239	2.5929892365
		H	1.0	0.6522827654	4.1207618781	3.0522637333
		C	6.0	-1.8124319311	-0.5561481943	2.5989036763
		O	8.0	-2.9914668234	0.1711918974	2.8088004808
		H	1.0	-1.7777506653	3.3020841539	2.9902580780
		H	1.0	2.1684449030	1.9918502702	2.3798093066
		H	1.0	-2.0149126488	-1.5604085120	2.9917378786
		C	6.0	-0.4606914861	1.5724975467	3.0467893991
		C	6.0	-1.8295955089	2.2515214425	3.2922803733
		H	1.0	-4.5890480602	2.1384483531	3.6431241802
		H	1.0	0.2915205088	-0.4785834327	2.9833650512
		C	6.0	-0.6023470662	0.0586730469	3.3040099986
		C	6.0	0.5938830241	3.5759338016	4.0151358053
		H	1.0	-0.3068362861	3.8869942833	4.5470173152
		N	7.0	0.6226478511	2.1233200561	3.8759771994
		C	6.0	1.9362202099	1.6808489565	3.4167251883
		H	1.0	1.4536012765	3.8844905399	4.6173216482
		H	1.0	2.0223182162	0.5931147750	3.4658017228
		H	1.0	-2.4769556920	1.3591570754	4.8873231555
		O	8.0	-2.2132028029	2.2625773994	4.6615720188
		H	1.0	-0.7100282958	-0.0977044326	4.3838060116
		H	1.0	2.7049902973	2.0977548420	4.0740603332
N,N-dimethyl-daunomycin	70095-84-0	H	1.0	5.3007942795	-1.8974865987	-2.2928685657
		H	1.0	1.5135367622	-1.2228323937	-3.5580628374
		H	1.0	0.5572395857	0.7107114334	-2.3742802239
		H	1.0	5.5018436524	-3.4537614162	-3.1686523032
		C	6.0	4.9306544463	-2.9210436646	-2.4077096385
		H	1.0	2.8374825485	-0.2715247979	-2.8944309172
		H	1.0	2.9899782489	1.5435748488	-1.7596472183
		C	6.0	1.9880901246	-0.9073116467	-2.6231063591
		H	1.0	1.0568037624	-3.6679164977	-2.4594724460
		C	6.0	0.9813689855	-0.1094033984	-1.7881853247

C	6.0	3.4704305325	-2.9132790895	-2.7921928721
H	1.0	5.0552122710	-3.3940935137	-1.4287513168
O	8.0	-1.4876936482	0.9512415852	-1.0721012867
O	8.0	3.0550408054	-3.4506226793	-3.8029000799
H	1.0	-2.4222213785	1.1733261523	-0.7698251831
C	6.0	-0.1377341472	-0.9852956187	-1.2632791422
H	1.0	3.7834644361	1.0138783635	0.6070383287
C	6.0	2.4849932232	-2.1610675435	-1.8691392362
C	6.0	1.2850487483	-3.0772280724	-1.5636695040
C	6.0	-1.3701438179	-0.3696803838	-0.8927144903
C	6.0	2.3708530779	1.6678824143	-0.8630520017
H	1.0	4.0073147057	2.6766943334	0.0841271403
C	6.0	0.0315652118	-2.3553698704	-1.1332635131
C	6.0	3.2502143261	1.9346603765	0.3586247056
O	8.0	1.6300560001	0.4705251692	-0.6166330824
O	8.0	-3.8068192562	0.7494279050	-0.1600827162
H	1.0	4.4112743797	0.9979297286	2.6264165908
C	6.0	-2.4237394125	-1.1416471558	-0.3726456529
C	6.0	-1.0345007490	-3.1460953150	-0.6094178822
C	6.0	-3.6803708707	-0.4842834394	0.0001996771
H	1.0	1.5764486734	-3.7943858918	-0.7901393655
H	1.0	-8.2689283340	0.7600081650	0.6464531678
O	8.0	1.5244286425	2.7514402881	-1.1715014733
C	6.0	-2.2452708316	-2.5459433917	-0.2268231588
O	8.0	-0.8279517973	-4.4635524550	-0.5037558166
H	1.0	-7.3212118216	2.2238005149	1.0243533684
O	8.0	-6.1945465173	0.5717806670	0.8359554058
H	1.0	2.7017105249	-1.0638702005	-0.2769210055
O	8.0	3.1860315745	-1.8033760013	-0.6826435531
C	6.0	-4.7729922280	-1.3144422139	0.5639723296
H	1.0	-1.6685020681	-4.8433124811	-0.1225017007
C	6.0	-7.4294763854	1.1586756621	1.2287114066
C	6.0	-3.3161938565	-3.3695327259	0.3087530279
C	6.0	-6.0199177350	-0.7587001343	0.9712197396
C	6.0	-4.5888586458	-2.7118922995	0.7091516377
H	1.0	2.6705848928	4.6066958141	-0.2220998941
C	6.0	3.9169397071	1.6759523754	3.3268398004
O	8.0	-3.1872307987	-4.6061225094	0.4387237378
H	1.0	3.1318369742	1.1006464458	3.8561412341
H	1.0	4.6642104295	1.9834668154	4.0646114685
C	6.0	2.4649046736	2.4908335671	1.5644379137
C	6.0	-7.0167268005	-1.5978752559	1.4956041617
C	6.0	-5.5923222794	-3.5300219715	1.2326404030
H	1.0	-7.9660733795	-1.1808894202	1.8057671881

		H 1.0 1.7564153353 1.7146526066 1.9161802129 C 6.0 0.6813982978 3.1691955190 -0.0679494610 C 6.0 -6.8010753423 -2.9671763316 1.6229164226 H 1.0 -5.3995549301 -4.5920773274 1.3211981756 N 7.0 3.4027013259 2.8542280189 2.6384382109 H 1.0 -7.6250916396 1.0117149324 2.2977054757 O 8.0 2.3416397955 4.7980179004 0.6682422325 H 1.0 0.0999049534 2.3066434225 0.2708592928 H 1.0 -0.8129504814 3.8314982831 -1.4648100703 H 1.0 0.3004129114 5.1168579784 -0.9339281671 H 1.0 -7.5883081400 -3.5937215468 2.0312130809 C 6.0 1.5826193997 3.6640006061 1.0728534870 C 6.0 -0.2558580816 4.2321957426 -0.6149999737 H 1.0 0.9400007290 4.0063792406 1.8901864499 C 6.0 2.8931407356 3.8265700470 3.5994465860 H 1.0 -0.9686233950 4.5363658394 0.1578653419 H 1.0 3.6690026795 4.0124474655 4.3484943936 H 1.0 1.9856139102 3.4926290694 4.1397852301 H 1.0 2.6824244919 4.7739628420 3.1010624485
Doxorubicin / Adriamycin	25316-40-9 / 23214-92-8	H 1.0 -2.8772485779 -4.6502763132 -0.6886418945 H 1.0 -2.7986664526 -3.9643471811 0.7949805328 H 1.0 7.3885981685 -1.1018134409 2.3941352183 H 1.0 6.6033080397 -3.3831842697 -1.5392507530 N 7.0 -2.8114742562 -3.7597029746 -0.2013175347 H 1.0 7.3216725637 -1.9907646121 0.1088403613 O 8.0 -4.2353305650 -4.2565304986 -2.5177025706 C 6.0 6.4917959093 -0.9685787497 1.7965343815 H 1.0 -1.8667202455 -3.5313730697 -3.6157653864 C 6.0 6.4552626311 -1.4731479136 0.4996700339 H 1.0 -4.3983939549 -4.2414123376 -3.4696406544 H 1.0 -1.3409238309 -2.9392878906 -2.0406615156 H 1.0 -4.9250007817 -3.4030089835 -0.0990277222 H 1.0 5.3964493461 0.1011165512 3.3297070037 C 6.0 6.3615335779 -2.4788009968 -2.1106522241 C 6.0 -4.0043906044 -2.9655265151 -0.5229061491 C 6.0 5.3939778925 -0.3005277295 2.3239702890 C 6.0 -1.7933715322 -2.6391615841 -2.9862395847 H 1.0 6.0609893030 -2.7595434357 -3.1200996433 H 1.0 7.2464184282 -1.8329294467 -2.1623405987 C 6.0 5.3115614513 -1.3174008004 -0.3008440158 C 6.0 -4.2156856701 -2.9099999755 -2.0453318693 O 8.0 5.2431758585 -1.7937884530 -1.5608730455 H 1.0 -1.1483645692 -1.9104782297 -3.4842465904

C	6.0	4.2474080285	-0.1367792820	1.5431374033
H	1.0	-3.5711680069	-1.5597560833	1.0793072343
C	6.0	4.1742353863	-0.6361182689	0.2199728995
H	1.0	-1.8114478540	-1.2031926649	-0.6476273045
C	6.0	-3.1824465308	-2.0264863195	-2.7883480984
C	6.0	-3.8506348253	-1.5354161388	0.0198404846
H	1.0	-5.1976416317	-2.4365242667	-2.2019700731
C	6.0	3.1021813437	0.5841739428	2.1590251774
O	8.0	3.2027127055	1.0252858818	3.3262291708
H	1.0	-3.5957957602	-1.8113076973	-3.7838459022
C	6.0	-2.8075996048	-0.7577754956	-0.7722951203
H	1.0	-4.7996446865	-0.9941506744	-0.0613406469
C	6.0	2.9347714688	-0.4372579923	-0.5734785836
H	1.0	1.7540602786	1.7195603307	3.5441867027
C	6.0	1.8857048427	0.7572214211	1.3845280157
O	8.0	0.8429296054	1.9455187608	3.2000784192
O	8.0	-3.1536357158	-0.7401022570	-2.1580797912
C	6.0	1.8072320262	0.2645373780	0.0507960952
C	6.0	0.7912828357	1.4335029480	1.9584936690
O	8.0	2.8367311396	-0.8500352893	-1.7479713760
H	1.0	-2.4425280341	1.6694146016	1.8482164908
H	1.0	1.3658152860	-0.4044435710	-2.1742788703
C	6.0	0.6250094283	0.4655016043	-0.6920392682
C	6.0	-0.3994416101	1.6029969761	1.2089592788
O	8.0	-2.8247280372	0.5687482043	-0.3245295355
O	8.0	0.4957067630	0.0414753226	-1.9542677227
H	1.0	-1.3773987353	2.7730026573	2.7317905849
C	6.0	-0.4731434915	1.1421343096	-0.0967365969
C	6.0	-1.5892691220	2.3475077163	1.7515584752
C	6.0	-1.7668100319	1.4059587665	-0.8479506332
H	1.0	-1.6422207157	1.1850974665	-1.9088473419
C	6.0	-2.0261043422	3.4492674007	0.7460678461
O	8.0	-1.6934612560	5.2506317655	3.0019977789
H	1.0	0.2707015101	4.7955734193	2.4539998165
C	6.0	-2.2215190886	2.8632697998	-0.6694395607
H	1.0	-1.3276187279	5.2252072545	3.8938804248
H	1.0	-3.1149669200	4.4427289280	2.0132429990
H	1.0	-3.2874210437	2.9091661997	-0.9017762816
O	8.0	-3.2604946289	4.0448037365	1.1381782868
C	6.0	-0.6248032090	5.2936080483	2.0562319808
C	6.0	-0.9513324514	4.5711419642	0.7401988390
H	1.0	-1.6838216074	3.4874423430	-1.3870820666
O	8.0	-0.3142560182	4.8889118880	-0.2435625627
H	1.0	-0.3552213350	6.3257878168	1.8033945331

Duborimycin	NSC 180510	H	1.0	0.2444309909	3.7353204729	-7.9991227196
		H	1.0	-1.0452247867	1.8053400851	-7.0486192505
		C	6.0	0.4327603081	3.3884314696	-6.9875178143
		H	1.0	1.9483492321	4.8594686581	-6.6383819665
		C	6.0	-0.2865603833	2.3186182904	-6.4707373473
		C	6.0	1.3998912266	4.0273857545	-6.2163130765
		H	1.0	3.9232990743	5.0258406324	-5.5237879983
		O	8.0	-1.6883615593	0.2015658456	-5.4115328931
		C	6.0	-0.0336070090	1.8835577288	-5.1675824682
		H	1.0	2.6708163684	6.1450513402	-4.9042125818
		C	6.0	1.6685077315	3.6041197084	-4.9044468683
		C	6.0	3.3295348683	5.3071393993	-4.6455541271
		C	6.0	-0.8373598273	0.7368232324	-4.6667809387
		C	6.0	0.9446657260	2.5074539704	-4.3545866923
		H	1.0	-2.2884496120	-0.9633133137	-4.4415885478
		O	8.0	2.5973801024	4.2028930202	-4.1299118893
		H	1.0	3.9994607319	5.6109954705	-3.8410633062
		O	8.0	-2.2871035399	-1.4321573920	-3.5596730980
		C	6.0	-0.6110750766	0.2683256034	-3.3110950129
		C	6.0	1.1836949572	2.0079764538	-2.9760872928
		C	6.0	-1.3634369655	-0.8094690914	-2.8170930966
		C	6.0	0.3726902424	0.8886498863	-2.4896231714
		O	8.0	2.0508072886	2.5181183646	-2.2342233072
		C	6.0	-1.1636503022	-1.2839128543	-1.4864604507
		H	1.0	-3.0477717082	-2.2793583395	-1.3059974083
		H	1.0	-1.6903976437	-3.3348176278	-1.6129780203
		C	6.0	0.5737195138	0.4083056013	-1.1825310995
		H	1.0	1.9268579450	1.6644090007	-0.8987331571
		C	6.0	-2.0031275127	-2.4563934206	-1.0326554247
		C	6.0	-0.2045739371	-0.6828049036	-0.6866853812
		H	1.0	-1.5603587180	-5.3652284504	-0.7327327530
		O	8.0	1.4929859001	0.9306241008	-0.3695233790
		C	6.0	-1.6905177546	-5.3497561493	0.3528907379
		C	6.0	-1.9274137094	-2.7482341403	0.4727983184
		H	1.0	-3.5008969977	-4.1887942388	0.3370985531
		H	1.0	-2.2106065952	-6.2662058198	0.6440901134
		H	1.0	-0.7056762816	-5.3642037870	0.8284237149
		C	6.0	0.0277300639	-1.1413020643	0.7420800811
		H	1.0	0.1762409649	-3.2435525604	0.4028863703
		C	6.0	-2.5068242618	-4.1493521566	0.8165112520
		H	1.0	1.0894155952	-1.0648268393	0.9780890958

		C	6.0	-0.4836834696	-2.5694167947	0.9617822613
		O	8.0	-2.8092960078	-1.8541116162	1.1803633223
		H	1.0	-2.3131130269	-1.0432339390	1.3897574098
		O	8.0	-0.6841826001	-0.1681608355	1.5668771544
		H	1.0	-0.4182916194	-2.8549058267	2.0133463574
		O	8.0	-2.6452395411	-4.2574768958	2.2263278136
		H	1.0	-3.0286727556	-3.4039368666	2.4883532474
		O	8.0	1.2322390815	0.2960762363	2.7582949712
		C	6.0	-0.1740005390	0.2020696039	2.8385546709
		H	1.0	-0.6141983615	1.1969192938	2.9984851793
		H	1.0	-0.1754138910	-1.7384914365	3.7541441453
		C	6.0	-0.5795913822	-0.7460876458	3.9725312995
		H	1.0	2.0122433822	2.8362800784	3.1279673462
		H	1.0	-1.6693465049	-0.8299888948	4.0304960241
		H	1.0	2.9479687251	0.6688005344	3.7187113877
		C	6.0	1.8853680553	0.8391636035	3.9186091853
		C	6.0	1.6876328650	2.3508356512	4.0522426910
		H	1.0	1.9832822561	-0.9932126920	4.9999258876
		H	1.0	0.6516615290	2.6378615176	4.2438576025
		C	6.0	1.5115259919	-0.0094425904	5.1521099648
		C	6.0	-0.0098157157	-0.2623262602	5.3162814046
		H	1.0	-0.9971703994	1.5442104240	5.1430542634
		H	1.0	2.2921431872	2.7244092559	4.8817943221
		H	1.0	-0.1093982598	-1.0859222612	6.0401561991
		N	7.0	-0.7810759141	0.8585393416	5.8605396143
		O	8.0	2.0666321136	0.6314778946	6.3003814813
		H	1.0	-0.2102456224	1.3387208108	6.5536369718
		H	1.0	2.0650849795	-0.0064124775	7.0265637234
Epirubicin	56390-09-1	H	1.0	-3.3120034484	6.0982230793	-0.2678702510
		H	1.0	-4.0548126334	4.4719316284	-1.7824460597
		O	8.0	-3.0298982986	5.1905260988	-0.0996230400
		H	1.0	7.5967452923	-0.9814068507	-2.5939975760
		C	6.0	-3.0519237991	4.4672825374	-1.3294741628
		H	1.0	-2.3526098266	4.8889232816	-2.0615135912
		O	8.0	-2.3491445559	2.3625155021	-2.1273718593
		H	1.0	8.0175481825	0.2929446076	-0.7580501206
		H	1.0	8.0397752523	2.3764622519	0.5355792603
		C	6.0	7.0780634896	0.7294263050	-0.4445922679
		C	6.0	7.0893921974	1.9120819932	0.2900632150
		C	6.0	7.0335373703	-1.6438263753	-1.9255098085
		C	6.0	-2.6686319867	2.9933695646	-1.1387672864
		H	1.0	6.7341646763	-2.5376845825	-2.4729524756
		O	8.0	5.8205592058	-1.0430704113	-1.4907262429

H	1.0	5.8801275170	3.4144954937	1.2774566674
C	6.0	5.8667200286	0.1031506722	-0.7801260521
C	6.0	5.8991647005	2.4948656978	0.7057697562
H	1.0	7.6686549110	-1.9330987212	-1.0793886980
C	6.0	4.6843063245	1.8857015750	0.3828628641
C	6.0	4.6337611945	0.6826603480	-0.3632841384
H	1.0	1.6782240737	-1.2146705745	-1.4415363195
C	6.0	3.4419632899	2.5555862624	0.8521593447
H	1.0	-1.3432676573	3.7928806383	1.1087600816
C	6.0	3.3191274185	0.0729461887	-0.6876821527
O	8.0	0.7355619516	-0.9566704525	-1.2062682294
O	8.0	3.5192081235	3.6259047743	1.4969180480
C	6.0	2.1636166409	1.9433825910	0.5440613563
C	6.0	2.1036596171	0.7308324488	-0.1997282756
H	1.0	-5.8972088174	-1.6396220905	-0.7782383257
H	1.0	-3.8655258383	3.8100454045	0.9677970015
H	1.0	1.9507833952	3.9610438363	1.7570228131
C	6.0	0.8487607402	0.1597549536	-0.4804367986
C	6.0	0.9773301903	2.5661849257	0.9663407798
C	6.0	-2.7746070228	2.3655626212	0.2667985178
O	8.0	0.9872780487	3.7167126848	1.6517918225
O	8.0	3.2328217829	-0.9773744333	-1.3606756747
H	1.0	-1.7436341250	-0.0136144583	-1.4128632213
C	6.0	-0.2890153979	1.9809629388	0.6737947467
C	6.0	-1.5320413184	2.7167210375	1.1137387330
C	6.0	-0.3525271992	0.7785141632	-0.0121249228
O	8.0	-3.9655110066	2.8466995030	0.8845248499
H	1.0	-3.7808914306	0.5687449495	-0.3992174239
C	6.0	-1.6748898438	0.0943572838	-0.3262560709
C	6.0	-5.6537433706	-2.6150384561	-0.3477362255
C	6.0	-2.9088853058	0.8442833056	0.1982144293
H	1.0	-6.3647765504	-2.8416599264	0.4500694320
H	1.0	-5.7525057999	-3.3710802677	-1.1335251875
H	1.0	-1.7834356289	2.4541714497	2.1502827700
O	8.0	-3.3551619945	-2.3334447109	-0.8937489986
H	1.0	-4.1409597238	-1.8271603919	0.9690343422
C	6.0	-4.2396325374	-2.6137493280	0.2086390039
H	1.0	-3.0946155776	0.5107289694	1.2238181157
O	8.0	-1.6467896769	-1.2124682043	0.2779094652
H	1.0	-1.4763991715	-2.1533644197	-1.5455433513
C	6.0	-1.9736722937	-2.2891416793	-0.5801802051
C	6.0	-3.8531499955	-3.9443387173	0.8640265676
H	1.0	-3.9677859677	-4.7422848263	0.1042315022
O	8.0	-4.7018500982	-4.1809715701	1.9715655852

		C	6.0	-1.4975058713	-3.5719555836	0.1077561427
		H	1.0	-2.2932604521	-3.1142158694	2.0570262604
		H	1.0	-1.5476385384	-4.3876361561	-0.6253195868
		C	6.0	-2.3861308070	-3.9110740234	1.3099445941
		H	1.0	-4.2066671390	-4.8170978389	2.5163889291
		H	1.0	-0.4507243746	-3.4482178898	0.4020191861
		N	7.0	-2.0950314996	-5.1764943171	2.0017356842
		H	1.0	-1.9707513499	-5.9243892944	1.3204862725
		H	1.0	-1.2223592081	-5.1082414730	2.5189152964
		H	1.0	3.0327740592	2.1307010399	-5.7351560118
		O	8.0	2.7259396543	1.4572556843	-5.1156759517
		H	1.0	3.0638846522	2.7164773055	-3.4677290139
		H	1.0	-0.3365135733	6.5431523830	-1.1968339316
		C	6.0	3.3215974909	1.7233462316	-3.8689827897
		H	1.0	4.4232046261	1.6942183237	-3.9050368826
		H	1.0	-2.8158594142	3.5620784578	0.7094226373
		H	1.0	-1.5532945054	2.2542275170	-0.8834999692
		O	8.0	-0.5055723942	3.9494073484	-0.7464121650
		H	1.0	1.1908713143	5.7346156862	-1.5890400342
		H	1.0	-1.6339530927	5.8372301569	0.8955147920
		C	6.0	0.5521746042	6.0705459548	-0.7670792101
		C	6.0	-0.9936170978	2.7829853913	-0.1060331179
		H	1.0	0.2561400447	1.3408082560	-1.6052074663
		C	6.0	-1.8951778758	3.1014288434	1.0846955623
		C	6.0	2.8712181196	0.6627167378	-2.8664496708
		O	8.0	2.2673346083	-0.3314644366	-3.2075245488
		C	6.0	0.1536440284	4.8968638135	0.1162051878
		H	1.0	2.1180833999	2.8059830705	-1.2643712607
		H	1.0	1.0995141792	6.8198860373	-0.1865650392
		H	1.0	-2.1642400313	2.1596981466	1.5736799780
		C	6.0	-0.7561470994	5.3022710183	1.2794169367
		H	1.0	-2.3199053210	-0.8454300516	-0.0138941504
		C	6.0	0.7793124277	1.2341940338	-0.6453292043
		C	6.0	-1.2323015201	4.0745829518	2.0630396664
		O	8.0	0.0594208743	1.9557133733	0.3628490105
		C	6.0	2.1816624136	1.8492061881	-0.7395399345
		N	7.0	-2.2066001360	4.4819107651	3.0841009232
		H	1.0	-0.2131547337	5.9936411335	1.9379527135
		H	1.0	1.0591984537	4.4243627231	0.5251389893
		O	8.0	4.4661916683	1.6620328648	-1.3244633415
		C	6.0	3.2300825612	0.9367590099	-1.3862512232
		H	1.0	5.1837684648	1.0413118897	-1.5151458435
		O	8.0	-1.5744427686	-0.2021837254	-0.2192128382
Esorubicin	63950-06-1					

		H	1.0	-2.5110058558	3.6625650951	3.6073887131
		H	1.0	-1.7528306629	5.0926735581	3.7616158761
		C	6.0	0.7970728181	-0.2434888571	-0.2794441715
		H	1.0	-0.3449710005	3.5760265314	2.4907915164
		H	1.0	2.5300135974	2.0596505802	0.2771183177
		C	6.0	-0.4493844769	-0.9019275285	-0.0424538513
		H	1.0	3.9068292004	-1.1155546284	-1.1112668131
		C	6.0	3.3197397314	-0.3621790929	-0.5757817886
		H	1.0	-6.1500756769	-4.2868676869	1.3355893705
		C	6.0	1.9789707335	-0.9639378073	-0.2256961400
		H	1.0	-5.5277924804	-5.8789851926	0.8263258574
		O	8.0	-2.8312789952	-2.2602527089	0.4434477913
		C	6.0	-0.4797978802	-2.2566046987	0.3383434110
		O	8.0	-4.1470156950	-4.3562239542	1.2130082300
		C	6.0	-5.3671994976	-5.0276193338	1.4987808655
		C	6.0	-1.7698164955	-2.9041730952	0.5920687865
		H	1.0	3.8725062745	-0.1319151801	0.3444623349
		C	6.0	1.9594912548	-2.3337547792	0.1627561405
		C	6.0	0.7444430275	-2.9722695387	0.4566354559
		H	1.0	2.9180620729	-3.9061239412	0.5188836678
		C	6.0	-2.9805130597	-5.0253996858	1.3227897421
		C	6.0	-1.7763879669	-4.3249603520	1.0245625899
		H	1.0	-5.4056435581	-5.3731363917	2.5390664612
		O	8.0	3.1350307226	-2.9716035896	0.2387192687
		H	1.0	-3.8341830481	-6.9076578633	1.9473642947
		C	6.0	-2.9220909301	-6.3714465841	1.7193671521
		C	6.0	-0.5526100878	-5.0282207090	1.1442874564
		C	6.0	0.7474858958	-4.3685033360	0.8510621202
		C	6.0	-1.7006973608	-7.0313843793	1.8242626763
		C	6.0	-0.5144976615	-6.3676350309	1.5387306362
		O	8.0	1.8116579709	-5.0198542956	0.9491181566
		H	1.0	-1.6836337613	-8.0726505213	2.1319421983
		H	1.0	0.4487959849	-6.8572763698	1.6114923956
11-Hydroxy aclacinomycin A	NSC 670121	H	1.0	-7.9779550316	-7.1198213142	-0.0107488774
		H	1.0	-6.5460451080	-6.1745483199	-1.7503395328
		H	1.0	-7.5423389873	-8.4819939777	-1.0305030955
		H	1.0	-5.3251666367	-7.4365912020	-1.5385019289
		H	1.0	-5.5875274875	-2.5711826668	-1.8265554746
		C	6.0	-7.1296640081	-7.7356911850	-0.3469171170
		H	1.0	-4.8081887536	-3.9179318064	-2.6879517291
		C	6.0	-6.0773794005	-6.8368892570	-1.0160119702
		H	1.0	-4.3107091300	-2.2444075901	-3.0119056488
		C	6.0	-4.6403701811	-2.9382575412	-2.2360693609

H	1.0	-2.9855028481	-0.1742593712	-3.4824231664
O	8.0	-7.0618890492	-9.5324854075	1.2515702624
C	6.0	-6.6228104081	-8.4570438420	0.8957175763
H	1.0	-3.5055263938	1.3496059103	-1.9708107919
H	1.0	-6.0460056643	-5.3591312079	0.5857900436
C	6.0	-5.3473361663	-6.0078716859	0.0311488729
O	8.0	-4.3602340540	-5.2499810809	-0.5780185712
H	1.0	-4.8850160000	-3.5608340547	0.5151978334
C	6.0	-3.5924627495	-3.0351394276	-1.1373135905
H	1.0	-6.9896745396	-6.2315083497	2.5348186477
C	6.0	-1.9824027703	-0.3645822065	-3.0912089784
H	1.0	-1.7786976912	-1.4270057316	-3.2294779664
H	1.0	-1.2680348164	0.2242411347	-3.6981507823
H	1.0	-3.4129517810	-2.0418398030	-0.7066322122
C	6.0	-4.0039755102	-3.9781646392	0.0059185039
C	6.0	-2.5277953378	1.3195083183	-1.4822215561
C	6.0	-5.5779880814	-7.7276452432	1.7518296165
O	8.0	-2.3753055858	-3.4819417130	-1.7662620690
O	8.0	-4.7055694941	-6.9112735466	0.9538456678
H	1.0	-1.9117058022	2.1325339924	-1.9121415723
C	6.0	-6.2408031524	-6.9437405824	2.8950863533
H	1.0	-6.7369965486	-7.6387027787	3.5775012858
N	7.0	-1.9494897177	-0.0112636825	-1.6701590759
H	1.0	-2.6878292135	1.5345011102	-0.4242121188
H	1.0	-4.9290855193	-8.4969566855	2.1792329511
H	1.0	-5.4760716831	-6.3853217735	3.4413713639
C	6.0	-2.8501861309	-4.1151448781	1.0126081123
H	1.0	-3.4679498829	-5.7881177852	1.7827787751
C	6.0	-1.2710355766	-3.6485746630	-0.8961199088
H	1.0	-1.7772901036	-5.5894948460	-0.1363398051
H	1.0	-2.6612849029	-3.1146408610	1.4176328228
H	1.0	-0.0352800849	-1.9460613246	-2.1939966488
O	8.0	-3.1702410811	-4.9259125341	2.1254041288
H	1.0	-0.4900972552	-4.0719044317	-1.5393969428
C	6.0	-0.5882820421	-0.1264654858	-1.1218781791
C	6.0	-1.5968206633	-4.5876335017	0.2668967574
H	1.0	0.1049781587	0.4826710841	-1.7370793922
O	8.0	-0.8277902478	-2.4254915764	-0.3339591202
C	6.0	-0.0382965058	-1.5714757059	-1.1639237137
H	1.0	-0.7683779134	1.4041581942	0.4412119695
H	1.0	-1.1413477243	-0.2519123102	0.9562473074
C	6.0	-0.4814322734	0.3574565818	0.3321102200
H	1.0	-0.7497331323	-4.6358200604	0.9555533442
C	6.0	1.4216985107	-1.5588902346	-0.6662831085

H	1.0	1.9941910162	-0.9035737930	-1.3388182699
H	1.0	2.0821120541	-3.3860184384	-1.6236560000
C	6.0	0.9442234206	0.2303508336	0.8692046345
H	1.0	2.5639318356	1.4422457320	-1.4317743977
H	1.0	-0.4264439901	10.2031166130	3.7407377840
H	1.0	1.5285605043	-3.5887095667	0.0588320099
O	8.0	-0.5784477957	7.6783983798	4.0710287873
C	6.0	2.0704794524	-2.9335238536	-0.6270853521
C	6.0	0.2570791545	9.6524178566	3.1036681035
O	8.0	1.7220138681	1.2638163286	0.2595032803
H	1.0	1.0918106691	11.3799736830	2.1554526636
H	1.0	-0.4388962457	6.7003433080	4.0039885405
C	6.0	0.2611769608	8.2484866784	3.1996153275
O	8.0	3.3776350987	1.4123872013	-1.9624671592
O	8.0	1.5072798319	-1.0428360675	0.6753908170
C	6.0	1.1070194200	10.2960091021	2.2173763394
H	1.0	0.9591225920	0.3862870611	1.9532138977
O	8.0	0.3859430374	5.4338351837	3.2737763127
C	6.0	1.1427851971	7.4944171008	2.3811689937
C	6.0	1.9837079978	9.5677204551	1.4028375309
C	6.0	1.1594831605	6.0371581250	2.4665612167
H	1.0	2.6530111952	10.0589000292	0.7067798013
C	6.0	2.0024519792	8.1796398054	1.4827514409
H	1.0	0.7734834540	3.8546720655	3.0121858442
H	1.0	4.5147152715	-0.7129412677	-2.7936878649
O	8.0	1.3156150654	3.1865980348	2.5133078848
C	6.0	2.0701635075	5.2866068515	1.6183724242
C	6.0	2.9358682310	7.4195391529	0.6160152001
C	6.0	2.1027667241	3.8843142089	1.6837191250
H	1.0	3.1027002899	-2.8511418297	-0.2769249722
C	6.0	2.9390117475	5.9644077492	0.7106585885
O	8.0	3.6962842659	8.0223972200	-0.1726625398
H	1.0	4.7635657082	3.4961085234	-1.9295251600
C	6.0	3.0013475606	3.1444644779	0.8588382350
C	6.0	3.8149445879	5.2234106464	-0.0969842777
C	6.0	2.9484620250	1.6342158841	0.9405079700
C	6.0	3.8382193842	3.7961564416	-0.0273011449
O	8.0	4.6590420037	5.8089924812	-0.9515265330
C	6.0	4.4939258240	1.5343252359	-1.0779143130
H	1.0	4.4998437639	6.7930702017	-0.8639272026
C	6.0	5.3846014220	-0.6515933801	-2.1363199318
C	6.0	4.8186826697	3.0647354898	-0.9277016911
H	1.0	5.9319284463	1.3647183544	-2.6622778137
H	1.0	2.8605849231	1.3333658966	1.9899238525

		H	1.0	3.9817835660	-0.1104672270	0.2636056629
		C	6.0	4.1705329344	0.9635807217	0.3122717535
		C	6.0	5.6699471628	0.8039772176	-1.7577412871
		H	1.0	5.1946798799	-1.2778981102	-1.2585648613
		H	1.0	6.2440688761	-1.0802571263	-2.6612601061
		H	1.0	5.0307939831	1.1305913502	0.9693633847
		H	1.0	6.5438203295	0.8485924813	-1.0974254555
		C	6.0	6.2354946841	3.3036534027	-0.4023952067
		O	8.0	7.0818132449	3.6353998439	-1.3955366093
		O	8.0	6.5743969411	3.1832611994	0.7575322755
		H	1.0	8.9798087674	4.1194743538	-1.9058056255
		C	6.0	8.4456316479	3.8536301901	-0.9942750870
		H	1.0	8.5031817623	4.6639564325	-0.2640940993
		H	1.0	8.8671393101	2.9478103000	-0.5514186432
11-Hydroxy aclacinomycin X	NSC 670122	H	1.0	-7.4335322131	-6.3091678388	-2.4150155867
		H	1.0	-7.5223080116	-8.4219178730	-1.0421682531
		N	7.0	-6.8461891731	-5.8805887293	-1.7152856445
		H	1.0	-6.2577503804	-5.1178103990	-2.0182046502
		C	6.0	-6.7783343751	-7.9229315128	-0.4272861058
		C	6.0	-6.3593832606	-6.6590430042	-0.7133651377
		H	1.0	-5.7331995244	-2.5282151593	-1.8028726267
		H	1.0	-4.8295405185	-3.7204571701	-2.7814951648
		O	8.0	-6.7056463174	-9.7410369831	1.0853373638
		H	1.0	-4.4645747340	-1.9989407972	-2.9211428338
		C	6.0	-4.7541078186	-2.7847221250	-2.2208537490
		C	6.0	-6.2915071545	-8.6407726279	0.7309595845
		C	6.0	-5.3676159170	-5.9533751780	0.2061693813
		H	1.0	-5.9266694954	-5.3679513253	0.9555486555
		H	1.0	-3.0263422774	-0.0847618483	-3.5150208438
		O	8.0	-4.5638734594	-5.1044951595	-0.5562027539
		H	1.0	-6.5906056726	-6.7491615581	2.7810195146
		H	1.0	-4.9968788021	-3.4038602563	0.5551637602
		H	1.0	-3.5442712580	1.4395860761	-2.0037717456
		C	6.0	-3.7126732186	-2.9205979207	-1.1185878535
		C	6.0	-5.2125505169	-7.9530602004	1.5789625804
		O	8.0	-4.5340571432	-6.9049430612	0.8501209463
		H	1.0	-6.1863604510	-8.3324398002	3.4541105894
		C	6.0	-4.1403218911	-3.8510799602	0.0295259726
		C	6.0	-5.7795606365	-7.4717218380	2.9177661930
		C	6.0	-2.0322662250	-0.2957603815	-3.1112877665
		H	1.0	-1.8480760208	-1.3621197187	-3.2473678405
		H	1.0	-3.5097712571	-1.9335843092	-0.6838243440
		O	8.0	-2.5124797056	-3.3904474952	-1.7588736814

H	1.0	-1.2995337354	0.2784450480	-3.7099477190
H	1.0	-4.4328357573	-8.6972161769	1.7624129961
C	6.0	-2.5706782074	1.3965061439	-1.5079150967
N	7.0	-2.0092060374	0.0571823330	-1.6897000535
H	1.0	-1.9401137744	2.2000190137	-1.9341677963
H	1.0	-4.9983188274	-7.0057169852	3.5241380077
H	1.0	-2.7354803854	1.6149124631	-0.4514099143
H	1.0	-3.4912550270	-5.7109171327	1.8146038710
C	6.0	-2.9724834491	-4.0185698098	1.0176059445
H	1.0	-1.9465775004	-5.5144265061	-0.1489123113
C	6.0	-1.4013234465	-3.5802939838	-0.8992325994
O	8.0	-3.2967078120	-4.8130382524	2.1400106747
H	1.0	-0.6350358341	-4.0151107279	-1.5522406753
H	1.0	-2.7573349797	-3.0198083987	1.4139704882
C	6.0	-1.7390454377	-4.5197031279	0.2590570074
H	1.0	-0.1189131533	-1.9074082426	-2.1913699027
C	6.0	-0.6538109063	-0.0757659100	-1.1295152421
O	8.0	-0.9348082418	-2.3689524260	-0.3364494285
H	1.0	0.0529229846	0.5206961240	-1.7415029679
C	6.0	-0.1255263831	-1.5286927380	-1.1627953811
H	1.0	-1.2281453097	-0.1799631937	0.9446907980
H	1.0	-0.8882541289	-4.5920033924	0.9410209940
H	1.0	-0.8181747595	1.4654690298	0.4242567450
C	6.0	-0.5507946057	0.4128112146	0.3231916765
H	1.0	1.9687077241	-3.3762686305	-1.6021998421
C	6.0	1.3292887221	-1.5387190623	-0.6506991351
H	1.0	1.9187998103	-0.8927401068	-1.3174478877
H	1.0	1.3977967418	-3.5700632157	0.0756150652
C	6.0	1.9555755799	-2.9234991698	-0.6057494994
C	6.0	0.8672094083	0.2613905058	0.8749690034
H	1.0	2.5451698308	1.4300803820	-1.4098924422
O	8.0	1.4076761993	-1.0235663999	0.6912892954
O	8.0	1.6702817750	1.2772187445	0.2703914665
O	8.0	3.3664885428	1.3802321793	-1.9269334039
H	1.0	0.8721487672	0.4206090904	1.9585409952
H	1.0	4.4645922871	-0.7829314508	-2.7142772869
H	1.0	2.9858914280	-2.8574912976	-0.2469034232
O	8.0	-0.5755529985	7.7715905828	3.9653940066
H	1.0	-0.4539505114	6.7903436577	3.9116105848
H	1.0	-0.3636908384	10.2901864553	3.6180870636
O	8.0	0.3636952804	5.5012155057	3.2121134858
C	6.0	0.2959140647	8.3167772069	3.1096570260
H	1.0	0.7237110053	3.9145202430	2.9731384419
C	6.0	0.3226004244	9.7196373968	3.0018317862

		O	8.0	1.2613057608	3.2298775299	2.4911647605
		C	6.0	1.1660540397	6.0818688765	2.4163549162
		C	6.0	1.1808589982	7.5380841054	2.3184040785
		C	6.0	1.2055381038	10.3380153661	2.1300138888
		H	1.0	1.2134752906	11.4214771245	2.0587539833
		C	6.0	2.0797424889	3.9031078277	1.6717294439
		C	6.0	2.0782185414	5.3052348350	1.5936009597
		C	6.0	2.0745754759	8.1977924755	1.4341129577
		C	6.0	2.8945351247	1.6296200747	0.9659602628
		C	6.0	2.0856208399	9.5851335788	1.3417839913
		H	1.0	4.8078029972	3.4305720909	-1.8826434723
		C	6.0	2.9785577718	3.1376924272	0.8707858083
		C	6.0	4.4710176163	1.4816100160	-1.0246595679
		C	6.0	5.3310926472	-0.7318756257	-2.0515232008
		C	6.0	2.9781320913	5.9568801302	0.6973527515
		H	1.0	2.7804054715	10.0568088142	0.6572848365
		C	6.0	3.0105597336	7.4113267847	0.5941856534
		H	1.0	3.8988755696	-0.1426921198	0.3177518672
		C	6.0	3.8461606950	3.7644006300	-0.0039256160
		C	6.0	3.8535721129	5.1908357312	-0.0870004733
		O	8.0	3.8024094498	7.9913609598	-0.1804545617
		H	1.0	5.9239331781	1.2688912367	-2.5886716332
		H	1.0	5.1248452201	-1.3475309111	-1.1699445301
		H	1.0	2.7844620992	1.3413953177	2.0168842061
		H	1.0	6.1858337869	-1.1802423116	-2.5676075003
		O	8.0	4.7269957572	5.7510638022	-0.9290699105
		C	6.0	4.1115238558	0.9269948839	0.3628672235
		C	6.0	4.8290716045	3.0043293588	-0.8774004029
		C	6.0	5.6405398014	0.7211878616	-1.6826131866
		H	1.0	4.5884320603	6.7392223722	-0.8512965871
		H	1.0	4.9637158423	1.0784206981	1.0339611261
		H	1.0	6.5071585375	0.7544851234	-1.0122665656
		C	6.0	6.2388590414	3.2122924678	-0.3205541761
		O	8.0	7.1146682432	3.5219307463	-1.2949695126
		O	8.0	6.5484797775	3.0874925243	0.8470241283
		H	1.0	9.0336031923	3.9667322072	-1.7614946361
		C	6.0	8.4736325416	3.7107531039	-0.8627435028
		H	1.0	8.8655292364	2.7953112221	-0.4125358279
		H	1.0	8.5322101714	4.5183524934	-0.1296806430
3'-Hydroxy daunorubicin	64842-75-7	O	8.0	5.3085405758	-0.4244607283	-2.6455138686
		H	1.0	0.3207910677	3.1088384775	-3.6135895054
		H	1.0	2.1101550990	0.1387544274	-3.5287899356
		O	8.0	0.9476209347	2.3563642811	-3.4221832146

O	8.0	-0.8803383769	4.0985423667	-3.1052573708
H	1.0	5.7241006836	-2.6807828652	-3.7093358879
C	6.0	4.4608093193	-1.2981649411	-2.6831910773
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C	6.0	2.5188800217	0.2850110520	-2.5244618857
H	1.0	3.9865847871	-2.7853148539	-4.1529905275
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H	1.0	3.3451963984	0.9990058228	-2.6294199844
C	6.0	0.6919587643	1.9750111249	-2.1655793728
C	6.0	3.0854716401	-1.0560237127	-2.0172148678
H	1.0	1.6167457593	-2.2780033938	-1.6137463007
C	6.0	-1.0674074429	3.6942458458	-1.9373550587
C	6.0	-2.8414369487	5.3782598261	-1.6603774990
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H	1.0	-4.4030825932	6.8234675839	-1.3470802475
C	6.0	-0.2912229811	2.5991743476	-1.3793423713
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C	6.0	-2.1062998877	4.3374911170	-1.0889437323
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C	6.0	1.2314808450	0.4736722461	-0.3385946606
H	1.0	3.7488222845	-1.9031133535	-0.1255112095
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C	6.0	-0.5219821166	2.1661236676	-0.0433792556
H	1.0	4.0241682170	-0.1687660212	-0.2854761421
O	8.0	1.1070951010	-1.8331633911	0.1786717096
H	1.0	-1.7531168846	-5.5399767799	-0.8119924159
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O	8.0	0.9262469994	-4.0852580853	0.5625031529
C	6.0	-2.3385454451	3.9108745334	0.2422195344
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H	1.0	-0.4841481290	-6.3240395952	0.1425779577
C	6.0	-4.0811142420	5.6200225523	0.3979541387
H	1.0	2.4043855282	-2.9786217732	1.3258165600
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		C	6.0	0.2861953354	1.2733588468	0.1321009781
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		O	8.0	-0.2861580853	3.7365455508	-1.0882118101
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H	1.0	-1.2918758908	1.4973836520	-1.1109891272
H	1.0	0.0455232742	6.0037817622	2.5016999970
C	6.0	-0.5435702475	5.4576112988	1.7471001207
O	8.0	-1.9289329254	5.5354199318	2.0727945870
C	6.0	0.6520704153	1.7212015671	-2.9155992233
O	8.0	-0.3005885017	3.9150020770	-0.6656132094
H	1.0	-0.0575659262	2.4436369151	-2.5129567016
H	1.0	0.1213822530	1.0239035945	-3.5942801754
H	1.0	-2.8710730299	5.0269267681	-0.1425002082
H	1.0	-2.1960948008	6.4494264328	1.8958633821
H	1.0	1.3750142418	2.2816997908	-3.5154065921
H	1.0	2.9093148591	8.4030782280	2.1795793784
H	1.0	0.8353504004	6.1735120524	0.2759338410
C	6.0	-0.2529649885	6.0927907972	0.3797270260
H	1.0	2.3753247853	9.7249941706	3.2397349709
H	1.0	0.4090737397	8.5857634544	2.2564979852
C	6.0	-0.7932543756	5.2549676592	-0.8050427873
C	6.0	-2.3074933746	5.3247084290	-1.0275228676
C	6.0	2.4145271150	9.3771598426	2.2030858298
H	1.0	-2.5788937642	4.6755370304	-1.8653698297
O	8.0	-0.8333779153	7.4092857613	0.4017374672
H	1.0	-2.5997199954	6.3479647598	-1.2784740410
C	6.0	1.0077848006	9.2663058225	1.6375509061
H	1.0	-0.3050410512	5.6118091768	-1.7196487915
H	1.0	3.0109641863	10.0888199307	1.6273063396
H	1.0	0.1599670680	11.0597843796	2.5229826456
O	8.0	1.1273508517	8.7061441143	0.3083123777
H	1.0	-1.7432849543	9.8232065536	1.6131898925
C	6.0	0.2672092606	10.6038655125	1.5327661335
C	6.0	-0.1189352890	8.4038526921	-0.3089360872
H	1.0	0.1625688267	8.0284977208	-1.3004577395
C	6.0	-1.1277779134	10.4024740274	0.9155727389
C	6.0	-1.0086833800	9.6423789795	-0.4176292162
O	8.0	1.0003938346	11.5465826655	0.7417653298
H	1.0	-1.9990375703	9.3632723748	-0.7860854468
O	8.0	-1.7746215563	11.6494237354	0.7400403116

		H	1.0	1.3851109428	11.0430834673	0.0079631688
		H	1.0	-1.0853406730	12.2451278543	0.4040846151
		H	1.0	-0.5638953147	10.3135621079	-1.1614446624
		H	1.0	7.7029446676	1.0150980091	-0.3151042160
		H	1.0	6.6856704192	2.4565621179	-0.1823968547
		H	1.0	4.0475078482	4.8508416590	2.8688669713
		H	1.0	5.3114626921	3.0573052196	1.7642205619
		C	6.0	6.6700814605	1.3731519954	-0.2736837376
		H	1.0	3.4845011498	5.2134105654	1.2290038349
		H	1.0	7.2872849306	-0.9030235262	0.6662119420
		C	6.0	3.2500193029	4.6681051024	2.1439068696
		O	8.0	4.5737531404	3.3121118891	-0.0990575602
		N	7.0	6.0176560098	0.7385701154	0.8749237221
		H	1.0	6.1917128294	1.1216249039	-1.2401234552
		C	6.0	4.4740327235	2.6756058904	1.1702199638
		H	1.0	2.3093584068	5.0351296950	2.5607446726
		C	6.0	6.2155772314	-0.7126498541	0.7752956522
		H	1.0	4.9354062065	0.4636754810	3.1024324303
		H	1.0	3.9966550038	2.8402422157	-0.7160223702
		C	6.0	3.1691403803	3.1677929793	1.8740779652
		C	6.0	4.6110415842	1.1287413199	1.0935931220
		H	1.0	5.8606716967	-1.2309019752	1.6627376050
		O	8.0	3.0903847416	2.5540083321	3.1761204820
		H	1.0	5.6997715486	-1.1561527360	-0.0965025368
		C	6.0	4.0931284380	0.4467203347	2.4012107233
		H	1.0	1.9092605431	4.4780558289	-0.2432557620
		H	1.0	3.9596424311	0.7771299216	0.2634835895
		C	6.0	2.9318060368	1.1774660021	3.0944216361
		H	1.0	2.8179904682	0.7997780758	4.1115332604
		C	6.0	1.9439904304	2.7647571393	1.0627897206
		C	6.0	1.4635780603	3.5234528391	0.0089871455
		O	8.0	3.7202164695	-0.9087427062	2.2314717420
		O	8.0	1.6979844935	0.8103812165	2.4485187498
		H	1.0	2.7840452059	-0.9367124011	1.9667295818
		C	6.0	1.3206894270	1.5255987861	1.3607564762
		C	6.0	0.3601121088	3.1011274354	-0.7580208005
		O	8.0	-0.0657391891	3.9259153692	-1.7232062086
		C	6.0	0.2893648108	1.0268350950	0.5541215334
		H	1.0	-0.8384063910	3.4806431654	-2.1546456771
		C	6.0	-0.2266891424	1.8419666018	-0.4968803726
		O	8.0	0.3984016950	-1.2141010789	1.3745928963
		C	6.0	-0.1967172155	-0.3716385308	0.7064749204
		C	6.0	-1.3763815024	1.4051509265	-1.2879217627
Menogaril	71628-96-1					

		O	8.0	-1.8410276142	2.1552898278	-2.2007853822
		C	6.0	-1.4340771436	-0.7493412591	-0.0414383220
		C	6.0	-1.9940351658	0.1207126985	-1.0070638313
		H	1.0	-3.1372292488	1.2877414264	-2.7323641392
		H	1.0	-1.5300918675	-2.6473806903	0.9102064846
		C	6.0	-2.0045525372	-1.9883779889	0.1909295945
		C	6.0	-3.1560314501	-0.2931163628	-1.7078902612
		O	8.0	-3.7037531177	0.4748942927	-2.6617343697
		C	6.0	-3.1630503993	-2.3980587060	-0.4975204680
		C	6.0	-3.7635234789	-1.5403622485	-1.4261487173
		H	1.0	-5.7318388993	0.4567089968	-0.7868116393
		H	1.0	-2.8925543779	-4.4817150118	-0.6860296948
		H	1.0	-3.7072208349	-4.0223152770	0.7988771140
		C	6.0	-3.6613303281	-3.8115390308	-0.2749867681
		H	1.0	-5.0654971202	-1.4788688445	-3.1350196643
		C	6.0	-5.0499992385	-1.9334011868	-2.1370539004
		C	6.0	-6.4662279425	-0.0850280753	-1.3952117792
		H	1.0	-6.4593348852	0.3362296166	-2.4073880547
		O	8.0	-6.2201060583	-1.4837868991	-1.4185021563
		H	1.0	-4.4294425525	-3.8245856868	-2.9386782198
		H	1.0	-7.4571815439	0.0432660075	-0.9538080768
		C	6.0	-5.0375431675	-4.1650519752	-0.8837961965
		C	6.0	-5.1926147286	-3.4539113027	-2.2437475056
		O	8.0	-6.0783868462	-3.7858571960	0.0166986703
		H	1.0	-6.3060615647	-2.8602599281	-0.1733702902
		H	1.0	-4.4022830161	-6.0836253563	-1.7204220615
		H	1.0	-5.0556677459	-6.1694186292	-0.0698345946
		C	6.0	-5.1634565694	-5.6821525258	-1.0438410013
		H	1.0	-6.1739598880	-3.6858117951	-2.6692950038
		H	1.0	-6.1533944731	-5.9308286224	-1.4358259004
		H	1.0	-1.6755327775	-1.1783348926	-4.6943858571
		O	8.0	-0.7443547402	-1.1519990569	-4.3325076609
		O	8.0	-3.2681269411	-0.9103212356	-4.4842588432
		H	1.0	-5.6371681459	-0.6473829155	-4.4838858482
		H	1.0	3.4625181694	0.9816155329	-4.8831271569
		H	1.0	1.5861718103	-0.6522044952	-4.0853108237
		H	1.0	4.8106007094	1.4033888734	-3.8430809547
		C	6.0	3.7534001060	1.6390953071	-4.0509870918
		C	6.0	-5.7427010255	-0.2255067584	-3.4919846302
		H	1.0	-7.8805273747	-0.0039224651	-3.5667658138
		H	1.0	1.8199046428	-1.9566049694	-2.9494375350
		C	6.0	-3.2964684750	-0.4449183581	-3.3235708604
		C	6.0	1.6496940762	-0.8743121156	-3.0164554398
4'-O-methylodoxorubicin	77121-90-5	H	1.0	-1.6755327775	-1.1783348926	-4.6943858571
		O	8.0	-0.7443547402	-1.1519990569	-4.3325076609
		O	8.0	-3.2681269411	-0.9103212356	-4.4842588432
		H	1.0	-5.6371681459	-0.6473829155	-4.4838858482
		H	1.0	3.4625181694	0.9816155329	-4.8831271569
		H	1.0	1.5861718103	-0.6522044952	-4.0853108237
		H	1.0	4.8106007094	1.4033888734	-3.8430809547
		C	6.0	3.7534001060	1.6390953071	-4.0509870918
		C	6.0	-5.7427010255	-0.2255067584	-3.4919846302
		H	1.0	-7.8805273747	-0.0039224651	-3.5667658138
		H	1.0	1.8199046428	-1.9566049694	-2.9494375350
		C	6.0	-3.2964684750	-0.4449183581	-3.3235708604
		C	6.0	1.6496940762	-0.8743121156	-3.0164554398

C	6.0	-0.8479363122	-0.6509213712	-3.0949850594
O	8.0	4.0089349739	-0.9036571075	-2.9334452683
O	8.0	3.5793669722	2.9879460366	-4.3798678295
C	6.0	-6.9809024270	0.1346266881	-2.9747094310
H	1.0	4.7873075831	-0.6859915889	-2.4018137942
C	6.0	-4.5939899096	-0.0418001784	-2.7194756558
C	6.0	-2.0846339295	-0.2845374594	-2.5398415185
C	6.0	2.8860297715	-0.2059157322	-2.3867028378
C	6.0	0.3521252374	-0.4982287736	-2.3429568165
C	6.0	2.9452501984	1.2683832495	-2.8138809244
H	1.0	3.0514063074	3.3647767777	-3.6534310187
O	8.0	2.3591817117	2.1501809207	-2.2051798890
C	6.0	-7.0822771749	0.6749478089	-1.6959829463
C	6.0	-4.6582569022	0.5073260295	-1.4148741688
H	1.0	2.8816185350	-1.4579006251	-0.6783555568
C	6.0	-2.1404609993	0.2625036560	-1.2279688607
C	6.0	2.8236912557	-0.3805848967	-0.8655064552
C	6.0	0.2990652222	-0.0130724394	-1.0460309676
H	1.0	-8.0569040739	0.9476418328	-1.3125967797
C	6.0	-5.9382179421	0.8678865272	-0.9041238679
H	1.0	3.6890426501	0.0873425550	-0.3822419777
C	6.0	-3.4106985494	0.6923130142	-0.6326403301
C	6.0	-0.9497688387	0.4071219436	-0.4926976805
C	6.0	1.5450356206	0.1374571832	-0.1872747216
H	1.0	1.6560278980	1.1983690412	0.0571922524
O	8.0	-6.0014198785	1.3855667310	0.3398471591
O	8.0	-3.4212185372	1.2012607428	0.5090404124
O	8.0	1.3537539425	-0.6135893136	1.0231749705
H	1.0	-7.7451483289	2.5399020568	0.2826304792
O	8.0	-0.9419022270	0.9571651204	0.7258359259
H	1.0	-7.9377475614	0.8939827411	0.9608247844
H	1.0	1.1671716743	1.1001395786	2.1468529665
C	6.0	-7.2642123744	1.7556394563	0.8794722551
H	1.0	-1.9022784873	1.1877771821	0.9161103796
C	6.0	1.5838838848	0.0921065083	2.2281357164
H	1.0	-0.1086203473	-0.9254415105	3.0529785729
H	1.0	-7.0505775311	2.1417738148	1.8761823651
C	6.0	0.9163150718	-0.6919107225	3.3588948054
H	1.0	3.6329189142	-1.5540290435	1.8222903582
O	8.0	2.9710304432	0.2972661653	2.4660021813
H	1.0	1.6099239487	-2.6345337459	2.8151629239
H	1.0	0.8532138104	-0.0394933263	4.2346276010
C	6.0	3.7317457668	-0.9056135388	2.7053781195
C	6.0	1.6821338309	-1.9875224951	3.7001379472

		H	1.0	5.5134893395	0.0698229583	1.9761146982
		H	1.0	0.1624443491	-2.7860654051	4.8223595490
		N	7.0	1.1784237545	-2.7471103910	4.8420121992
		C	6.0	5.1887528713	-0.4929674479	2.8557572370
		C	6.0	3.1907437089	-1.7252119084	3.8916979420
		H	1.0	3.6917216140	-2.6998056833	3.8639138424
		H	1.0	5.8220358167	-1.3795513425	2.9566016485
		H	1.0	2.1543259461	0.1144737692	5.9760036243
		H	1.0	3.2777414448	0.8118286806	4.7825289413
		H	1.0	1.4529093993	-2.2824338105	5.7038847050
		H	1.0	5.3383819886	0.1304795329	3.7392847729
		C	6.0	3.1820738334	0.0792310866	5.5878052670
		O	8.0	3.5542226996	-1.2358236591	5.1855092196
		H	1.0	3.8579102773	0.3501541726	6.4043503246
Morpholino adriamycin	89196-04-3	H	1.0	-4.2141316191	4.2189006173	4.8690221537
		H	1.0	-5.6654406817	4.1416721489	3.8225975897
		C	6.0	-4.5690827444	4.1400638641	3.8346491050
		H	1.0	-4.2002077842	4.9895923397	3.2601866882
		H	1.0	-5.5525219137	2.4305358701	5.3214219373
		O	8.0	-4.0401367028	2.9879977694	3.1869160254
		C	6.0	-5.1345120071	1.5749163844	4.8071796099
		C	6.0	-4.3261313277	1.7641405159	3.6736804563
		H	1.0	-6.0352771474	0.1766160697	6.1594349366
		C	6.0	-5.4076817109	0.2954899552	5.2814114107
		O	8.0	-2.6404605928	1.8778251080	1.3062086242
		C	6.0	-3.7799064199	0.6330014032	3.0015453119
		C	6.0	-2.9234022238	0.7628845303	1.7996775614
		H	1.0	-1.7617564623	1.5081051937	0.0666348410
		C	6.0	-4.8844858249	-0.8218527726	4.6412330842
		C	6.0	-4.0788858814	-0.6548008746	3.5135009713
		O	8.0	-1.2732530677	0.8322648139	-0.5000370226
		H	1.0	-5.0828283053	-1.8272774276	4.9915566402
		H	1.0	5.9104026367	-0.4132062234	-1.0242367559
		C	6.0	-2.3970701595	-0.4579722629	1.1801624973
		C	6.0	-1.5742624627	-0.3535042167	0.0463783635
		C	6.0	-3.5467962015	-1.8862318823	2.8703152582
		H	1.0	5.5811179054	-0.7134355593	0.6898276792
		O	8.0	4.6820055865	1.8491026556	-1.3145874171
		H	1.0	4.5685964050	1.3262692228	-2.1227166158
		H	1.0	-0.4925116704	-0.5221214209	-2.3723714130
		C	6.0	5.2062360398	-0.8711256126	-0.3259375948
		C	6.0	-2.6976585197	-1.7484879542	1.6979310692
		H	1.0	1.8500279691	-0.4928446024	-3.1114297973

H	1.0	5.1613452500	-1.9458393978	-0.5188510465
O	8.0	-3.8318118683	-3.0079969282	3.3408727972
C	6.0	-1.0446595495	-1.5237871690	-0.5698905459
C	6.0	-0.1229749278	-1.3504203414	-1.7578139646
C	6.0	-2.1793867386	-2.8974259572	1.0773502086
H	1.0	-0.9562283910	-2.7938744406	-3.1337123443
C	6.0	3.7998893138	1.2777197418	-0.3451563988
C	6.0	2.0283578941	-0.2087099308	-2.0666044527
C	6.0	3.8254638633	-0.2535210905	-0.4687237179
H	1.0	2.3017767163	1.8312532536	-2.6649558664
H	1.0	4.1783188794	1.5880213203	0.6341934587
H	1.0	1.1458424448	4.3528369264	1.2446956046
C	6.0	-1.3371092168	-2.7818734318	-0.0682641815
H	1.0	2.0978419632	5.7105535264	-2.4497966242
H	1.0	-3.0338640050	-4.0140233047	2.3200321042
O	8.0	1.1703335452	-0.9864543253	-1.2111055270
O	8.0	3.3515090561	-0.5987827477	-1.8001672813
C	6.0	-0.0132461965	-2.6225867529	-2.6041533804
O	8.0	-2.4452196959	-4.1301327324	1.5228429813
O	8.0	0.5383348181	5.2841875640	-1.2286198718
C	6.0	1.7934416811	1.2933079704	-1.8564715743
N	7.0	2.1754256346	3.1702769754	-0.1340117863
H	1.0	0.7684348836	-2.4954797450	-3.3612286121
H	1.0	-1.6760463555	-4.5595899267	-1.1948694385
H	1.0	3.1443915567	-0.6906165855	0.2712954040
C	6.0	2.3357439358	1.7641145219	-0.4830729451
C	6.0	0.9177786005	3.5920727305	0.4824927429
C	6.0	1.6863512049	4.8318928061	-1.9418340478
H	1.0	-0.9287464204	4.6439057075	0.0176282636
C	6.0	-0.8351202331	-4.0557584403	-0.7019404835
C	6.0	-0.0701256804	4.2158359022	-0.5100004233
H	1.0	3.0975491841	5.0299502116	-0.3458927331
C	6.0	2.7260117985	4.2222846398	-0.9943191089
H	1.0	0.7251630489	1.5043047745	-1.9384901303
C	6.0	0.2987303266	-3.8553734311	-1.7271785241
H	1.0	1.3828056005	4.1018906724	-2.7114850175
H	1.0	0.4491231603	2.7448716863	0.9927734800
H	1.0	1.7743814653	1.2120652184	0.2799041568
O	8.0	-0.6284010041	-5.5247295521	-3.1939244871
H	1.0	-0.4854590679	-4.7371514617	0.0792859072
H	1.0	1.7415663400	-2.7843134289	-0.9628239623
H	1.0	-0.4446502297	3.4540013269	-1.2139692635
C	6.0	0.3693283179	-5.0827151910	-2.6449826929
O	8.0	1.5619732416	-3.7322183487	-1.0888833578

		H	1.0	3.5816649908	3.8300931986	-1.5454495548
		C	6.0	1.7149567799	-5.7359817989	-2.8931638258
		H	1.0	0.6561043879	-6.8535565668	-4.0171316093
		H	1.0	2.4180277022	-4.9647213677	-3.2427829039
		O	8.0	1.6049998821	-6.7909903594	-3.8084785853
		H	1.0	2.1107383840	-6.0701744240	-1.9213064128
		H	1.0	-2.7778643250	3.2183676172	-4.5064436301
		H	1.0	-3.8444055276	1.8748886603	-4.9604454630
		H	1.0	-1.5441394476	1.0165536480	-4.6588414453
		C	6.0	-3.2201804963	2.2818275655	-4.1588121197
		H	1.0	-0.0573583045	2.8966401755	-3.8766536694
		O	8.0	0.7472256646	0.8066542053	-3.8302827888
		O	8.0	-0.6168065505	3.0761532276	-3.1043158146
		C	6.0	-2.1273483516	1.2817279346	-3.7701974071
		H	1.0	0.8847226898	-0.1136799139	-4.1003166584
		H	1.0	-3.8819810129	2.5211523692	-3.3192827152
		H	1.0	0.6585187314	-2.8369848824	-3.8750366480
		H	1.0	-2.5831246910	0.3521141196	-3.4056319377
		O	8.0	0.5900714502	-1.8535802144	-3.6650445965
		C	6.0	-1.1371003952	1.8088765316	-2.7048832568
		C	6.0	0.0854860278	0.8404821487	-2.5779283663
		O	8.0	0.3484389103	-4.3357798208	-3.5168424348
		H	1.0	0.7583913789	1.3110235261	-1.8494933255
		C	6.0	-0.1112764425	-1.7606181097	-2.5194288655
		H	1.0	0.0146412715	-6.7474428217	-3.2298676871
		C	6.0	-0.3686227231	-0.4742478772	-1.9716234896
		C	6.0	-0.3053112669	-4.2255785153	-2.4553698174
		H	1.0	-2.8914801181	1.9008637528	-1.4160764763
		C	6.0	-1.8061566209	1.9985178231	-1.3219159465
		C	6.0	-0.5844116710	-2.9153625093	-1.8713969066
		C	6.0	-0.5540620158	-6.6847297430	-2.3099348247
		H	1.0	-1.5994342185	3.0139066832	-0.9761010910
		C	6.0	-0.8131886421	-5.4322425177	-1.7643039537
		H	1.0	-0.8290519923	-8.8112721135	-2.0876647314
		C	6.0	-1.0954061150	-0.3674013747	-0.7890918251
		C	6.0	-1.0307801724	-7.8326830702	-1.6628777132
		C	6.0	-1.3313288621	-2.8011947655	-0.6633623604
		C	6.0	-1.3393695576	1.0242194708	-0.2259124569
		H	1.0	5.8000841708	2.7077101675	0.3495956544
		C	6.0	-1.5552583513	-5.3047327630	-0.5609034912
		C	6.0	-1.5836802097	-1.5229372571	-0.1262341550
		H	1.0	3.5517309780	3.9061968145	0.3941947379
		C	6.0	-1.8275680347	-3.9904270960	0.0125114436
MX2	NCI 619003					

		C	6.0	-1.7567883945	-7.7372132141	-0.4862592165
		O	8.0	-0.1080733649	1.5344861403	0.3359556978
		H	1.0	4.4551726318	1.6053826408	0.7315094311
		H	1.0	-2.0880105523	0.9809795389	0.5671506967
		C	6.0	-2.0296557246	-6.4778641479	0.0815634864
		H	1.0	-2.1318006532	-8.6167459052	0.0256197316
		O	8.0	-2.2755739581	-1.3480152377	1.0081810576
		C	6.0	5.0299201349	2.4756601960	1.0928642456
		H	1.0	1.5848739007	3.4756765081	1.1329422729
		C	6.0	4.1052760977	3.6792009646	1.3116522780
		O	8.0	-2.4915969884	-3.8879214679	1.0891268525
		H	1.0	-2.5334553437	-2.2534543849	1.3254373855
		H	1.0	-0.7219507544	3.6875825410	1.5067242991
		H	1.0	4.7425569454	4.5485921280	1.5341174835
		O	8.0	-2.7343092802	-6.4447153856	1.2168943341
		H	1.0	-2.8292232552	-5.4921966748	1.4688565671
		H	1.0	2.2052602173	1.0685727662	1.2538071824
		O	8.0	5.7176167880	2.1429684353	2.2938439449
		C	6.0	0.1084232549	1.2009113658	1.6963698520
		C	6.0	1.8169708713	3.0500512978	2.1165264651
		C	6.0	1.5713453978	1.5223693771	2.0197823471
		C	6.0	-0.6419952523	3.3282791410	2.5400899263
		H	1.0	0.9167516438	4.7291067128	3.1393948332
		N	7.0	3.1705960916	3.5011060039	2.4213319327
		H	1.0	-0.1157089404	0.1419031031	1.8697699150
		H	1.0	-2.7388414020	3.5515572444	2.9962842864
		C	6.0	0.7617336884	3.6468174088	3.0810973822
		O	8.0	-0.7992908808	1.8874062963	2.5491811999
		H	1.0	-1.7584959335	4.9950616786	3.3292460855
		H	1.0	4.2276525863	0.9380067743	3.0918408689
		C	6.0	-1.7753002392	3.9018311041	3.3753093136
		C	6.0	4.8026043678	1.8441889026	3.3463077358
		H	1.0	1.8190289127	1.0480990012	2.9754137238
		C	6.0	3.8636154767	3.0248223756	3.6222635179
		H	1.0	4.4764925568	3.8526727611	4.0088657331
		H	1.0	5.4138122448	1.6219476559	4.2273330544
		H	1.0	-1.6772912027	3.6031146113	4.4215981029
		O	8.0	0.8774496684	3.1498857268	4.4172384866
		H	1.0	3.1295481895	2.7760131592	4.3896101844
		H	1.0	0.3985854022	2.3068786516	4.4287220290
NSC 286628	NSC 286628 / 67903-59-7	H	1.0	-0.3374915892	-1.6051806595	-6.2974900014
		H	1.0	-2.1221541211	-2.2617139599	-7.8061109043
		H	1.0	-4.4957332679	-2.8653292578	-8.1659034087

H	1.0	-0.8878105439	0.0203893531	-5.8788708448
C	6.0	-2.8547274141	-2.0618449306	-7.0270835480
C	6.0	-4.1931992050	-2.4010664461	-7.2318694958
H	1.0	-0.7634657938	-3.5312432682	-5.4279144951
C	6.0	-1.0071284158	-1.0403067409	-5.6369475931
C	6.0	-2.4491574276	-1.4638111790	-5.8290897482
C	6.0	-5.1363588580	-2.1529920450	-6.2342105902
H	1.0	-6.1770593023	-2.4216955193	-6.3888336210
C	6.0	-3.4005997698	-1.2136979666	-4.8330421232
C	6.0	-4.7359325301	-1.5606213854	-5.0344017542
H	1.0	-3.0853276431	-0.7521540520	-3.9023285420
H	1.0	-0.0485545489	-5.6432940596	-4.4075165591
H	1.0	-5.4661009537	-1.3665920540	-4.2541700524
C	6.0	-0.3429441100	-3.5207036234	-4.4313794060
O	8.0	-0.5606529418	-1.1174520978	-4.2790324804
C	6.0	0.0522269704	-4.7194672511	-3.8459891498
C	6.0	-0.2259912881	-2.3077363344	-3.7327299742
C	6.0	0.5665658772	-4.7396450954	-2.5550907247
C	6.0	0.2695245809	-2.3077212269	-2.3976753564
H	1.0	0.8871922346	-5.6587391428	-2.0802562737
O	8.0	0.0185219234	0.0426776793	-2.0423415563
C	6.0	0.6685479326	-3.5470527019	-1.8367769713
C	6.0	0.3683667379	-1.0682679558	-1.5872402639
H	1.0	0.3172352259	1.0193988513	-0.8499168249
C	6.0	1.2194941793	-3.6271686720	-0.4594374380
O	8.0	1.5987167131	-4.7285639880	-0.0027102204
C	6.0	0.8810741216	-1.1654429453	-0.2156159585
H	1.0	-0.4584713917	5.5744201660	-0.2737565781
O	8.0	0.6168438151	1.1930036896	0.0942693119
C	6.0	1.3036980700	-2.4099301049	0.3290199337
H	1.0	-2.5784682771	4.2697041865	0.7183315408
C	6.0	0.9632954742	-0.0033888454	0.5754536014
N	7.0	-0.0657023281	5.5290808963	0.6650776101
H	1.0	-0.2596531450	3.4519329076	0.6239113284
H	1.0	-0.5012323169	6.2942664560	1.1806661248
C	6.0	-0.4836766204	4.2791981552	1.3050157359
H	1.0	-4.4037195123	2.7073823303	1.9132987283
H	1.0	2.1134470734	-4.3124083618	1.4794815776
C	6.0	-1.9920934589	4.2281033348	1.6452595328
C	6.0	1.8248549066	-2.4648697417	1.6314846478
H	1.0	-2.0064507853	2.0771207773	1.8095760682
C	6.0	1.4519150677	-0.0751645530	1.9178079717
O	8.0	2.2577067510	-3.6096221334	2.1760916420
O	8.0	-2.3749896814	5.3771943291	2.4073161335

		C	6.0	-2.3185107089	2.9389627253	2.4103698080
		H	1.0	2.0415701257	1.9496008149	2.1674020985
		C	6.0	1.9061745133	-1.2837769024	2.4239801229
		H	1.0	5.2453819187	-1.5294470364	2.5767348916
		C	6.0	-3.7789791635	2.7980377691	2.8074806818
		H	1.0	1.3954352999	3.9788298086	2.3403205234
		C	6.0	0.3354683180	4.0756725070	2.5899172755
		C	6.0	1.4736656215	1.2067412953	2.7393358586
		H	1.0	6.4498182984	-0.2980431964	3.0080663514
		O	8.0	0.1054527292	1.6143187978	2.8592433412
		H	1.0	-4.1155750159	3.6721700137	3.3703911966
		H	1.0	-3.9179340202	1.9053720338	3.4226116939
		H	1.0	-2.1406547369	5.1705654901	3.3251610573
		C	6.0	5.5166319252	-0.7695031045	3.3192451631
		H	1.0	0.2521952624	4.9749883985	3.2141511137
		O	8.0	4.5503392248	1.3763913046	2.8807478489
		C	6.0	-0.1568303041	2.8929199170	3.4348432542
		O	8.0	-1.5501109862	2.9522961694	3.6392788220
		C	6.0	4.4264525302	0.2792688014	3.3950901945
		H	1.0	3.2469012129	-2.2036345876	3.8195401657
		C	6.0	2.5214483681	-1.3884137576	3.7986942390
		H	1.0	5.6391446356	-1.2750024092	4.2800830283
		C	6.0	2.1102313345	1.0411467701	4.1366010035
		C	6.0	3.1601607048	-0.0656423256	4.2244296204
		H	1.0	1.7609679751	-1.6434513506	4.5479819008
		H	1.0	0.2756638522	2.9423810694	4.4433993001
		H	1.0	2.5552719045	1.9914986725	4.4491157448
		H	1.0	1.3173602902	0.7813680450	4.8457951905
		O	8.0	3.5954697225	-0.2561345629	5.5785654780
		H	1.0	3.8610816886	0.6070819961	5.9269625213
		C	6.0	5.3755924936	2.6915009715	1.9463591201
		C	6.0	4.6667848500	1.3374979602	1.8301486558
		C	6.0	5.2893290137	0.1915664190	2.6622441454
		C	6.0	4.8615781837	0.2235990982	4.1577129908
		C	6.0	3.3210447764	0.3513929119	4.2359367445
		C	6.0	2.8537726195	1.5728607942	3.4341369859
		O	8.0	3.2591999212	1.4322961261	2.0696335083
		O	8.0	1.4575118869	1.6025123129	3.4414746323
		C	6.0	0.8598340150	2.7904199442	2.8837957467
		C	6.0	0.2720594280	2.4202564265	1.5193755413
		C	6.0	-0.7932387953	3.4053030884	1.0450575336
		C	6.0	-1.9770979152	3.3348163304	2.0612645549
		C	6.0	-1.5128018450	3.5391177492	3.5058434615
Nogalamycin	1404-15-5	C	6.0	5.3755924936	2.6915009715	1.9463591201
		C	6.0	4.6667848500	1.3374979602	1.8301486558
		C	6.0	5.2893290137	0.1915664190	2.6622441454
		C	6.0	4.8615781837	0.2235990982	4.1577129908
		C	6.0	3.3210447764	0.3513929119	4.2359367445
		C	6.0	2.8537726195	1.5728607942	3.4341369859
		O	8.0	3.2591999212	1.4322961261	2.0696335083
		O	8.0	1.4575118869	1.6025123129	3.4414746323
		C	6.0	0.8598340150	2.7904199442	2.8837957467
		C	6.0	0.2720594280	2.4202564265	1.5193755413
		C	6.0	-0.7932387953	3.4053030884	1.0450575336
		C	6.0	-1.9770979152	3.3348163304	2.0612645549
		C	6.0	-1.5128018450	3.5391177492	3.5058434615

C	6.0	-0.1797615981	3.3153446872	3.8605783726
C	6.0	0.2325524751	3.6158219155	5.1842974310
C	6.0	-0.7061232710	4.0442129998	6.1576185836
C	6.0	-2.0609176160	4.1889978019	5.7830030867
C	6.0	-2.4476908081	3.9449198349	4.4765472077
C	6.0	-3.1018073230	4.5905906504	6.7753418389
O	8.0	-4.2931312613	4.5150149287	6.4770471995
C	6.0	-2.6292103007	5.0225517505	8.1180075079
C	6.0	-3.5145259235	5.5646915469	9.0594194209
C	6.0	-3.1178964686	5.7499708666	10.4106497763
C	6.0	-1.8159705542	5.4668592078	10.7749890770
C	6.0	-0.8684834906	5.0254037502	9.8314230762
C	6.0	-1.2732905423	4.7864038387	8.4985401910
C	6.0	-0.2891080639	4.3183103863	7.5234557121
O	8.0	0.9207629425	4.1602361965	7.8683759276
O	8.0	0.3833274303	4.8326619157	10.2658029093
C	6.0	-4.1734632366	6.1830243642	11.4192212867
C	6.0	-4.8897437783	4.9620408251	12.0564626855
C	6.0	-5.5319047028	4.0715104416	10.9724539648
C	6.0	-6.4473805354	4.9154062749	10.0594694322
C	6.0	-5.7426733974	6.2258431422	9.6488638276
O	8.0	-4.7624519367	5.9130098552	8.6465306977
O	8.0	-5.1962510206	6.9334562913	10.7178498897
O	8.0	-6.8884836957	4.2209868494	8.9074775189
N	7.0	-6.1145362349	2.8813648102	11.6149341298
C	6.0	-7.4102636815	3.0888007527	12.2616968454
C	6.0	-6.1445536615	1.6954295189	10.7537688715
O	8.0	-3.9836537854	4.2098980014	12.8303169168
C	6.0	-3.6410835683	7.1246283810	12.4936785786
O	8.0	1.5305037410	3.4942025846	5.4719897315
C	6.0	-3.0524558293	4.3511687448	1.6947272453
O	8.0	-2.8357760576	5.4890930549	1.3141464969
O	8.0	-4.2908871063	3.8479757029	1.8242852904
C	6.0	-5.3719652839	4.7504270640	1.5076647171
C	6.0	-1.2679774828	3.0598848340	-0.3743117490
O	8.0	-0.1852077135	4.6930503404	1.0666894505
O	8.0	2.9510720060	0.4299290370	5.6003463368
C	6.0	1.7141106100	-0.1869028867	5.9193749857
C	6.0	5.3229605379	-1.0299020781	4.9065421587
O	8.0	5.3659561547	1.4342409070	4.7493119244
C	6.0	6.7129780512	1.4579242860	5.1834233347
O	8.0	4.8855278789	-1.0748646619	2.1419074151
C	6.0	5.6646044700	-1.5464463286	1.0615765759
H	1.0	4.7230946989	1.0251741879	0.7809409430

H	1.0	6.3872936665	0.2720989350	2.6138949149
H	1.0	2.8868429447	-0.5354251803	3.7538234221
H	1.0	3.2570087428	2.4932327641	3.8724828772
H	1.0	1.6316376882	3.5573944936	2.7598523035
H	1.0	-2.4384473874	2.3430743081	1.9842739776
H	1.0	-5.6803885014	5.3975776709	12.6918251749
H	1.0	-4.7108392480	3.6879478574	10.3569255222
H	1.0	-7.3487366595	5.2031091967	10.6126781117
H	1.0	6.4179212966	2.6034215639	1.6192976572
H	1.0	4.8773793426	3.4167623435	1.2965695090
H	1.0	5.3728430295	3.0683416557	2.9690806190
H	1.0	1.0878075044	2.3631613360	0.7950772073
H	1.0	-0.1630844590	1.4179872799	1.5975319744
H	1.0	-3.4952491374	4.0646761275	4.2280126477
H	1.0	-1.4842986001	5.5790367779	11.7995220925
H	1.0	0.9100737204	4.5329919851	9.4812510705
H	1.0	-6.4440570426	6.8918722864	9.1427092280
H	1.0	-6.1650195251	4.2476183214	8.2566491524
H	1.0	-8.2437350675	3.1893535630	11.5474397025
H	1.0	-7.6258596543	2.2334541433	12.9098925889
H	1.0	-7.3874558408	3.9823313432	12.8912608834
H	1.0	-5.1558039234	1.5342588409	10.3146505687
H	1.0	-6.3903050786	0.8187091047	11.3627308379
H	1.0	-6.8760306817	1.7760802771	9.9373670132
H	1.0	-4.3931203186	3.3252476676	12.8689950011
H	1.0	-3.1148748879	7.9687378687	12.0419634211
H	1.0	-4.4829282259	7.5073732514	13.0766558652
H	1.0	-2.9696460428	6.5934865243	13.1700917449
H	1.0	1.6412410112	3.6991947423	6.4343801118
H	1.0	-6.2840619020	4.1841014557	1.6893542565
H	1.0	-5.3318241479	5.6320979324	2.1503759742
H	1.0	-5.3099345174	5.0646828912	0.4636697537
H	1.0	-1.7080071501	2.0580160630	-0.4234608772
H	1.0	-2.0105474484	3.7818395080	-0.7286513365
H	1.0	-0.4146091536	3.0976696088	-1.0563603462
H	1.0	-0.9038431655	5.3431053458	0.9806467320
H	1.0	1.5743727726	-0.0637722231	6.9967487121
H	1.0	0.8771945946	0.2762368420	5.3880040480
H	1.0	1.7296488557	-1.2634928213	5.6877896651
H	1.0	6.4019860917	-1.1835912644	4.8114530978
H	1.0	5.0633664424	-0.9374912347	5.9628028461
H	1.0	4.8283112477	-1.9090574939	4.4920055464
H	1.0	6.9162317225	2.4893485417	5.4817807249
H	1.0	6.8838977609	0.8060107504	6.0488498296

		H	1.0	7.4265137341	1.1822316548	4.3931958460
		H	1.0	5.2450486258	-2.5095917198	0.7617003018
		H	1.0	5.6378076211	-0.8728791959	0.1925084659
		H	1.0	6.7166913027	-1.6908025396	1.3532323916
Pirarubicin	72496-41-4	H	1.0	3.3374727201	3.4481079269	-2.5831414204
		H	1.0	3.8464905902	1.6673764941	-0.8968077248
		O	8.0	4.5515006844	4.0754944832	-0.3942812922
		O	8.0	0.8187877122	4.6346038842	-3.7974909395
		H	1.0	0.0674843808	4.8371589054	-4.4244729939
		C	6.0	2.6061118100	3.8316387867	-1.8605933213
		H	1.0	-3.5737892985	4.2788383980	-5.9810675272
		H	1.0	3.0862294313	-2.2763597864	-0.9262667639
		H	1.0	2.4715769573	4.8958581045	-2.0703378463
		H	1.0	-5.8726511604	3.3318885602	-6.3148244533
		H	1.0	4.5846923831	4.9769922672	-0.7472789334
		C	6.0	0.3873989564	3.6277681721	-3.0275399743
		C	6.0	3.2118314829	2.1389524073	-0.1392368396
		O	8.0	-1.4310274154	4.5092177202	-4.9676795455
		C	6.0	-3.9514795308	3.4764961900	-5.3593613186
		C	6.0	1.2763326116	3.1352243078	-2.0293117706
		H	1.0	1.8533108319	-4.7729789915	0.3695946799
		C	6.0	3.1868517254	3.6312925002	-0.4608690248
		C	6.0	-5.2225809458	2.9454633632	-5.5355752722
		H	1.0	3.6885551027	1.9654868133	0.8295868318
		C	6.0	-1.7759742169	3.5743790322	-4.2108276168
		C	6.0	-0.8859525689	3.0582070848	-3.1861502168
		C	6.0	-3.1263104241	2.9686762924	-4.3528371941
		O	8.0	1.9823714195	0.0785302681	-0.5355694866
		C	6.0	0.8966115688	2.0677800350	-1.2315533496
		C	6.0	2.4448898793	-2.1868691689	-0.0420732922
		H	1.0	1.4136845013	-2.4028317214	-0.3403736466
		C	6.0	-5.6767825620	1.9145142890	-4.7173026087
		C	6.0	1.8273767661	1.4667995007	-0.1917154983
		H	1.0	-6.6705944337	1.5148705692	-4.8725757399
		C	6.0	-1.3055892436	2.0011792623	-2.3301487683
		C	6.0	-3.5548623443	1.9219627874	-3.5003395496
		H	1.0	-6.6927615172	-0.6070445940	-4.0543664382
		N	7.0	2.8053871383	-4.5859920293	0.6793882361
		C	6.0	-0.4203998519	1.5173463302	-1.3473322254
		C	6.0	-4.8623761228	1.3926681552	-3.6992055945
		H	1.0	3.5096301856	-0.4673944860	0.7511846853
		C	6.0	2.4733742301	-0.7550764379	0.4761115781
		C	6.0	-2.6460995220	1.4166610138	-2.4387461683

H	1.0	3.9385586575	-2.9686163842	1.3110837231
C	6.0	2.8884504468	-3.1716275196	1.0563048800
C	6.0	2.4450856428	4.4869883472	0.5915303745
H	1.0	3.4021960125	-4.7588234354	-0.1270257893
O	8.0	-5.2715651295	0.3933174884	-2.8899092718
H	1.0	3.7874510066	4.1438802124	2.2250673556
H	1.0	1.3300671458	1.5205688730	0.7833979379
C	6.0	-6.5711855496	-0.1560938180	-3.0618842282
O	8.0	-2.9996114882	0.5151098732	-1.6497758627
O	8.0	-0.7738472226	0.5677264723	-0.4843133771
O	8.0	1.7374268955	5.4291012482	0.2739819333
H	1.0	-0.9805380985	-5.1999636442	1.2744527646
H	1.0	-1.7160334569	0.3254114266	-0.7239314693
H	1.0	-6.6612348314	-0.9310288431	-2.3005104663
C	6.0	2.7025538623	4.2279264632	2.0704697544
H	1.0	1.6370291834	5.7945129154	2.2534058443
H	1.0	-7.3532605905	0.5970245080	-2.9064090785
O	8.0	1.6579974339	-0.6282478290	1.6276364010
H	1.0	1.0590711639	-5.3086019617	2.7165075372
O	8.0	2.1596700918	5.2456960210	2.8649418792
C	6.0	2.0744497242	-2.9326508244	2.3413994182
O	8.0	0.7205823340	-3.3619700398	2.1262058260
H	1.0	-0.9900965869	-6.9894257710	2.9841480588
H	1.0	2.2700024644	3.2447474357	2.3259290020
C	6.0	-1.0511581442	-4.9248318121	2.3324352795
H	1.0	3.1543745243	-1.1938983233	2.9445569382
C	6.0	0.3207418753	-4.4947630581	2.8401929898
C	6.0	2.0988407106	-1.4392469700	2.7212495941
H	1.0	2.5143967415	-3.5088794754	3.1624956386
H	1.0	-2.6179784698	-6.3322623262	2.8754175364
C	6.0	-1.5928282656	-6.0905837505	3.1757827214
H	1.0	-1.7128685538	-4.0542638203	2.4040357688
H	1.0	0.6008857134	-6.0851369418	4.9269562210
O	8.0	0.2626675625	-4.1556438885	4.2253393761
C	6.0	1.2302372840	-1.0886953956	3.9176490157
H	1.0	0.1920632401	-1.3537874235	3.7139542982
C	6.0	-1.5283571468	-5.7491301438	4.6721139071
H	1.0	1.2962005852	-0.0167915867	4.1225351117
C	6.0	-0.1255549111	-5.2613519206	5.0382230452
H	1.0	-1.7909400274	-6.6198300172	5.2849628779
H	1.0	1.5546279793	-1.6433160041	4.8017218909
H	1.0	-2.2483084672	-4.9549005800	4.9043773237
H	1.0	-0.0765019222	-4.9083009520	6.0720574223

Pyromycin	668-17-7	H	1.0	4.1865552180	-0.4965417497	-7.4982359136
		O	8.0	2.8116914367	1.4974323046	-6.6733414505
		C	6.0	3.6437055852	-0.7081720411	-6.5832400718
		H	1.0	2.2081494898	2.0860804561	-6.1404888155
		H	1.0	4.3303060534	-2.7339323250	-6.3873467427
		C	6.0	2.8455502464	0.3272198578	-6.0320140577
		C	6.0	3.7226818866	-1.9364470392	-5.9732784951
		O	8.0	1.2298072845	2.2726989319	-4.8283342893
		C	6.0	2.1285709779	0.0862303526	-4.8451978457
		C	6.0	3.0097933030	-2.2043307337	-4.7770723117
		C	6.0	1.3082685642	1.1537367673	-4.2799836529
		C	6.0	2.2105253978	-1.1927159222	-4.2098578292
		O	8.0	3.1387558836	-3.4252925254	-4.2452220921
		H	1.0	-5.5285052951	2.8558735820	-2.4452710088
		H	1.0	2.5818811502	-3.4375661466	-3.4262257125
		H	1.0	-0.2798057394	2.8341694532	-2.9731459631
		C	6.0	0.5618659367	0.8786158438	-3.0276431022
		C	6.0	1.4732243769	-1.4513396447	-2.9821681873
		H	1.0	-4.4793464353	2.3819825960	-3.7980735057
		C	6.0	-0.2261768922	1.8735359389	-2.4719717700
		C	6.0	-4.8400682803	2.0896740462	-2.8094759793
		C	6.0	0.6532497329	-0.3925584926	-2.4065012807
		O	8.0	1.5427870378	-2.5876818024	-2.4172702382
		H	1.0	-5.3328310059	1.1187933323	-2.8499012666
		O	8.0	-3.1850280257	4.0852005594	-2.2712499323
		C	6.0	-2.9700703052	3.0298140148	-1.7184910526
		O	8.0	-3.7365656497	1.9276333811	-1.8994799674
		C	6.0	-0.9423312991	1.6482973343	-1.2809560282
		C	6.0	-0.0674876495	-0.6153401031	-1.2084778940
		H	1.0	-1.2316792756	3.7021985924	-0.7701861937
		H	1.0	0.5611086155	-2.3881022437	-1.1200734105
		C	6.0	-1.8141079524	2.7778107968	-0.7491046522
		C	6.0	-0.8611841864	0.4108044927	-0.6418734319
		O	8.0	-0.0335223044	-1.7988891897	-0.5818591707
		H	1.0	-4.2603752185	3.3695219452	0.4974806127
		H	1.0	-3.5301481748	0.8975811963	0.3426410862
C	6.0	-2.2514510069	2.5943266713	0.7450177058		
H	1.0	-3.0291930483	4.5909817667	0.7853932732		
C	6.0	-1.5442325197	0.1426287156	0.6803265481		
H	1.0	-1.9351419832	-0.8812706146	0.6756874496		
C	6.0	-3.3704843897	3.5967454232	1.0968868361		
C	6.0	-2.6734805655	1.1340687612	0.9808004473		
H	1.0	2.2985838869	-3.5567228221	0.8063347588		
O	8.0	-1.1254540155	2.9363166956	1.5503841105		

		H	1.0	4.0037532790	-2.9437622774	2.7593102374
		H	1.0	-0.6710692175	2.1161798867	1.8080707917
		O	8.0	-0.4974881849	0.2336731660	1.6833879368
		H	1.0	1.7846781847	-1.4297004092	1.9417604174
		H	1.0	-2.9918914385	1.0057090440	2.0195969498
		C	6.0	1.7115589288	-4.0102912712	1.6294395526
		H	1.0	2.0309166711	-5.0516593220	1.7340784547
		H	1.0	1.5710421369	0.7671694292	2.9423702542
		C	6.0	-3.7393012487	3.6354656483	2.5825283305
		H	1.0	0.6624053002	-4.0197906819	1.3254473541
		H	1.0	-0.5104970156	-2.3796592205	1.8913201572
		C	6.0	3.2552065779	-3.4759391804	3.3787466533
		H	1.0	-4.4442661265	4.4494660594	2.7770899662
		H	1.0	-4.2160592726	2.7076919046	2.9161112995
		H	1.0	3.5135668884	-4.5390110906	3.3597417336
		C	6.0	1.4022799266	-1.9350784923	2.8504952812
		N	7.0	1.8821536390	-3.3254263581	2.9065238128
		C	6.0	-0.7194752617	-0.5015404535	2.9000993770
		H	1.0	-2.8467855614	3.7977390310	3.1907312953
		C	6.0	-0.1387464342	-1.9140094695	2.8055016561
		H	1.0	3.3411833287	-3.1362777259	4.4120685896
		H	1.0	2.9668903496	-0.9739703331	4.0164313691
		H	1.0	-1.7960929955	-0.5439926114	3.1068533882
		C	6.0	1.2774404851	0.3414909643	3.9100246892
		C	6.0	1.8767970261	-1.0678090536	4.0411524802
		O	8.0	-0.1681822449	0.2405356961	3.9540781980
		H	1.0	2.7596142982	1.4621126107	5.0028067770
		H	1.0	1.1650951003	2.2412047608	4.9216695827
		H	1.0	-0.5155826609	-2.5048017850	3.6485370689
		C	6.0	1.6803273428	1.2838970378	5.0317085729
		O	8.0	1.5655732693	-1.6372127573	5.3067036823
		H	1.0	1.4305240489	0.8528322274	6.0036521456
		H	1.0	0.6144902588	-1.5172883904	5.4405196073
		H	1.0	-3.5730168710	-2.5699024403	3.4702594334
		H	1.0	-1.9295136691	-3.2467163553	3.4400146332
		C	6.0	-2.8738003675	-3.1814836718	2.8947641206
		H	1.0	-3.2858413401	-4.1748906452	2.7207880625
		O	8.0	-1.8769067891	-0.7472270744	2.5805646151
		H	1.0	-2.9053579764	1.2951974242	1.5265424682
		O	8.0	-2.6617350712	-2.6174477168	1.5887849946
		C	6.0	-2.1473972872	-1.3730609554	1.5752550144
		H	1.0	-4.6164736237	-0.6311017313	1.1228421736
		H	1.0	-1.3524242624	2.9141896502	0.7585339626
Rhodomycinone	21288-60-8	H	1.0	-3.5730168710	-2.5699024403	3.4702594334
		H	1.0	-1.9295136691	-3.2467163553	3.4400146332
		C	6.0	-2.8738003675	-3.1814836718	2.8947641206
		H	1.0	-3.2858413401	-4.1748906452	2.7207880625
		O	8.0	-1.8769067891	-0.7472270744	2.5805646151
		H	1.0	-2.9053579764	1.2951974242	1.5265424682
		O	8.0	-2.6617350712	-2.6174477168	1.5887849946
		C	6.0	-2.1473972872	-1.3730609554	1.5752550144
		H	1.0	-4.6164736237	-0.6311017313	1.1228421736
		H	1.0	-1.3524242624	2.9141896502	0.7585339626

H	1.0	-3.7396503347	2.1637487831	0.2257516860
C	6.0	-2.9248623130	1.4695325746	0.4470606440
H	1.0	-5.8093902923	1.2770212500	0.0050485766
H	1.0	-6.6360822261	-0.2406627881	-0.3432248944
C	6.0	-1.6198197235	2.1407420280	0.0276849107
C	6.0	-4.5156091664	-0.4944593707	0.0393732865
C	6.0	-5.7029933038	0.3099992854	-0.4973353077
O	8.0	0.9030126837	3.0560482984	-0.4681914826
H	1.0	1.8644438447	3.2702193881	-0.6169392397
C	6.0	-0.4566887359	1.1677606259	-0.0800305360
C	6.0	-1.9857443169	-0.8485825346	0.1495553279
C	6.0	-3.1395303731	0.1291783236	-0.2715523956
C	6.0	0.8333771873	1.7179504944	-0.3193476777
C	6.0	-0.6229251231	-0.2032018186	-0.0048520522
O	8.0	3.4094344581	2.7277123695	-0.7724554895
H	1.0	1.2118648145	-2.8002874395	-0.0363037683
H	1.0	-4.5303937262	-1.4967634596	-0.4041711860
C	6.0	1.9625880154	0.8927500619	-0.4073737185
C	6.0	0.5195125561	-1.0563820396	-0.0824539206
C	6.0	3.2764669252	1.4715231154	-0.6393217067
C	6.0	1.8019969496	-0.5188244449	-0.2771487681
O	8.0	0.3127700039	-2.3705868355	0.0406843498
O	8.0	-1.8548142748	2.7684526057	-1.2501347400
H	1.0	-5.5822556869	0.4938150894	-1.5672331354
H	1.0	-2.0387602429	-1.7057101825	-0.5253402842
H	1.0	5.0699907620	2.8928051444	-1.0055725653
O	8.0	2.8251419335	-2.6490698045	-0.2391943626
H	1.0	-1.0376310491	3.2332544761	-1.4870754130
C	6.0	2.9530212346	-1.4112234830	-0.3527438934
C	6.0	4.4377656877	0.5922793769	-0.7143566413
H	1.0	-2.6530031867	1.1392618588	-1.8902110845
O	8.0	-3.0549018160	0.2771813783	-1.6884756948
O	8.0	5.9501158846	2.4456328665	-1.0740454150
C	6.0	4.2936904084	-0.8137266934	-0.5731065797
C	6.0	5.7322540426	1.1340576035	-0.9293841192
C	6.0	5.4024368759	-1.6490799202	-0.6424362935
H	1.0	5.2588658127	-2.7171597741	-0.5313415279
C	6.0	6.8421467979	0.2711690785	-0.9952485625
C	6.0	6.6732887113	-1.0972997790	-0.8529743827
H	1.0	7.8195827901	0.7113214862	-1.1599986793
H	1.0	7.5395433673	-1.7497886081	-0.9064382839

Steffimycin	11033-34-4	H	1.0	0.6452440786	-1.4093226640	-6.0584533401
		H	1.0	-0.6421296466	-0.1882621449	-5.9497683846
		H	1.0	0.1655372008	1.9163791913	-5.7328518094
		C	6.0	-0.0753266652	-0.9379597982	-5.3857722381
		H	1.0	-0.1865921805	3.4770427573	-4.9639763859
		H	1.0	-1.4241807219	2.2160165286	-4.9880976866
		C	6.0	-0.3495226983	2.4001007865	-4.8996532361
		H	1.0	-0.7516949537	-1.6992888409	-4.9874495815
		O	8.0	0.6909341331	-0.3529925049	-4.3302537048
		H	1.0	2.2709842180	-4.2460053641	-1.9320433936
		H	1.0	2.0076665396	1.4332986511	-4.0736621271
		C	6.0	0.2062594180	1.8880294890	-3.5725644694
		O	8.0	1.6191416780	2.1112202226	-3.4971207006
		H	1.0	-1.1139218980	0.1552294318	-3.4072498867
		C	6.0	-0.0423980043	0.3769820753	-3.3409620451
		H	1.0	2.0211002893	-5.9299896692	-1.4215602591
		H	1.0	0.8514452354	-2.5203968416	-2.5318580787
		C	6.0	1.8069449297	-4.8885297905	-1.1716806563
		H	1.0	2.2541415008	-4.6517016225	-0.1956658237
		O	8.0	-1.1091130803	3.6488351751	-2.5588780927
		C	6.0	-0.3915599694	2.6798669982	-2.3941699913
		C	6.0	-0.1030610501	-2.5003410327	-1.9968527053
		H	1.0	1.4906328342	-0.4819693650	-2.1106745680
		C	6.0	0.4646096473	-0.1210973154	-1.9652957941
		O	8.0	0.3954290220	-4.7531496595	-1.1436176207
		H	1.0	0.5812844574	-3.0116961172	-0.0182302699
		O	8.0	-1.0643834747	-2.8827153964	-2.9538896734
		O	8.0	-0.3549657295	-1.1995313024	-1.4891355769
		C	6.0	-0.0713260791	-3.4518396184	-0.7818774600
		C	6.0	0.0051168355	2.2123874016	-1.0331458480
		H	1.0	-0.9483364811	-5.3489764333	0.4855311103
		C	6.0	0.4744522564	0.9111296110	-0.8556283134
		H	1.0	-3.2781789407	-2.5848770526	-4.4040338821
		C	6.0	-2.4182964400	-3.0010518954	-2.4617385619
		H	1.0	-2.9472799647	-4.3031774262	-4.0999721891
		O	8.0	-1.5040452450	-4.6236095694	0.8139016219
		H	1.0	-0.4671554670	4.1140277602	-0.1254837063
		H	1.0	-2.7367177668	-2.0361609266	-2.0450362407
		C	6.0	-1.4814779877	-3.6501474707	-0.2249833756
		C	6.0	-3.2966763088	-3.3714551097	-3.6441221495
C	6.0	-0.0725437060	3.1183690145	0.0367647810		
H	1.0	-1.8253601352	-2.7098634847	0.2180101080		
H	1.0	-2.1195358707	-5.0090096041	-1.7662516223		
C	6.0	-2.4498378296	-4.0460692814	-1.3429606703		

		C	6.0	0.9726936564	0.5366760766	0.4178045912
		O	8.0	1.5183211033	-0.6791554069	0.5522568735
		H	1.0	-4.3255163223	-3.5113088674	-3.3049700814
		C	6.0	0.3685516041	2.7420448228	1.2937298223
		H	1.0	1.8151251918	-0.7495330435	1.4996063397
		C	6.0	0.9157232156	1.4500308347	1.4999147160
		O	8.0	-3.7718781605	-4.1380030940	-0.8374783603
		H	1.0	-3.6911915411	-4.6119900998	0.0043207610
		O	8.0	-0.1994958777	4.8385751673	2.2471501081
		C	6.0	0.2763828485	3.7231988640	2.4149212617
		C	6.0	1.4294064031	1.0604965977	2.8177790854
		O	8.0	1.9405909548	-0.0907352736	2.9832755775
		C	6.0	0.7885913768	3.2901328638	3.7513365892
		C	6.0	1.3476060548	1.9934553673	3.9213931546
		H	1.0	0.2808470463	5.1606059765	4.6549847146
		C	6.0	0.7090490524	4.1770673743	4.8046191022
		H	1.0	2.3516354738	-0.0691168450	4.6056804627
		C	6.0	1.8286893898	1.6310812874	5.2093318996
		O	8.0	2.3719157554	0.4356707332	5.4582302352
		C	6.0	1.1889227914	3.7982630385	6.0783862865
		C	6.0	1.7449697480	2.5369959688	6.2789759704
		O	8.0	1.0630070754	4.7374455383	7.0410970431
		H	1.0	2.1239511759	2.2125770133	7.2390228154
		C	6.0	1.5193877905	4.4376656038	8.3576445920
		H	1.0	2.5955506281	4.2300709389	8.3681521693
		H	1.0	0.9784827935	3.5836570771	8.7812206640
		H	1.0	1.3150760249	5.3283229292	8.9516727538
		H	1.0	-1.3776298036	-5.8645557372	-1.9659679170
		H	1.0	-1.9330585829	-4.1948515430	-2.2175573691
		H	1.0	-5.9843875763	-1.3321786838	-0.5727699038
		C	6.0	-1.1473505039	-4.8156433715	-1.7660933752
		H	1.0	-0.1881459082	-4.5604638013	-2.2388567327
		O	8.0	-1.0879826622	-4.6677570191	-0.3571388492
		C	6.0	-5.3038567950	-0.8644752426	0.1428383309
		H	1.0	-2.4580019611	-2.4294137651	-0.8164986341
		H	1.0	-4.8908495557	-1.6310999797	0.8044078589
		H	1.0	-5.8637402040	-0.1244916030	0.7265670472
		O	8.0	-4.2639127310	-0.2639977353	-0.6322588587
		H	1.0	-3.9628049223	-4.2706343822	2.9723153296
		H	1.0	-4.0107429165	1.5281967629	-1.9526906959
		O	8.0	-2.8598468036	-2.8237936837	1.0971130727
		H	1.0	-1.5806736805	-4.9407643537	2.2678669296
		C	6.0	-1.9165136430	-2.4168586605	0.1345220086
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H	1.0	-2.0432583451	-0.3918030292	-1.4439275260
C	6.0	-0.7062031386	-3.3642436815	0.0926933997
H	1.0	-5.6615086735	1.9868449542	-0.0937628846
H	1.0	0.5748113611	-5.2501967481	0.8769441489
H	1.0	0.0495807143	-2.9379818026	-0.5781034791
H	1.0	-4.3058601649	-2.5617904042	3.3064802221
C	6.0	-3.5274037736	-3.3298857787	3.3243369009
O	8.0	-3.4281384519	2.2006460958	-1.5638892529
C	6.0	-3.2692594625	0.4641313492	0.0952864040
C	6.0	-2.3550221076	-2.9292456228	2.4440216731
C	6.0	-1.1924915295	-3.9378635680	2.5072309800
C	6.0	-1.8958232324	-0.0337134233	-0.4172783053
O	8.0	-1.4195979155	-1.1143572778	0.3990690718
C	6.0	-0.1008128441	-3.5672713780	1.4877720159
H	1.0	-3.1835332880	-3.4605719408	4.3521050945
O	8.0	0.9373985463	-4.5353792334	1.4241071925
C	6.0	-4.8281643841	2.4848634260	0.4073412083
H	1.0	-3.3298820102	0.2429593318	1.1673433079
C	6.0	-3.5015444146	1.9751076594	-0.1512036510
O	8.0	0.6176831406	-0.5880688543	-1.4803564333
H	1.0	-4.9022815157	3.5587473517	0.2289155504
H	1.0	-4.9062152471	2.3160425652	1.4852535113
H	1.0	-1.9683884228	-1.9510892946	2.7593469848
H	1.0	1.5636973023	-0.6584799913	-1.7808123218
O	8.0	-0.7039779816	-3.8946228298	3.8398094937
C	6.0	-0.0713138109	-5.0808469526	4.2992059666
H	1.0	0.3599335584	-2.6299948358	1.8148966319
C	6.0	-0.7862164788	0.9987376226	-0.4271478459
C	6.0	0.4856710265	0.6256944380	-0.9301519620
C	6.0	-2.3224272666	2.7655289715	0.4467581466
O	8.0	3.0481406663	0.0017528850	-1.9084405914
C	6.0	-0.9622267369	2.2986158755	0.0467758065
C	6.0	1.5681007068	1.5387101067	-0.8731875863
H	1.0	4.6724094170	0.0198635530	-2.3132852152
O	8.0	-2.4863900120	3.7324728807	1.1672846992
C	6.0	2.8849800065	1.1498640318	-1.3899844573
C	6.0	0.1081182151	3.2040099927	0.1248857515
O	8.0	5.5262673504	0.5226658108	-2.3288353252
C	6.0	1.3637968635	2.8288865372	-0.3209742928
H	1.0	-0.0529798893	4.1985112565	0.5228942037
C	6.0	3.9906072735	2.0801695729	-1.3022791300
C	6.0	5.2787693637	1.7165441032	-1.7816664099
C	6.0	2.4856663878	3.8091771840	-0.2277606517
C	6.0	3.8223018237	3.3749742693	-0.7384699400

		C	6.0	6.3504885484	2.6194273082	-1.6913342551
		H	1.0	7.3108142270	2.2939469896	-2.0686862698
		O	8.0	2.3183985467	4.9246797535	0.2481313498
		C	6.0	4.8774230051	4.2592978413	-0.6534204102
		C	6.0	6.1514404811	3.8791716060	-1.1313772611
		H	1.0	4.7290344562	5.2416565106	-0.2220922481
		H	1.0	8.4444067106	4.3096908130	-2.5314904872
		O	8.0	7.1162502493	4.8155915614	-0.9993140109
		C	6.0	8.4327221814	4.5142823629	-1.4547541479
		H	1.0	8.8539081233	3.6577850875	-0.9158932936
		H	1.0	9.0283886013	5.4030909083	-1.2471516653
		H	1.0	0.1148833496	-4.9405014702	5.3672216274
		H	1.0	0.8734801839	-5.2670578132	3.7795641739
		H	1.0	-0.7253128311	-5.9570346637	4.1694389122
		O	8.0	-7.6821437903	-1.9537722787	-2.9143273995
		H	1.0	-7.8589867580	-2.4749533985	-2.1119390247
		H	1.0	-6.3142032017	-0.4169631185	-3.0066732811
		H	1.0	-5.6878402731	-1.9894013797	-3.4943528960
		C	6.0	-6.3680580130	-1.4914220151	-2.7804790506
		C	6.0	-5.8216879895	-1.7584074087	-1.3863741981
		H	1.0	-5.4601564648	0.7767259894	-1.2383223511
		H	1.0	-3.7184346011	-0.7808716905	-2.8896659374
		O	8.0	-6.4728901107	-2.4633472126	-0.6279635487
		C	6.0	-4.7314597081	0.3232821593	-0.5525207783
		H	1.0	-3.2370954337	-2.3402863910	-2.2283697412
		C	6.0	-3.3905938825	-1.2882231814	-1.9741545403
		C	6.0	-4.4850010098	-1.1699023514	-0.9008691591
		H	1.0	-5.1980530642	0.3664437648	0.4361016744
		O	8.0	-4.8507788527	2.8783351475	0.3840080323
		H	1.0	-1.3990709506	-0.6239582765	-2.4283481991
		H	1.0	6.8230393831	-3.6957344634	0.0849986175
		C	6.0	-3.4964744620	1.1936425828	-0.5692625598
		H	1.0	-4.8962345793	-2.2985045353	0.5953442170
		H	1.0	5.9408166058	-2.5157819895	-1.8853160748
		H	1.0	-4.7597026758	3.8277370412	0.6817631803
		H	1.0	-1.6873113325	-3.2454718929	-1.1651316301
		C	6.0	-2.0609067360	-0.6398991840	-1.5545967760
		O	8.0	-4.0841912114	-1.8908091555	0.2466917952
		C	6.0	-3.6461191228	2.5251410652	-0.0818840661
		O	8.0	4.4738846297	-3.7963647359	-1.3849412211
		C	6.0	-2.2738373387	0.7810253295	-1.0701823396
		H	1.0	5.0286180457	-5.3710351881	0.8890962475
		H	1.0	-0.1888492191	-4.2460541336	0.4119107720
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C	6.0	5.2848512741	-2.6719005878	-1.0237380358
O	8.0	0.0972437029	-2.6001898451	-1.7676818651
C	6.0	6.0899852074	-2.8962343046	0.2520166220
H	1.0	3.4956573444	-5.4211254804	-0.7988140071
H	1.0	2.5081470699	-2.9705197433	-2.8929900267
O	8.0	-1.3936914612	-1.3104920688	-0.4811494542
C	6.0	-0.8910937748	-2.6098358989	-0.7619166684
O	8.0	-3.8338515992	5.1591066662	0.8567190594
H	1.0	6.6503204379	-1.9850273574	0.4920033510
C	6.0	-2.5625286255	3.4173580098	-0.1041406719
H	1.0	1.6092995339	-1.5599101259	-3.5079948595
C	6.0	-0.3789573563	-3.1768933845	0.5573279115
C	6.0	3.6441130207	-4.4081568753	-0.4125582699
C	6.0	-1.1699602689	1.6857965664	-1.1099358814
C	6.0	4.3362520787	-4.5225865556	0.9635106786
C	6.0	-2.7377932145	4.7685781307	0.3976007580
H	1.0	-1.1475007889	-3.0627847721	1.3247109697
C	6.0	2.1845993411	-1.9538933029	-2.6658124078
H	1.0	4.6687996483	-1.7680938973	-0.9185005190
O	8.0	2.3071722707	-3.9256958145	-0.3813561248
H	1.0	5.7063122008	-3.5158473040	2.3053059203
C	6.0	5.1453133467	-3.2921307449	1.3909686774
H	1.0	1.6136087992	-4.0454104691	2.1181112543
C	6.0	-1.3074188971	3.0004044840	-0.6300235561
C	6.0	1.3215111492	-1.9249574078	-1.4150784906
O	8.0	-0.0229214747	1.2465914197	-1.6382126896
H	1.0	3.5864683749	-4.7958927735	1.7100516342
H	1.0	-2.7543655219	7.2465686222	1.2455509697
C	6.0	1.9534838502	-2.5541286491	-0.1535386933
H	1.0	3.0720802896	-1.3270384717	-2.5373092500
C	6.0	-1.5786476311	5.6994367493	0.3562031898
C	6.0	0.9195367533	-2.4954663782	1.0031873580
H	1.0	1.0838983212	-0.8838566504	-1.1616803889
H	1.0	4.4817604728	-2.4514374078	1.6303933254
H	1.0	0.6076860156	2.0275721042	-1.5830197308
N	7.0	1.3489645473	-3.0753013610	2.2745041179
C	6.0	-1.7777608116	6.9887365090	0.8547502392
C	6.0	-0.1611028882	3.9128482404	-0.6901452523
C	6.0	-0.3275721159	5.2934358402	-0.1708595664
H	1.0	2.8318944888	-1.9596502778	0.1235401943
O	8.0	0.9229334872	3.5184107201	-1.1720446764
H	1.0	2.1766737945	-2.5979621775	2.6253648018
H	1.0	0.7044531325	-1.4350453050	1.1830373653
C	6.0	-0.7289663146	7.8995176511	0.8370904118

		H	1.0	-0.8720868757	8.9043984711	1.2227947437
		C	6.0	0.7330910708	6.2443967775	-0.1806880217
		C	6.0	0.5137230338	7.5359342388	0.3258584345
		O	8.0	1.9243181477	5.8600391419	-0.6839716095
		H	1.0	1.3164717423	8.2618391622	0.3213802707
		H	1.0	2.7654484705	7.6639317327	-1.3278329301
		C	6.0	3.0021180923	6.7874444985	-0.7126595036
		H	1.0	3.8364068538	6.2474814693	-1.1605497835
		H	1.0	3.2816407170	7.1146783322	0.2960775675
		H	1.0	8.2202185260	3.2395579621	-2.0238190150
		C	6.0	7.3708537087	2.5688021646	-1.9361066990
		H	1.0	8.4252270546	0.9280012747	-2.8175746410
		H	1.0	6.0639062357	4.0328920780	-1.0179357366
		C	6.0	7.4881989664	1.2572983434	-2.3875465106
		C	6.0	6.1809612996	3.0180202127	-1.3774472153
		H	1.0	8.5343231150	-1.3306048283	-2.5604599924
		H	1.0	7.9748129987	-0.8341657152	-4.1873319945
		C	6.0	7.7076347430	-1.3871038719	-3.2787702716
		C	6.0	6.4089301609	0.3633525276	-2.2903227745
		C	6.0	5.0974010161	2.1431495102	-1.2704541318
		O	8.0	3.8011780270	3.8683712090	-0.2858742661
		H	1.0	7.5217201041	-2.4304922486	-3.5334205922
		O	8.0	6.4902557026	-0.9137784807	-2.7156375411
		C	6.0	5.1786812994	0.8028740934	-1.7221081248
		C	6.0	3.8512023685	2.6755829672	-0.6606357788
		H	1.0	2.2867353079	3.9723442856	0.2860117293
		C	6.0	3.9989607300	-0.0899517362	-1.5960652981
		C	6.0	2.7125638516	1.7857021664	-0.5123086760
		O	8.0	1.4058954742	3.5397083881	0.4790164057
		O	8.0	4.0204847073	-1.2666257799	-2.0154255327
		C	6.0	2.7854058330	0.4377393548	-0.9617055958
		C	6.0	1.5266725541	2.2717366620	0.0609073269
		C	6.0	1.6659394677	-0.4033860853	-0.8077039426
		C	6.0	0.4015953466	1.4133408777	0.2199748903
		H	1.0	2.5716089534	-1.7948133779	-1.6603647856
		H	1.0	-0.9136706113	3.0600625848	0.5745905602
		H	1.0	-2.9581365355	7.0596212588	0.0150655525
		H	1.0	-0.8424328917	1.9252259253	1.9055377951
		H	1.0	-2.7599058269	5.6954062242	1.1328634262
		C	6.0	0.4762657259	0.0891295856	-0.1824554874
		O	8.0	1.6654409623	-1.6602485161	-1.2506380515
		C	6.0	-0.8610344061	1.9948842377	0.8096479635
		C	6.0	-3.3125693569	6.0546900940	0.2577290158
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H	1.0	-4.8032346575	8.0089767780	1.5426890854
O	8.0	-2.7761020110	5.5446906208	-2.0565221521
H	1.0	-4.6119526513	6.6526263556	2.6409496587
C	6.0	-2.9943552348	5.1757429107	-0.9279609533
H	1.0	-1.9490942353	3.2764166178	-2.2714676456
C	6.0	-5.1626290931	6.9932828613	1.7539966766
O	8.0	-0.2098003542	-1.9333334083	0.8412404539
H	1.0	0.8263730851	-4.0749025913	1.5781596820
O	8.0	-3.0169731782	3.8473286115	-0.5811130073
C	6.0	-0.6896466933	-0.8686458276	-0.0138994658
C	6.0	-2.1247627555	1.2515234620	0.3420981129
C	6.0	-4.8240545809	6.0816900500	0.5684707773
C	6.0	-2.7754677101	2.9142051867	-1.6515240851
H	1.0	-0.4314781601	-3.7580923009	2.7749368826
H	1.0	-1.8762531472	-0.3472013822	1.7015842526
H	1.0	-3.3704684159	2.6164371633	0.9580897067
H	1.0	-0.9227032588	-1.2888664674	-0.9949688070
C	6.0	-2.4305626241	1.5087879246	-1.1510766692
C	6.0	-1.9473527560	-0.2405459496	0.6143477936
H	1.0	-5.3658307197	6.4208236584	-0.3235123792
C	6.0	-0.2542774840	-4.0997255590	1.7524240255
H	1.0	-6.8729941466	7.6879149294	2.9146028172
H	1.0	0.8873276260	-5.1780579403	-0.5896767410
O	8.0	-3.2732073142	1.6605010331	1.0858541533
H	1.0	-5.1716185581	5.0620241949	0.7764474365
H	1.0	0.8905679801	-6.7716966733	1.8571630860
C	6.0	-0.8985181064	-3.1375784790	0.7566927148
C	6.0	-6.6617423001	7.0328899906	2.0638542930
O	8.0	-2.4272268283	0.6218614719	-1.9816881988
H	1.0	-3.6575148557	2.8440317785	-2.2944665875
O	8.0	0.6406068199	-7.8089231262	4.0818132944
O	8.0	-0.7971945354	-3.6451902770	-0.5780818558
H	1.0	-7.2341576725	7.4050855517	1.2070532924
N	7.0	0.0277836745	-6.5011731404	2.3186086144
H	1.0	-2.8426742325	-0.7717769712	0.2830647158
H	1.0	-7.0431071106	6.0354526915	2.3090174342
O	8.0	0.5903736974	-6.0751785416	-0.3641236900
C	6.0	-0.1447984097	-7.0449832025	3.5481563696
H	1.0	-1.9749329301	-3.0061306331	0.9792720245
C	6.0	-0.7810756295	-5.5380343221	1.5753158580
F	9.0	-1.5686427251	-5.3256564763	4.4483437020
H	1.0	-0.5449573095	-5.3400954603	-2.6299380826
C	6.0	-0.7548760970	-5.9413427579	0.0842793904
C	6.0	-1.4999461537	-4.8829880130	-0.7451900447

		H	1.0	-1.8147082767	-5.6005151902	1.9225844794
		C	6.0	-1.4549226385	-6.6682689249	4.2891352225
		F	9.0	-1.4934516822	-7.2312621883	5.4928488826
		C	6.0	-1.5516798834	-5.1909021266	-2.2333443645
		H	1.0	-2.0232733209	-4.3644482905	-2.7701130432
		H	1.0	-2.5259685837	-4.7806810871	-0.3519116042
		H	1.0	-1.2246178454	-6.9241849382	-0.0311288518
		F	9.0	-2.5437920378	-7.0812224077	3.5938889849
		H	1.0	-2.1302046088	-6.1023737182	-2.4118672989
Zorubicin / Rubidazone	36508-71-1	H	1.0	8.5969652474	5.2086636079	1.2943412100
		H	1.0	9.2441517588	5.6140365242	3.6581389839
		C	6.0	8.0239030774	4.7606713613	2.1006746150
		H	1.0	6.6777069059	3.7559970489	0.7654722918
		C	6.0	8.3911455061	4.9822089114	3.4285974487
		H	1.0	2.8071160011	4.3835743764	-0.4268388688
		C	6.0	6.9259051756	3.9526742967	1.8046259720
		H	1.0	3.9947632846	3.3527159446	-1.2452965996
		H	1.0	2.3249068249	3.3797990732	-1.8129003281
		C	6.0	2.9482275745	3.4128633610	-0.9207634041
		H	1.0	-3.3211884521	3.7345075360	0.1596457387
		H	1.0	4.5529450662	3.5468189858	0.8897162279
		C	6.0	7.6668689854	4.3801874664	4.4607787288
		H	1.0	-0.0316788554	3.0601138049	-0.6323764685
		O	8.0	-2.3688980368	3.4340561123	0.1312905997
		C	6.0	6.1850060656	3.3587394704	2.8368362821
		H	1.0	7.9565528705	4.5424058233	5.4947297761
		N	7.0	4.3316056146	2.7060525371	1.4099922386
		O	8.0	-4.9065770299	3.3659473494	0.2228285700
		C	6.0	6.5752653887	3.5677800073	4.1664037939
		C	6.0	2.6015400434	2.2682507705	0.0032861102
		H	1.0	0.8833061217	0.4448926100	-1.9501104386
		H	1.0	0.2386679930	2.6711934193	1.0546315115
		C	6.0	4.9964353612	2.4667255686	2.6044485329
		C	6.0	0.1000725571	2.2241169710	0.0605194787
		H	1.0	-7.2765647793	3.1590482629	0.2973255920
		N	7.0	3.2439297606	1.9544137698	1.0686185656
		C	6.0	-2.4095224102	2.0954668190	0.1406332671
		C	6.0	1.3690656433	1.4289921031	-0.3309739905
		O	8.0	1.4115223834	1.2371684795	-1.7505881571
		C	6.0	-4.8752505560	2.1151705257	0.2363939992
		H	1.0	6.0079173771	3.0781300921	4.9504644864
		C	6.0	-1.1656277388	1.3993998924	0.0909899989
		C	6.0	-7.3354214478	2.0778424235	0.3189143064

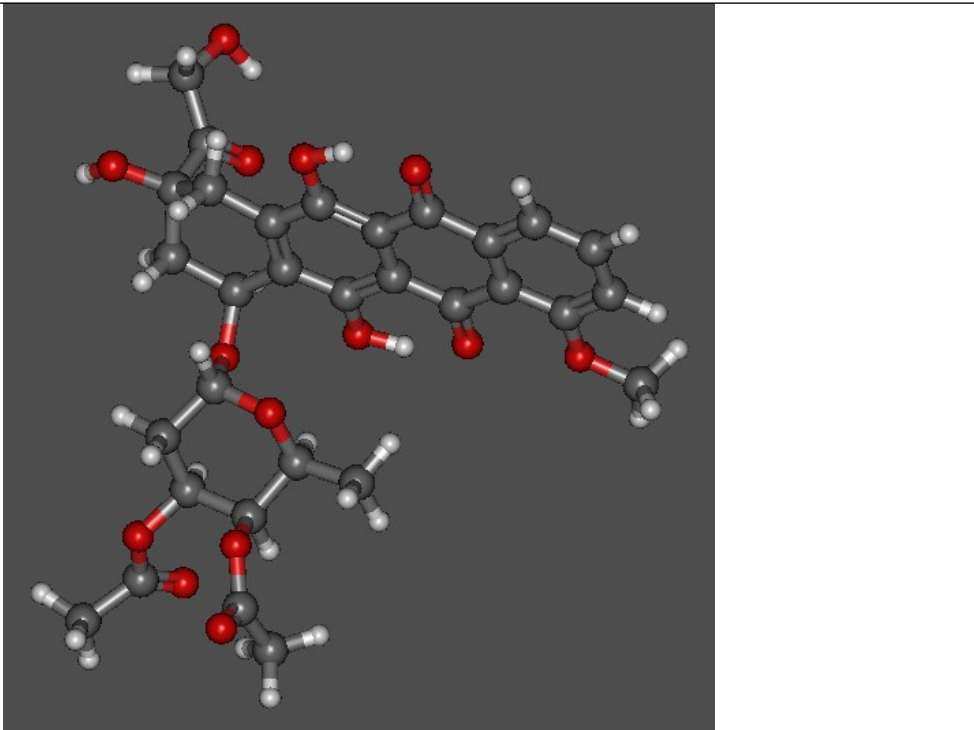
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C	6.0	-3.6201490084	1.3856003846	0.1966732605
H	1.0	-9.4818387047	1.9678966588	0.3911781938
C	6.0	-6.1462287838	1.3450705976	0.2931190126
C	6.0	-8.5513007241	1.4086075837	0.3704020635
H	1.0	1.3566220321	0.2536764163	1.4860064311
C	6.0	1.3581926862	0.0806672432	0.4061512759
C	6.0	-1.1589535475	0.0147364221	0.1108319764
H	1.0	2.2801193668	-0.4657870546	0.1902617051
C	6.0	-3.6145041519	-0.0382643658	0.2206319294
C	6.0	0.1379942651	-0.7621103518	0.0260811175
C	6.0	-6.1475944005	-0.0712045936	0.3188350943
O	8.0	0.2251761826	-1.2153675122	-1.3621904911
C	6.0	-2.3833436046	-0.7182262937	0.1817392449
H	1.0	1.6512688036	-1.6881030637	-3.5502207535
C	6.0	-8.5908393640	0.0171258234	0.3960238338
C	6.0	-4.8585685796	-0.8096673526	0.2925128723
C	6.0	-7.4060760210	-0.7365395714	0.3705773438
H	1.0	0.0670263153	-1.6515778611	0.6563563781
H	1.0	-9.5491973319	-0.4841954644	0.4363413466
H	1.0	2.0433539535	-2.1838550667	-1.1461845823
C	6.0	1.1510702724	-2.5500258351	-3.0917870863
H	1.0	0.1399073728	-2.6173427815	-3.5069263173
C	6.0	1.0402364346	-2.3376436318	-1.5861736225
O	8.0	-2.3031242119	-2.0477480044	0.2253034532
H	1.0	2.2717140325	-3.3535770064	-5.3336456217
O	8.0	-4.8169345761	-2.0577308608	0.3285578511
O	8.0	-7.4092584546	-2.0856975373	0.3925974249
H	1.0	-3.2504486686	-2.3700712438	0.2783332376
H	1.0	2.9487201024	-3.7288374563	-2.9704952647
N	7.0	1.9211238461	-4.1519485456	-4.8081042643
C	6.0	1.9252214381	-3.8414129842	-3.3746741441
O	8.0	0.4371589823	-3.4539178699	-0.9576853197
H	1.0	-9.2659432354	-2.5639706561	-0.4435874466
H	1.0	-9.2150286508	-2.5414873305	1.3455321418
C	6.0	-8.6488454533	-2.7803375468	0.4369948104
H	1.0	2.5855399836	-4.9056999732	-4.9716900474
H	1.0	2.2006367038	-4.5349274080	-0.7145643162
C	6.0	1.1783582924	-4.6697453974	-1.1093496977
C	6.0	1.2853726701	-5.0040316846	-2.6054528229
H	1.0	0.2702849563	-5.1601450354	-2.9968498318
H	1.0	-8.3876552556	-3.8386298580	0.4430846816
H	1.0	1.7026460423	-6.6956450025	-3.4853267173
O	8.0	2.0719922946	-6.1917618516	-2.7508190424

		H	1.0	0.4329823063	-5.4677331712	0.7529092633
		C	6.0	0.4594928276	-5.7400630996	-0.3053112615
		H	1.0	-0.5715738031	-5.8469821967	-0.6568089838
		H	1.0	0.9751947584	-6.6961413419	-0.4173897516
		H	1.0	-6.5560770275	4.7115768901	6.2380159943
		O	8.0	-6.8350000000	5.6340000000	6.2380000000
		C	6.0	-6.3370000000	6.2240000000	5.0360000000
		C	6.0	-7.1530000000	5.7650000000	3.8500000000
		O	8.0	-6.2830000000	5.6140000000	2.7070000000
		C	6.0	-7.8460000000	4.4140000000	4.0030000000
		O	8.0	-9.0400000000	4.3900000000	3.2110000000
		C	6.0	-6.8110000000	3.4360000000	3.4810000000
		C	6.0	-6.0740000000	4.2370000000	2.4190000000
		N	7.0	-4.6320000000	4.0120000000	2.3840000000
		C	6.0	-3.8400000000	3.4100000000	3.3270000000
		N	7.0	-2.5650000000	3.3960000000	3.0150000000
		C	6.0	-2.5200000000	4.0280000000	1.7790000000
		C	6.0	-1.4600000000	4.3360000000	0.9060000000
		N	7.0	-0.1820000000	4.0460000000	1.1470000000
		N	7.0	-1.7620000000	4.9660000000	-0.2450000000
		C	6.0	-3.0420000000	5.2600000000	-0.5020000000
		N	7.0	-4.1210000000	5.0240000000	0.2340000000
		C	6.0	-3.7870000000	4.4000000000	1.3750000000
		H	1.0	-5.2970000000	5.9330000000	4.8870000000
		H	1.0	-6.3970000000	7.3100000000	5.1100000000
		H	1.0	-7.9360000000	6.5020000000	3.6930000000
		H	1.0	-8.0960000000	4.2170000000	5.0410000000
		H	1.0	-6.1490000000	3.0970000000	4.2760000000
		H	1.0	-7.2810000000	2.5530000000	3.0470000000
		H	1.0	-6.4810000000	4.0360000000	1.4290000000
		H	1.0	-4.2310000000	2.9900000000	4.2430000000
		H	1.0	0.5340000000	4.3030000000	0.4820000000
		H	1.0	0.0780000000	3.5770000000	1.9940000000
		H	1.0	-3.2250000000	5.7670000000	-1.4480000000
		P	15.0	-9.8590000000	3.0180000000	3.0320000000
		O	8.0	-11.2920000000	3.3760000000	2.8880000000
		O	8.0	-9.4440000000	2.0700000000	4.0970000000
		O	8.0	-9.3520000000	2.4480000000	1.6320000000
		C	6.0	-9.1310000000	3.3160000000	0.5170000000
		C	6.0	-8.7530000000	2.5120000000	-0.7050000000
		O	8.0	-7.3060000000	2.4820000000	-0.8210000000
		C	6.0	-9.1880000000	1.0490000000	-0.6690000000
		O	8.0	-9.4480000000	0.5780000000	-1.9980000000
AG-TC base pairs						

C	6.0	-7.9720000000	0.3700000000	-0.0720000000
C	6.0	-6.8600000000	1.1370000000	-0.7540000000
N	7.0	-5.5830000000	1.1080000000	-0.0540000000
C	6.0	-5.3740000000	0.7080000000	1.2370000000
N	7.0	-4.1210000000	0.7520000000	1.5960000000
C	6.0	-3.4600000000	1.2130000000	0.4650000000
C	6.0	-2.0840000000	1.4530000000	0.2430000000
O	8.0	-1.1430000000	1.3070000000	1.0290000000
N	7.0	-1.8430000000	1.9090000000	-1.0500000000
C	6.0	-2.8100000000	2.1160000000	-2.0050000000
N	7.0	-2.3910000000	2.5650000000	-3.2000000000
N	7.0	-4.1000000000	1.9000000000	-1.8070000000
C	6.0	-4.3510000000	1.4480000000	-0.5600000000
H	1.0	-8.3240000000	4.0090000000	0.7490000000
H	1.0	-10.0380000000	3.8820000000	0.3060000000
H	1.0	-9.2440000000	2.9630000000	-1.5660000000
H	1.0	-10.0780000000	0.9140000000	-0.0540000000
H	1.0	-7.9490000000	0.4840000000	1.0120000000
H	1.0	-7.9640000000	-0.6930000000	-0.2880000000
H	1.0	-6.7070000000	0.7760000000	-1.7680000000
H	1.0	-6.1690000000	0.3730000000	1.8830000000
H	1.0	-0.8790000000	2.0950000000	-1.2860000000
H	1.0	-1.4170000000	2.7470000000	-3.4050000000
H	1.0	-3.0790000000	2.7250000000	-3.9210000000
H	1.0	-10.1859538275	1.1011808790	-2.3337575760
O	8.0	5.4980000000	1.2440000000	-6.6360000000
C	6.0	4.1520000000	1.1020000000	-7.1020000000
C	6.0	3.3930000000	2.3960000000	-6.9180000000
O	8.0	2.5140000000	2.2470000000	-5.7750000000
C	6.0	4.2630000000	3.6210000000	-6.6190000000
O	8.0	3.7120000000	4.8170000000	-7.1890000000
C	6.0	4.2030000000	3.7060000000	-5.1080000000
C	6.0	2.7640000000	3.2960000000	-4.8600000000
N	7.0	2.4430000000	2.8080000000	-3.5050000000
C	6.0	1.0990000000	2.7330000000	-3.1270000000
O	8.0	0.2240000000	3.0390000000	-3.9500000000
N	7.0	0.7860000000	2.3330000000	-1.8760000000
C	6.0	1.7550000000	2.0210000000	-1.0150000000
N	7.0	1.3980000000	1.6740000000	0.2170000000
C	6.0	3.1300000000	2.0610000000	-1.3790000000
C	6.0	3.4260000000	2.4480000000	-2.6220000000
H	1.0	3.6530000000	0.3150000000	-6.5370000000
H	1.0	4.1540000000	0.8380000000	-8.1620000000
H	1.0	2.8590000000	2.6020000000	-7.8460000000

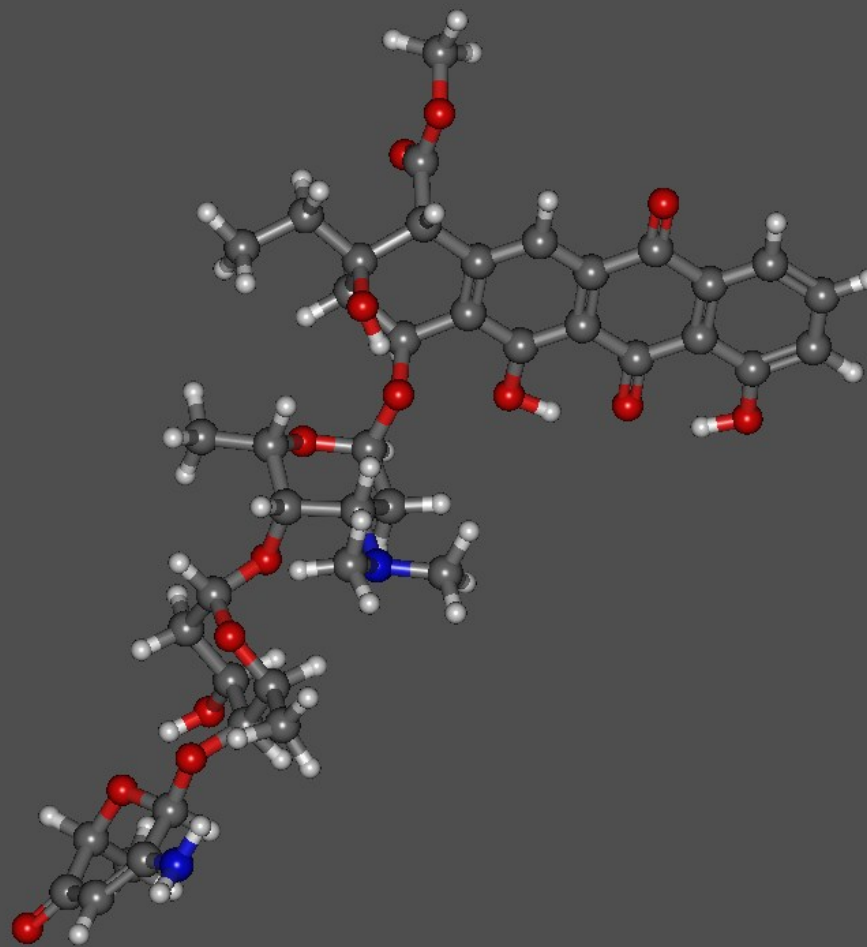
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H	1.0	4.915000000	3.020000000	-4.652000000
H	1.0	4.435000000	4.713000000	-4.753000000
H	1.0	2.083000000	4.114000000	-5.101000000
H	1.0	0.419000000	1.718000000	0.454000000
H	1.0	2.091000000	1.431000000	0.911000000
H	1.0	3.912000000	1.783000000	-0.673000000
H	1.0	4.467000000	2.462000000	-2.935000000
H	1.0	6.0007987932	1.6049866582	-7.3757594648
P	15.0	3.520000000	4.943000000	-8.782000000
O	8.0	3.935000000	3.665000000	-9.415000000
O	8.0	4.153000000	6.213000000	-9.218000000
O	8.0	1.942000000	5.094000000	-8.950000000
C	6.0	1.070000000	4.956000000	-7.825000000
C	6.0	0.712000000	6.313000000	-7.266000000
O	8.0	0.147000000	6.122000000	-5.951000000
C	6.0	1.894000000	7.266000000	-7.094000000
O	8.0	1.912000000	8.194000000	-8.192000000
C	6.0	1.628000000	7.960000000	-5.765000000
C	6.0	0.558000000	7.143000000	-5.060000000
N	7.0	0.978000000	6.489000000	-3.803000000
C	6.0	-0.011000000	6.134000000	-2.917000000
O	8.0	-1.191000000	6.339000000	-3.137000000
N	7.0	0.436000000	5.531000000	-1.765000000
C	6.0	1.743000000	5.279000000	-1.416000000
O	8.0	1.994000000	4.763000000	-0.330000000
C	6.0	2.732000000	5.683000000	-2.391000000
C	6.0	4.181000000	5.571000000	-2.040000000
C	6.0	2.308000000	6.247000000	-3.531000000
H	1.0	1.563000000	4.372000000	-7.049000000
H	1.0	0.159000000	4.447000000	-8.126000000
H	1.0	0.024000000	6.788000000	-7.967000000
H	1.0	2.834000000	6.718000000	-7.081000000
H	1.0	2.534000000	8.057000000	-5.172000000
H	1.0	1.216000000	8.956000000	-5.910000000
H	1.0	-0.311000000	7.768000000	-4.843000000
H	1.0	-0.239000000	5.172000000	-1.096000000
H	1.0	4.310000000	5.752000000	-0.972000000
H	1.0	4.749000000	6.310000000	-2.605000000
H	1.0	4.540000000	4.573000000	-2.284000000
H	1.0	3.047000000	6.508000000	-4.285000000
H	1.0	2.5782171538	7.8157226091	-8.7999646631

6. Optimized 3D chemical structures of anthracyclines and 3D structure of AG-TC base pairs

Name	NSC No. / CAS No.	3D chemical structures	
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5		 A 3D ball-and-stick model of the anthracycline derivative 3'-Acetoxy-4'-O-acetyldoxorubicin. The molecule is shown in a perspective view against a dark gray background. It features a complex polycyclic core with several hydroxyl groups and two acetoxy groups attached to the sugar moiety. The atoms are represented by spheres: carbon (gray), oxygen (red), and hydrogen (white).

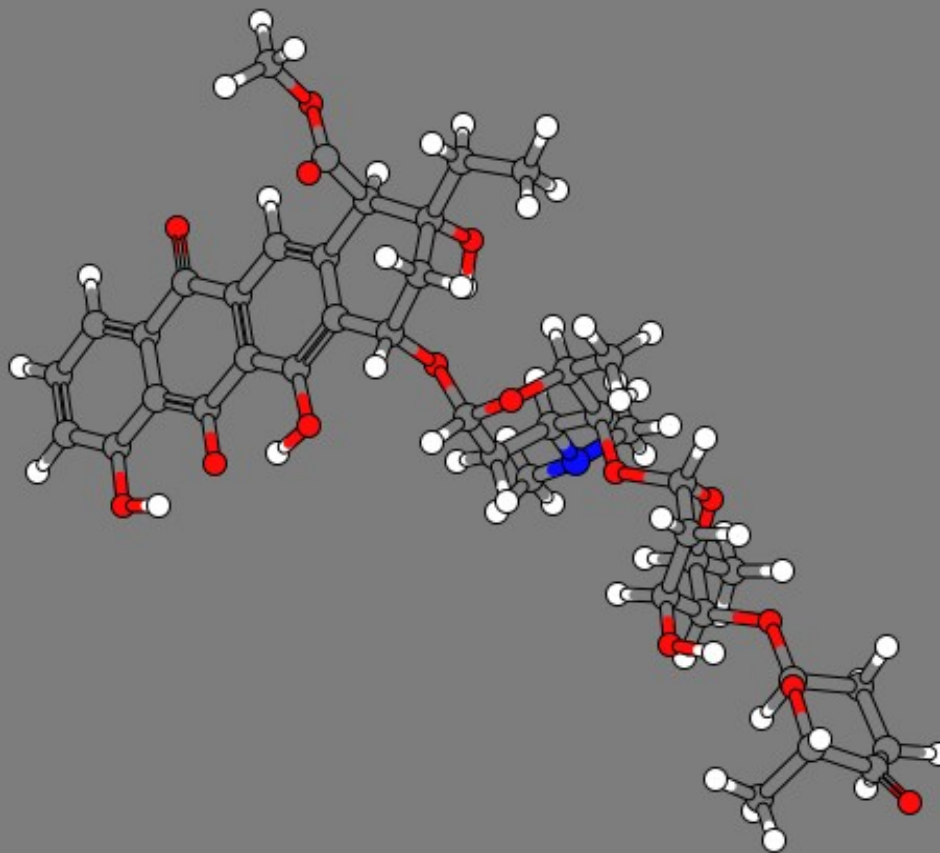
Aclacinomycin X

NSC 670120



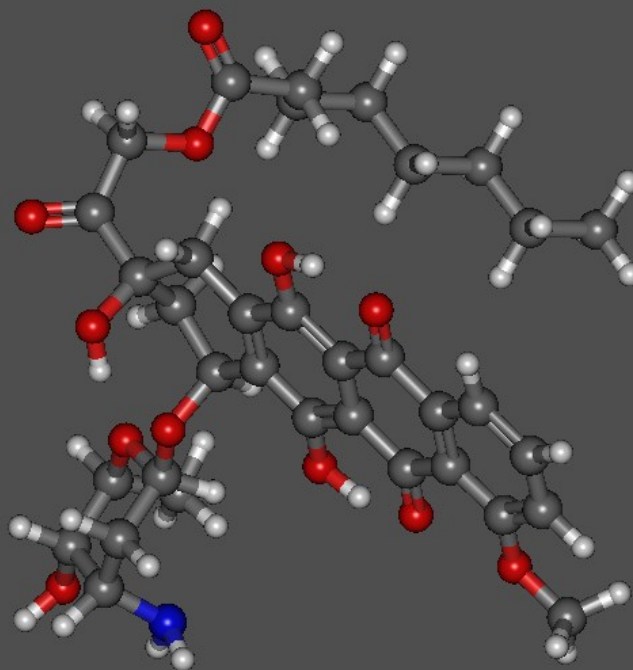
Aclarubicin

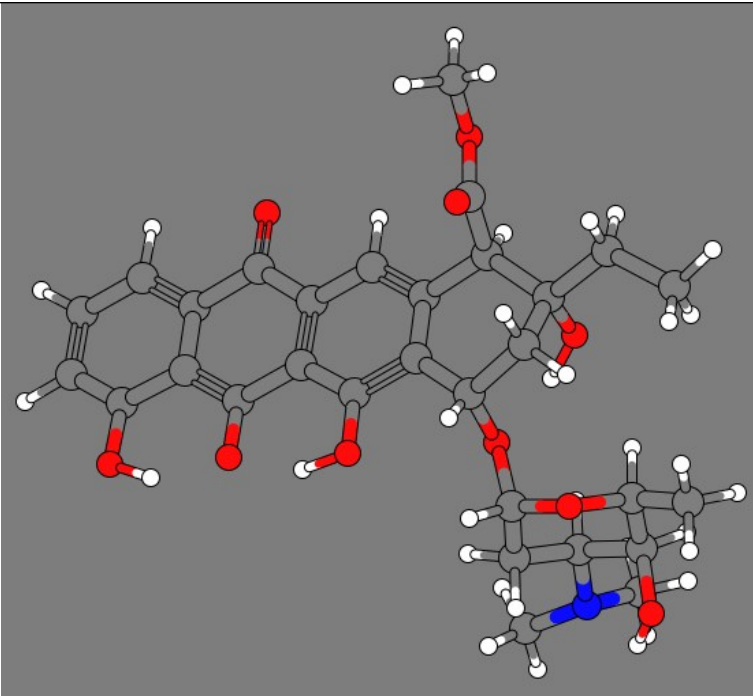
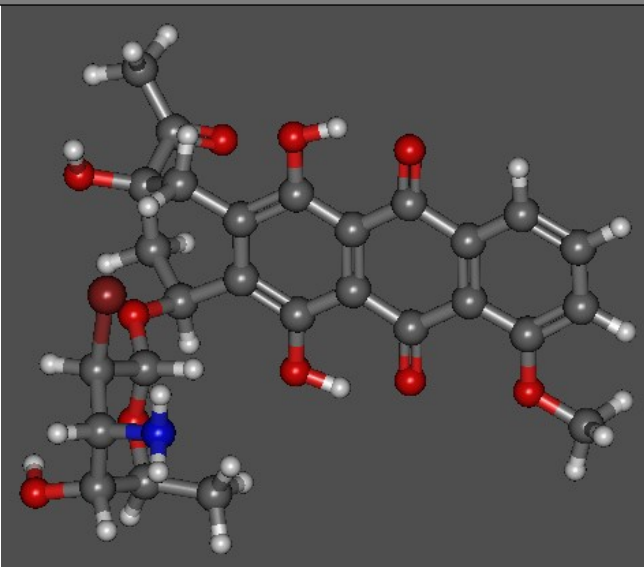
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Adriamycin 14-octanoate

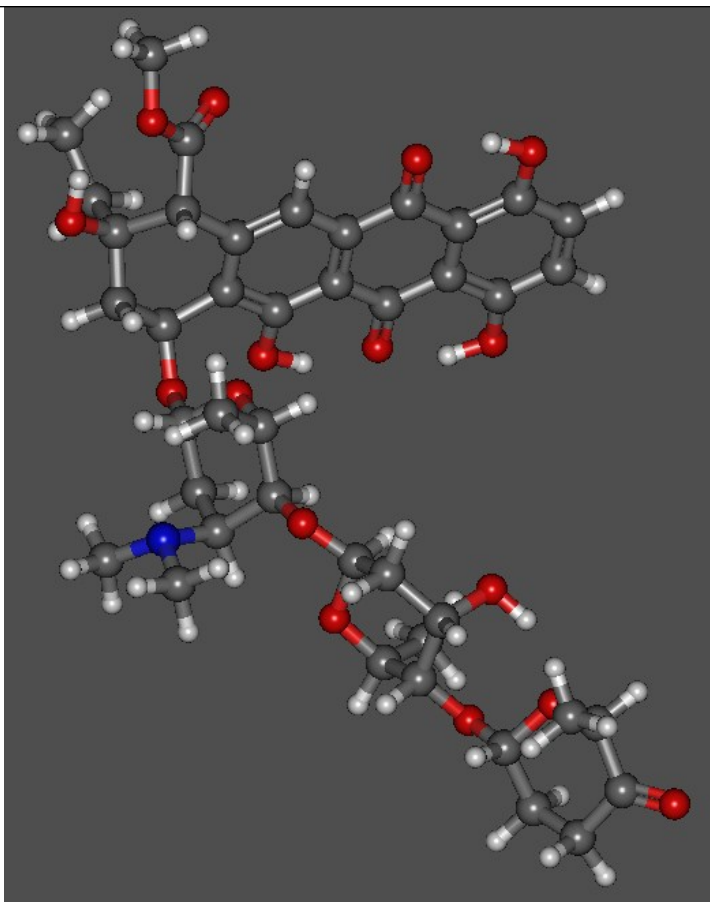
51898-39-6

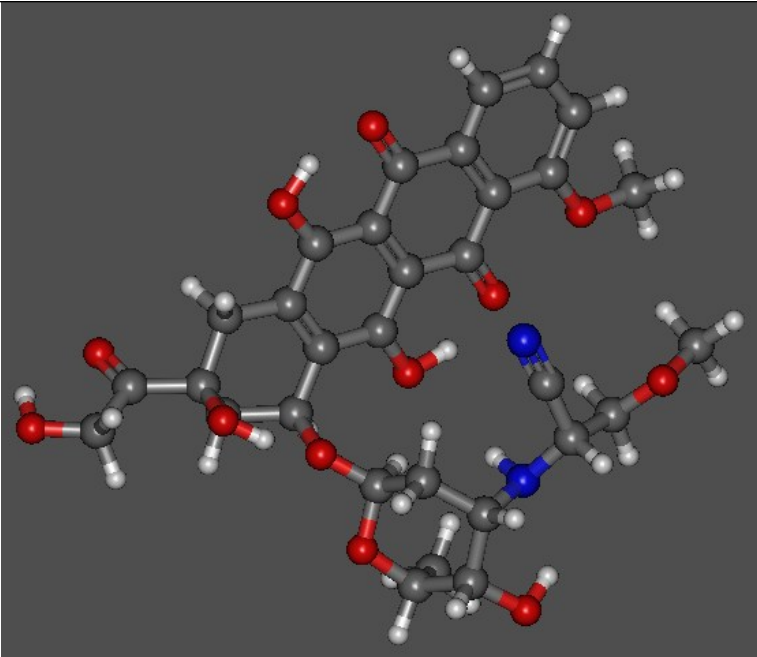
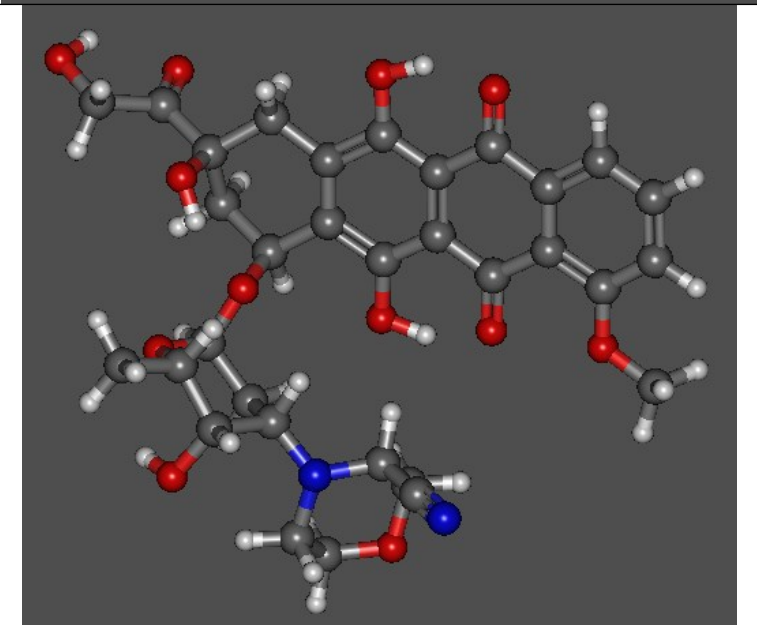


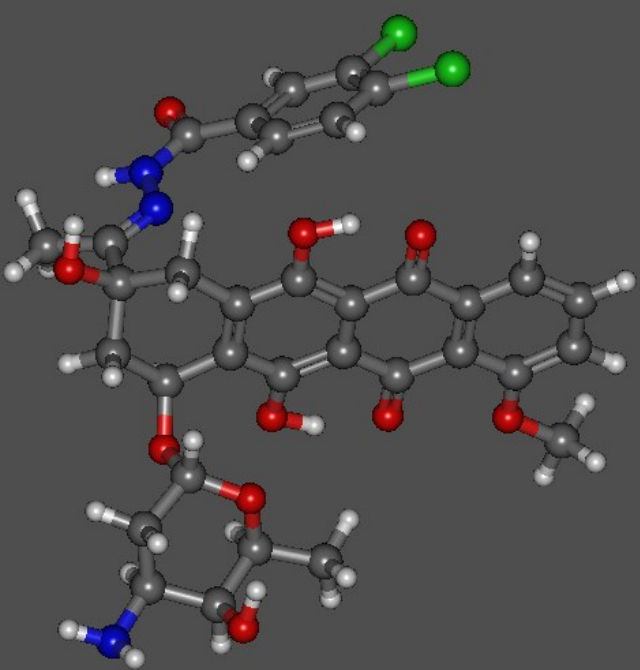
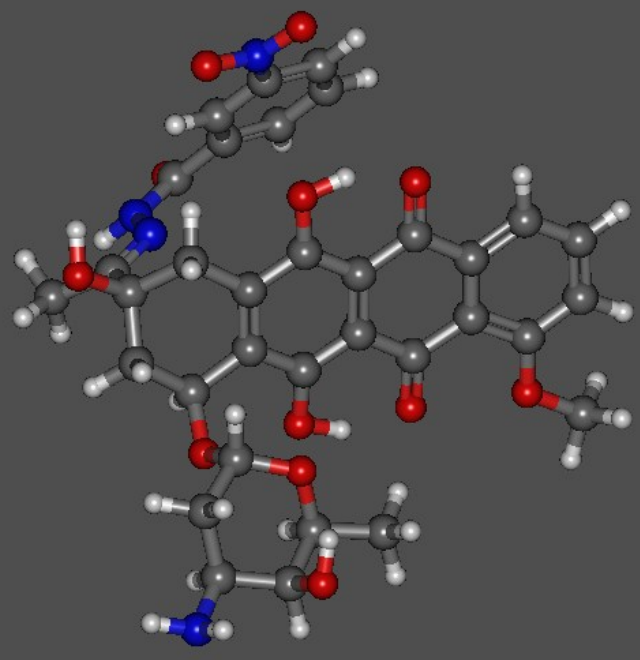
<p>Aklavin</p>	<p>60504-57-6</p>	 A 3D ball-and-stick model of the molecule Aklavin. The structure features a complex polycyclic core with several fused rings. It includes multiple hydroxyl groups (red and white spheres) and a side chain with a nitrogen atom (blue sphere) and a methyl group (grey and white spheres). The model is set against a dark grey background.
<p>2'-Bromo-4'-epi-daunorubicin</p>	<p>NSC 650931</p>	 A 3D ball-and-stick model of the molecule 2'-Bromo-4'-epi-daunorubicin. The structure is a complex polycyclic molecule with a central ring system and several hydroxyl groups. A bromine atom (dark red sphere) is attached to the 2' position. The model is set against a dark grey background.

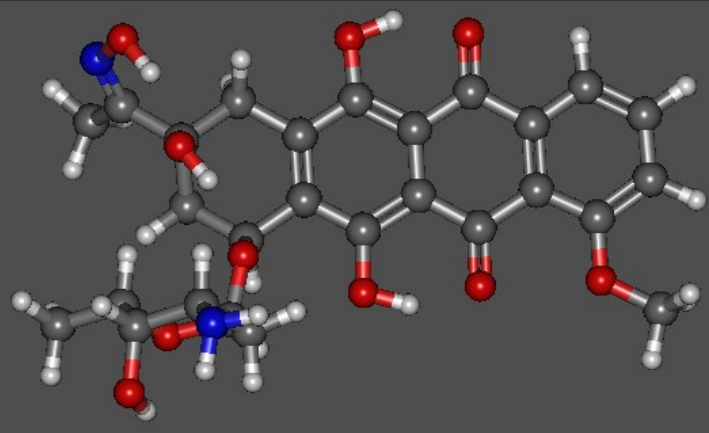
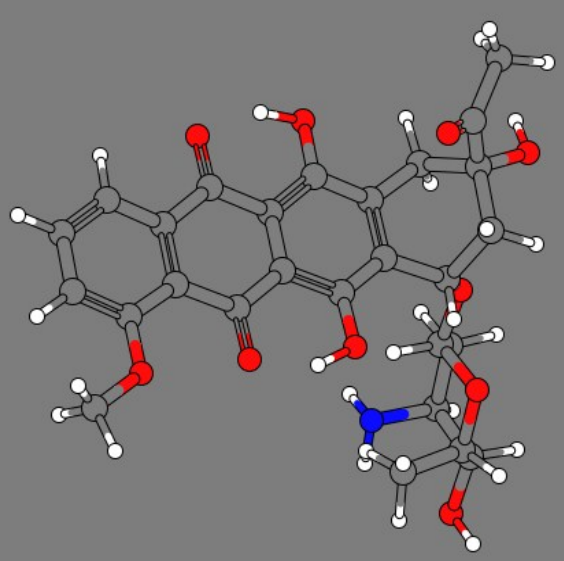
Cinerubin A

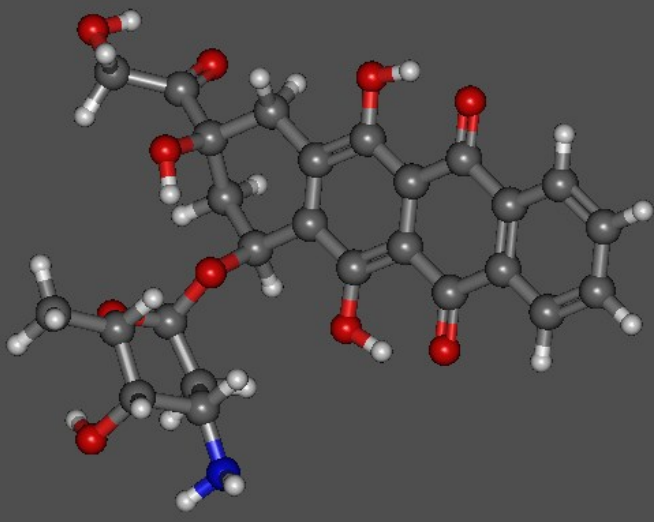
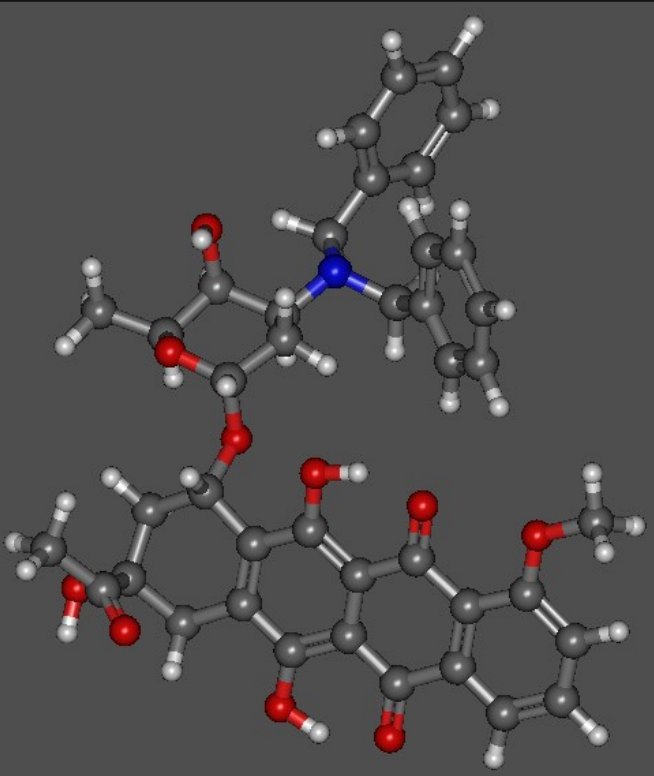
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34044-10-5

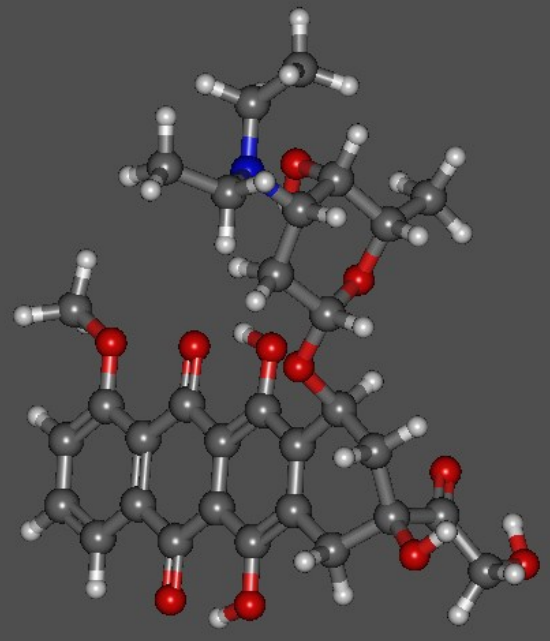
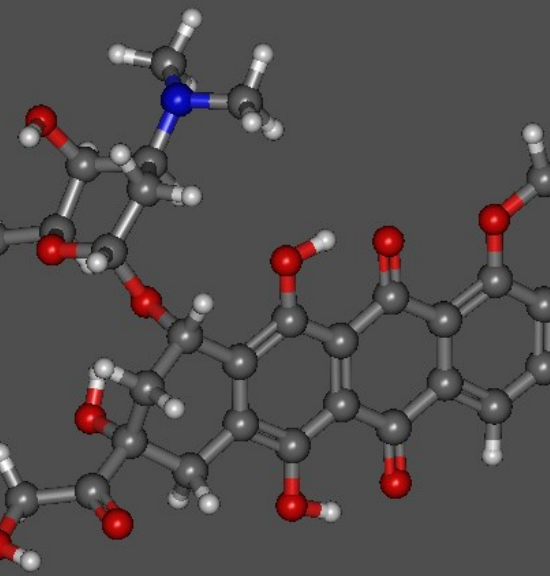


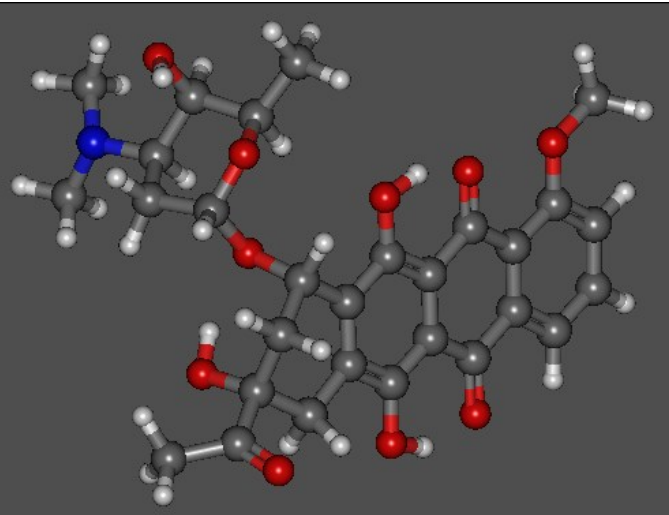
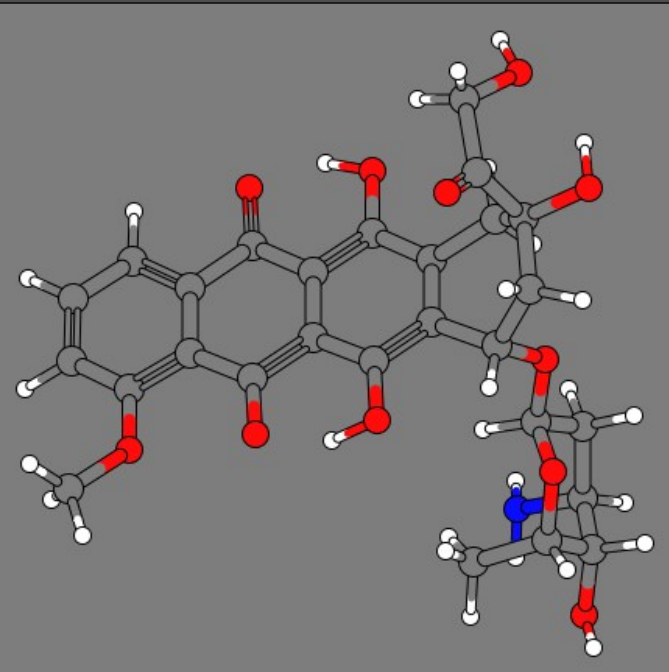
<p>N-(1-Cyano-2-methoxyethyl) doxorubicin</p>	<p>NSC 639659</p>		 A 3D ball-and-stick model of N-(1-Cyano-2-methoxyethyl)doxorubicin. The molecule features a tetracyclic doxorubicin core with a cyanoethyl group at C-13 and a methoxy group at C-10. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	
<p>Cyanomorpholino doxorubicin</p>	<p>88254-07-3</p>		 A 3D ball-and-stick model of Cyanomorpholino doxorubicin. The molecule features a tetracyclic doxorubicin core with a cyanomorpholino group at C-13 and a methoxy group at C-10. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

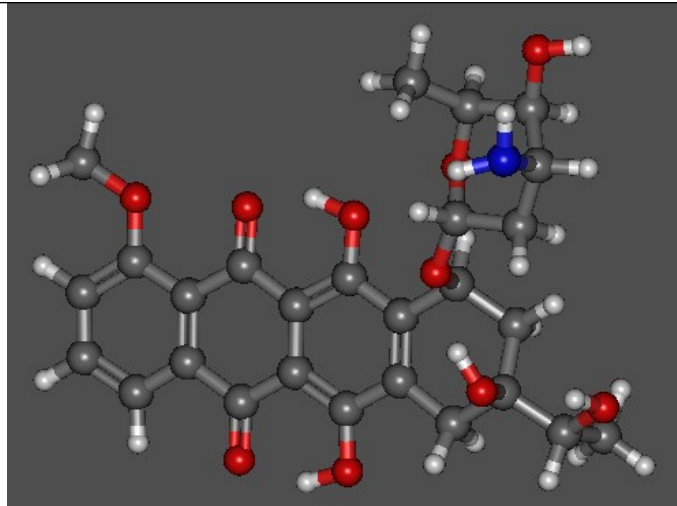
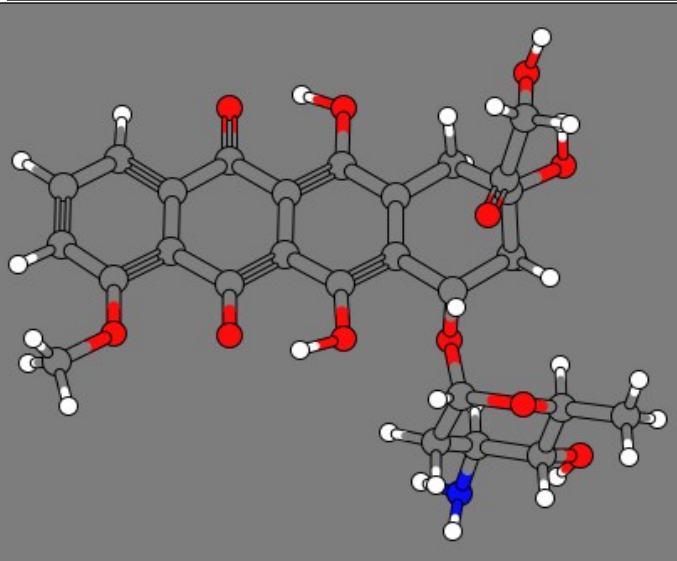
<p>Daunomycin 3,4-dichlorobenzoyl hydrazone</p>	<p>66996-54-1</p>			
<p>Daunomycin 4-nitrobenzoylhydrazone</p>	<p>66996-56-3</p>			

Daunomycin 3-oxime	34610-60-1		 A ball-and-stick model of Daunomycin 3-oxime. The molecule features a complex polycyclic core with a central nitrogen atom (blue) bonded to a hydrogen atom (white) and two oxygen atoms (red). The structure is highly branched and includes several hydroxyl groups (red and white) and a carbonyl group (red and grey).	
Daunorubicin / Daunomycin	20830-81-3 / 23541-50-6		 A ball-and-stick model of Daunorubicin / Daunomycin. The molecule is a complex polycyclic structure with a central nitrogen atom (blue) bonded to a hydrogen atom (white) and two oxygen atoms (red). It features a highly branched core with multiple hydroxyl groups (red and white) and a carbonyl group (red and grey).	

<p>4-Demethoxyadriamycin / Medorubicin</p>	<p>64363-63-9</p>		 <p>A ball-and-stick model of the anticancer drug 4-Demethoxyadriamycin (Medorubicin). The molecule features a tetracyclic anthracycline core with a dimethylamino group at position 10 and a hydroxyl group at position 4. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).</p>	
<p>N,N-dibenzyl-daunorubicin</p>	<p>70878-51-2</p>		 <p>A ball-and-stick model of the anticancer drug N,N-dibenzyl-daunorubicin. The molecule features a tetracyclic anthracycline core with a dimethylamino group at position 10 and two hydroxyl groups at positions 1 and 4. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).</p>	

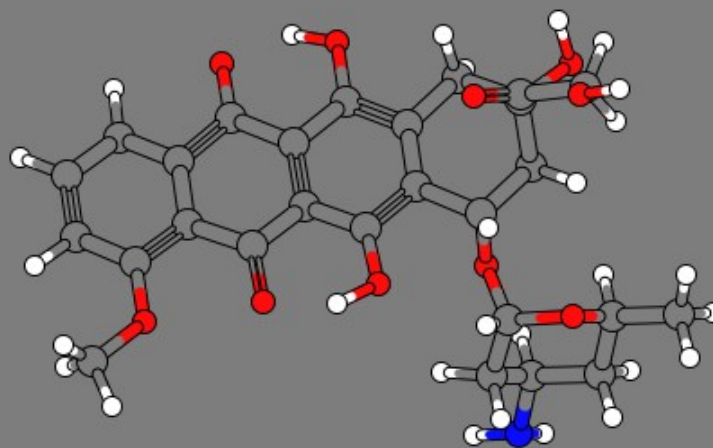
N,N-diethyladriamycin	70844-09-6		 A 3D ball-and-stick model of N,N-diethyladriamycin. The molecule features a complex polycyclic core with a central nitrogen atom (blue) bonded to two ethyl groups (grey and white). The core includes several oxygen atoms (red) and hydrogen atoms (white) attached to carbon atoms (grey).	
N,N-dimethyladriamycin	67106-76-7		 A 3D ball-and-stick model of N,N-dimethyladriamycin. The molecule features a complex polycyclic core with a central nitrogen atom (blue) bonded to two methyl groups (grey and white). The core includes several oxygen atoms (red) and hydrogen atoms (white) attached to carbon atoms (grey).	

<p>N,N-dimethyldaunomycin</p>	<p>70095-84-0</p>		 A ball-and-stick model of N,N-dimethyldaunomycin. The molecule features a complex polycyclic core with a central nitrogen atom (blue) bonded to two methyl groups (grey and white). It has several hydroxyl groups (red and white) and a dimethylamino group (blue and grey) attached to the structure.	
<p>Doxorubicin / Adriamycin</p>	<p>25316-40-9 / 23214-92-8</p>		 A ball-and-stick model of Doxorubicin / Adriamycin. The molecule consists of a tetracyclic anthracycline core with a dimethylamino group (blue and grey) and a D-glucopyranoside sugar moiety (grey, white, and red) attached to the structure.	

<p>Duborimycin</p>	<p>NSC 180510</p>		 A 3D ball-and-stick model of the molecule Duborimycin. The structure features a complex polycyclic core with several hydroxyl groups and a nitrogen atom. The atoms are color-coded: carbon is grey, oxygen is red, hydrogen is white, and nitrogen is blue.	
<p>Epirubicin</p>	<p>56390-09-1</p>		 A 3D ball-and-stick model of the molecule Epirubicin. The structure is a complex polycyclic system with multiple hydroxyl groups and a nitrogen atom. The atoms are color-coded: carbon is grey, oxygen is red, hydrogen is white, and nitrogen is blue.	

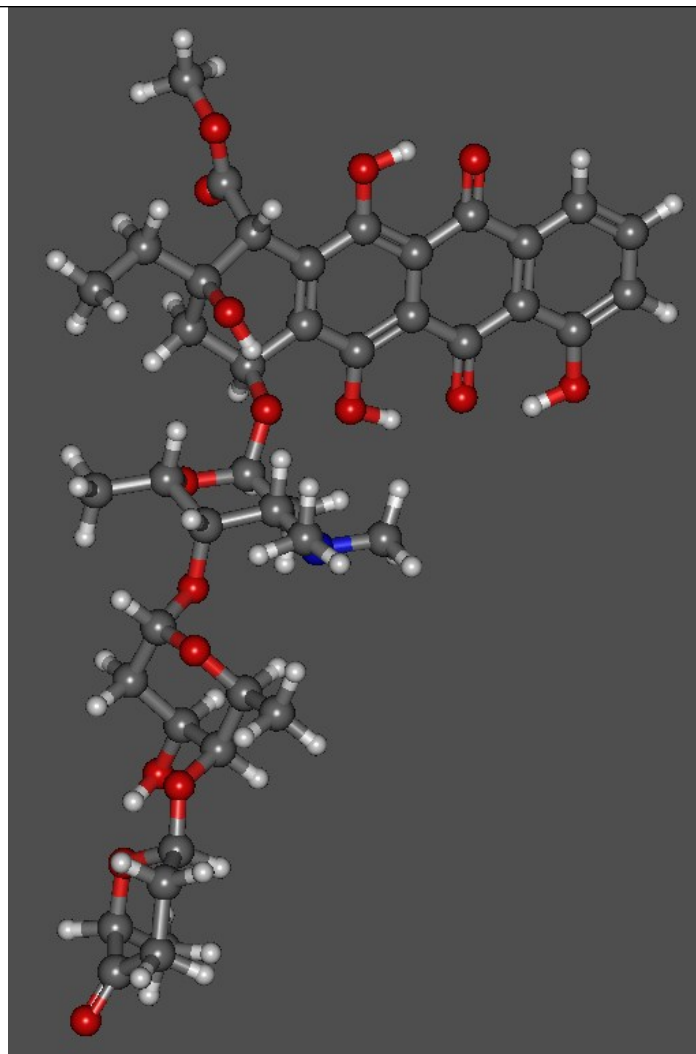
Esorubicin

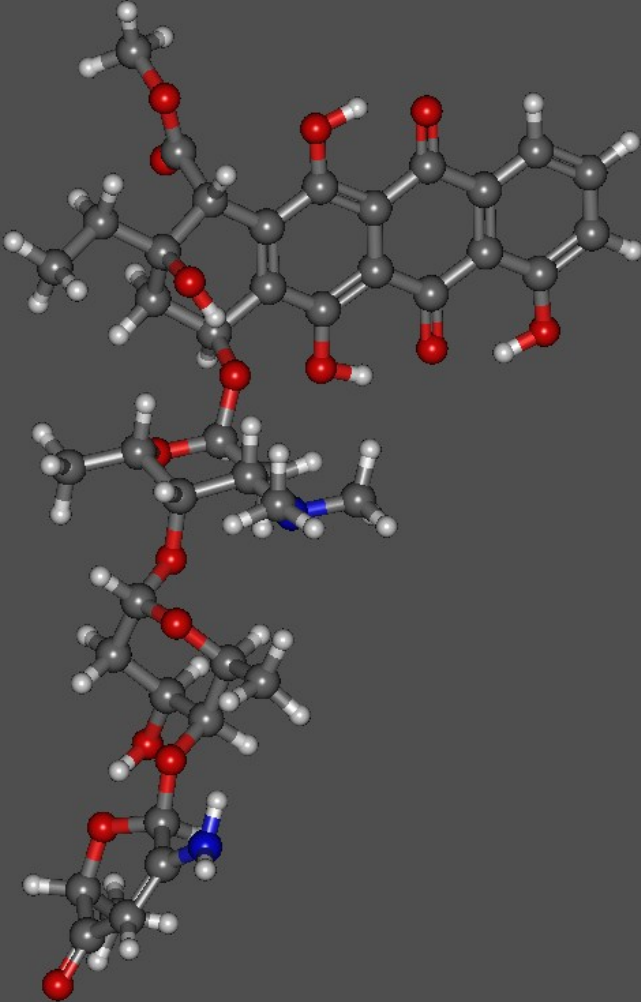
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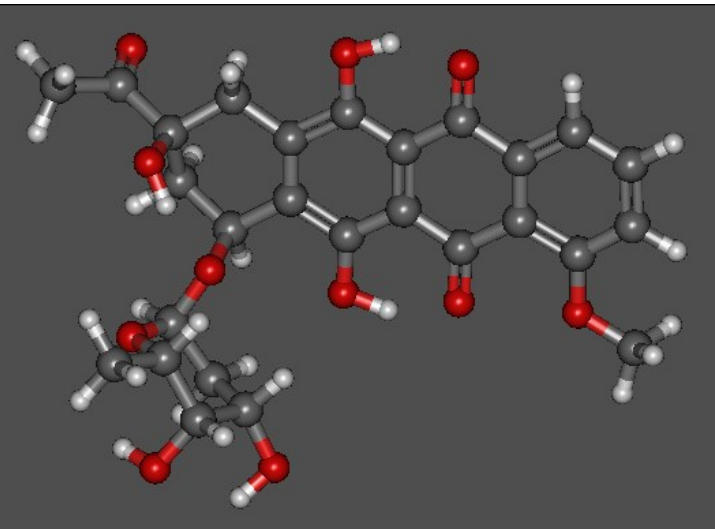
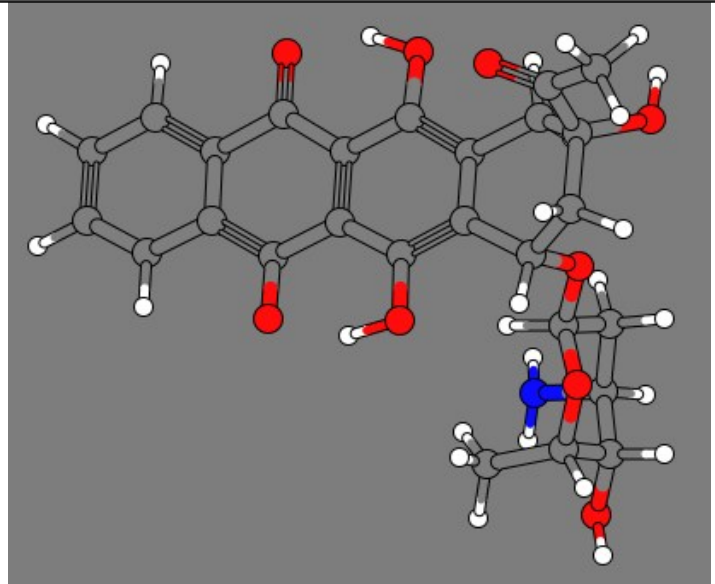


11-Hydroxy aclacinomycin A

NSC 670121

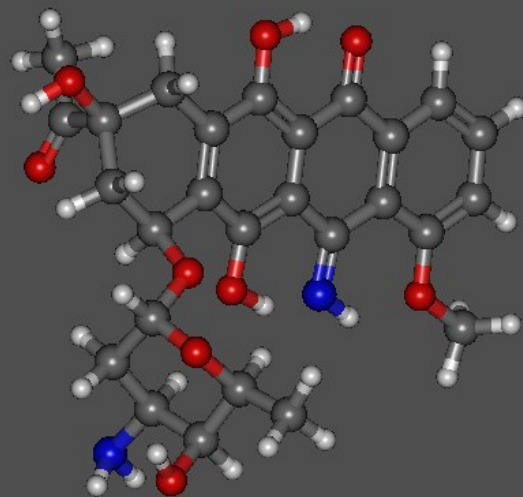


<p>11-Hydroxy aclacinomycin X</p>	<p>NSC 670122</p>		 <p>A 3D ball-and-stick model of the molecule 11-Hydroxy aclacinomycin X. The structure is a complex polycyclic molecule with a central fused ring system. It features several hydroxyl groups (red oxygen atoms bonded to white hydrogen atoms) and a nitrogen atom (blue) within the ring system. The model is rendered in a perspective view against a dark gray background.</p>	
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<p>3'-Hydroxy daunorubicin</p>	<p>64842-75-7</p>		 A ball-and-stick model of 3'-Hydroxy daunorubicin. The molecule features a tetracyclic anthracycline core with a hydroxyl group at the 3' position of the aglycone moiety. The atoms are color-coded: carbon (grey), oxygen (red), and hydrogen (white).	
<p>Idarubicin</p>	<p>57852-57-0</p>		 A ball-and-stick model of Idarubicin. The molecule features a tetracyclic anthracycline core with a 4-oxo-1,2,3,4-tetrahydrophthalazine ring system at the 12-position. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

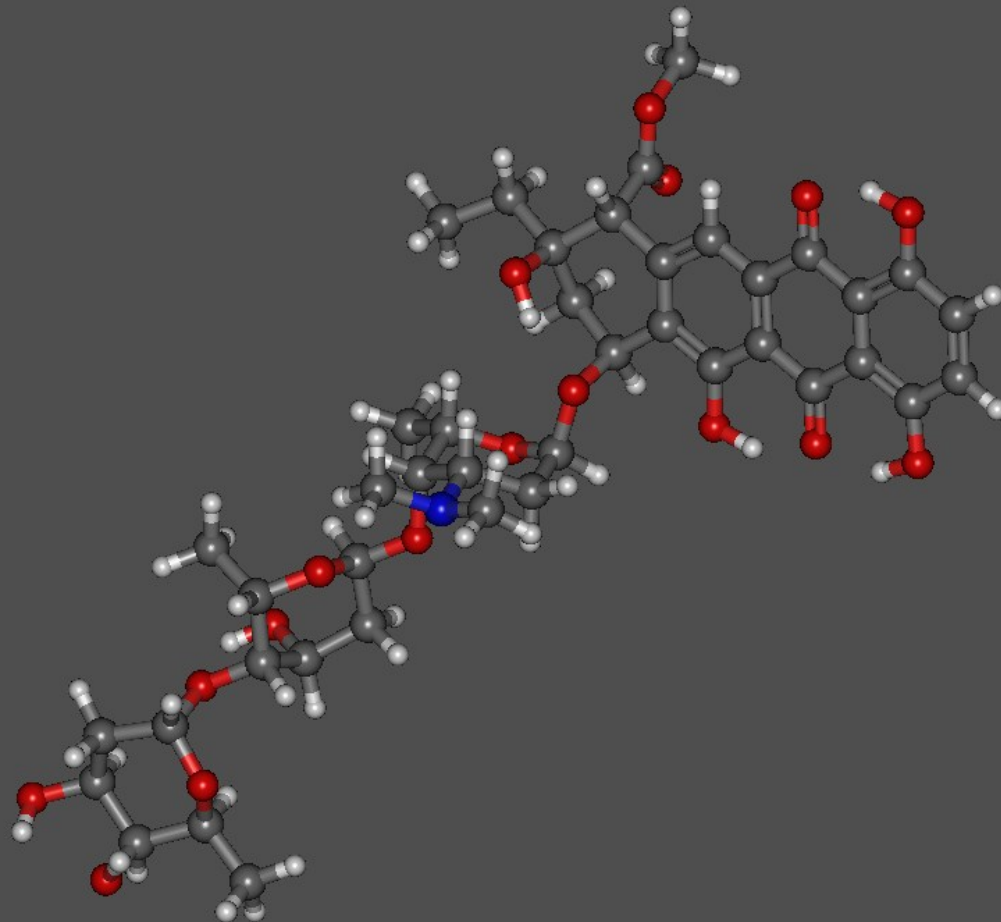
5-Imino daunorubicin

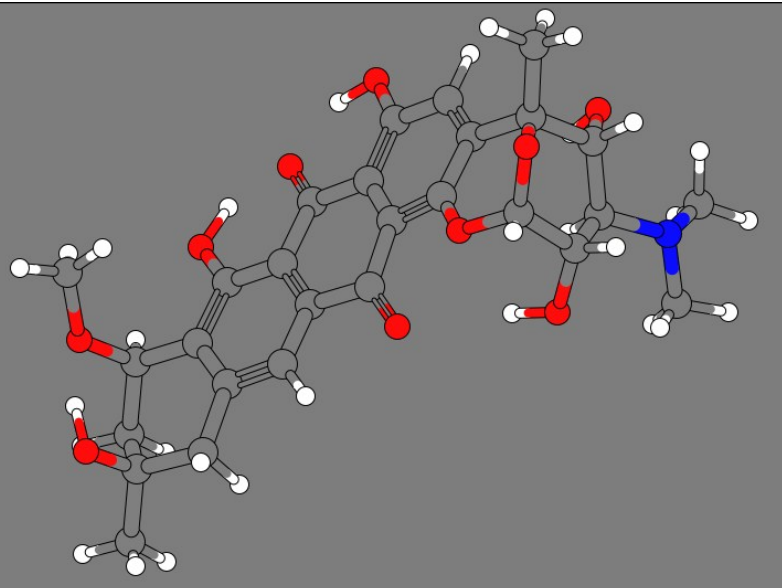
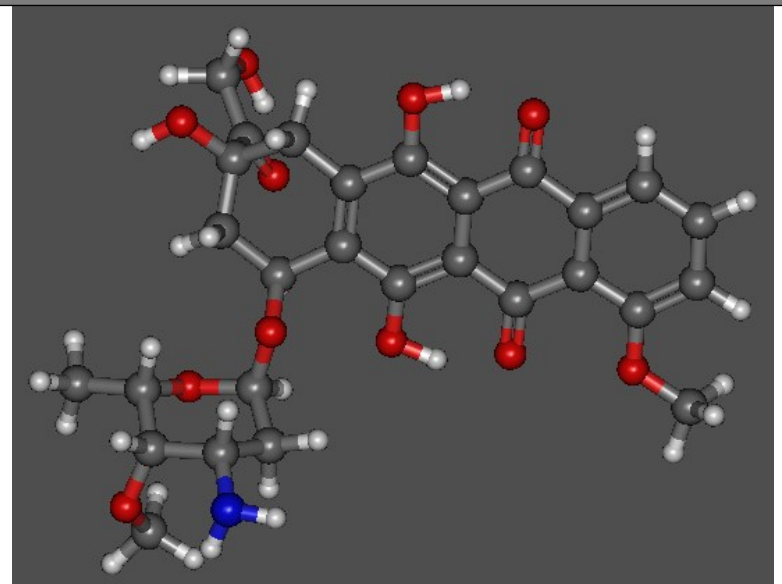
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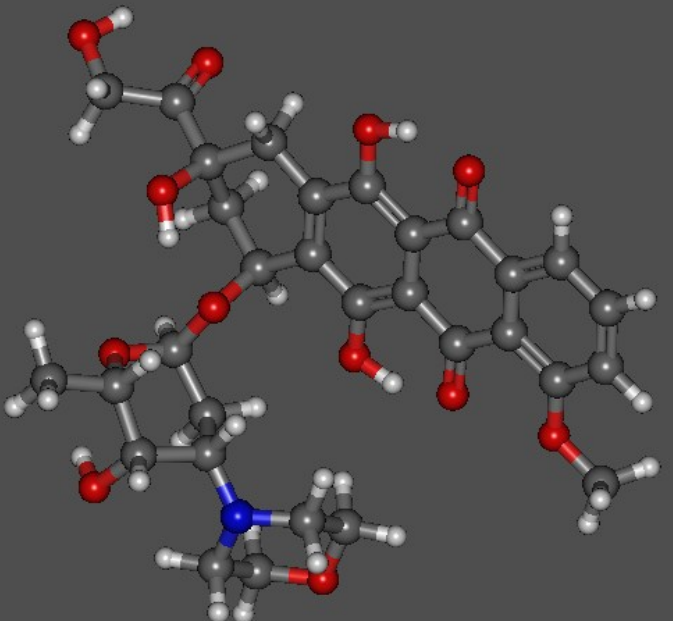
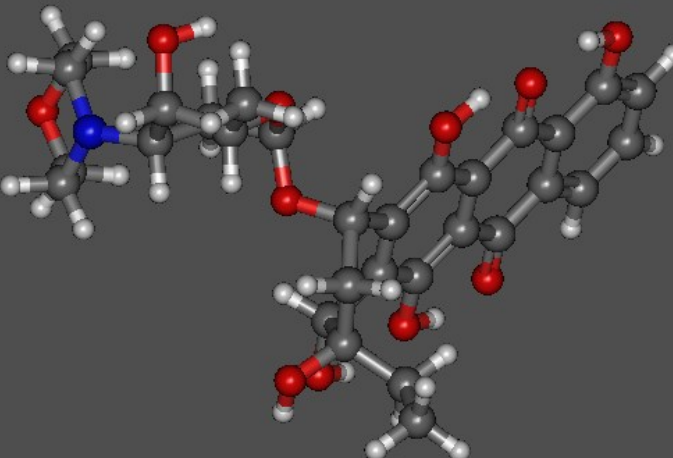


Marcellomycin

63710-10-1

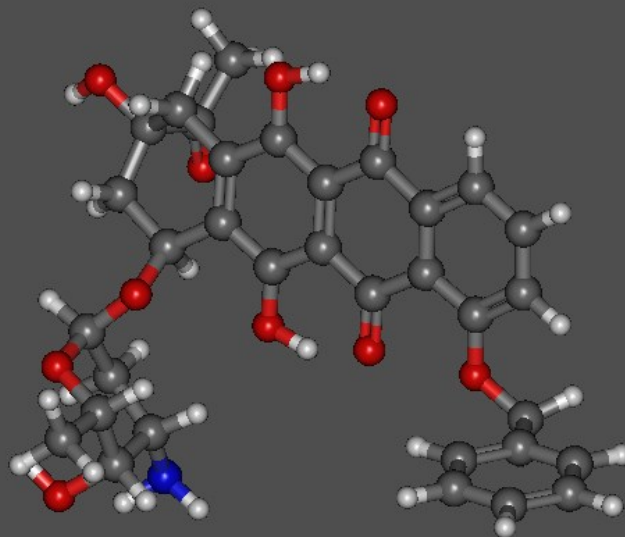


<p>Menogaril</p>	<p>71628-96-1</p>	 <p>A 3D ball-and-stick model of the Menogaril molecule. The structure features a complex polycyclic core with multiple hydroxyl groups (red and white) and a methylamino group (blue and white). The atoms are color-coded: carbon is grey, oxygen is red, hydrogen is white, and nitrogen is blue.</p>
<p>4'-O-methylodoxorubicin</p>	<p>77121-90-5</p>	 <p>A 3D ball-and-stick model of the 4'-O-methylodoxorubicin molecule. It shows a tetracyclic anthracycline core with several hydroxyl groups and a methylamino group. The atoms are color-coded: carbon is grey, oxygen is red, hydrogen is white, and nitrogen is blue.</p>

<p>Morpholino adriamycin</p>	<p>89196-04-3</p>		 A 3D ball-and-stick model of Morpholino adriamycin. The molecule features a complex polycyclic core with multiple hydroxyl groups (red and white spheres) and a morpholine ring system (blue and white spheres) attached to the side chain. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).	
<p>MX2</p>	<p>NCI 619003</p>		 A 3D ball-and-stick model of MX2. The structure is similar to Morpholino adriamycin but with a different side chain configuration. It shows a complex polycyclic core with multiple hydroxyl groups and a morpholine ring system. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).	

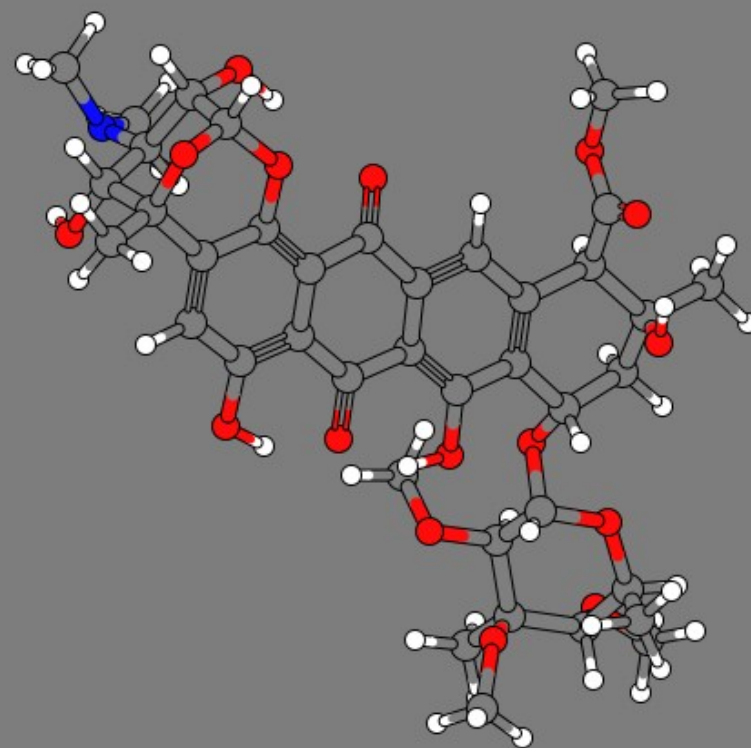
NSC 286628

NSC 286628 /
67903-59-7



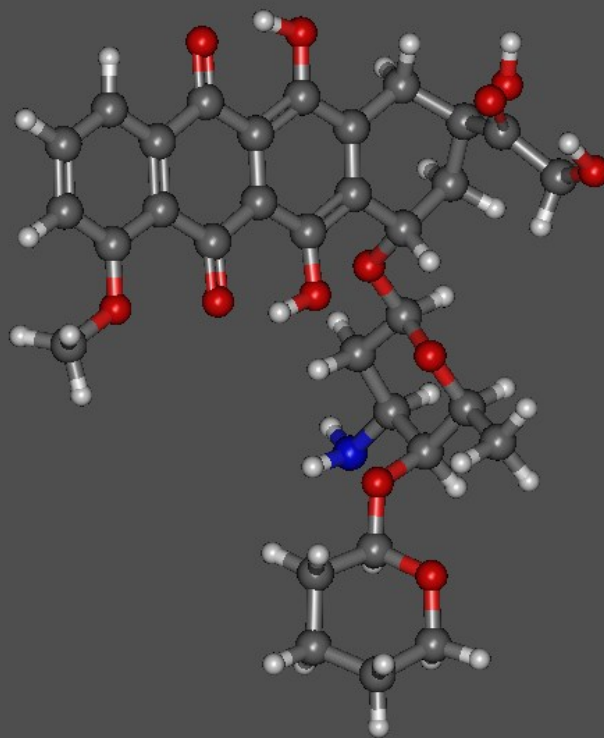
Nogalamycin

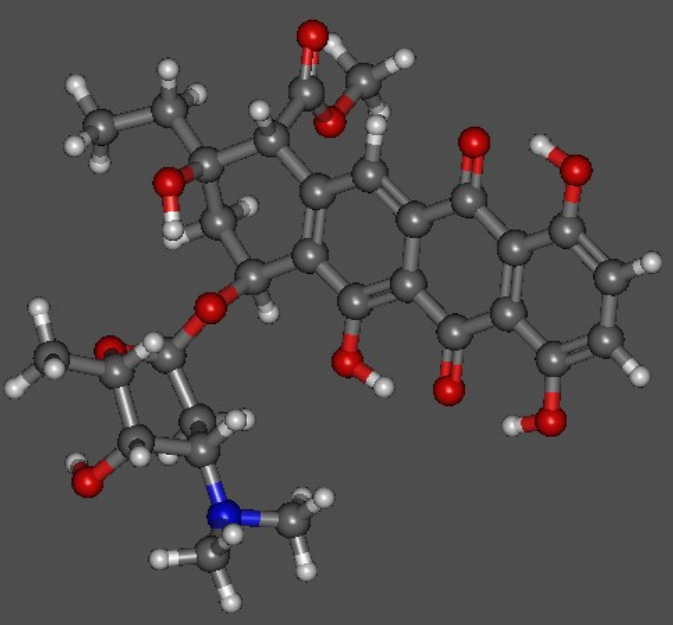
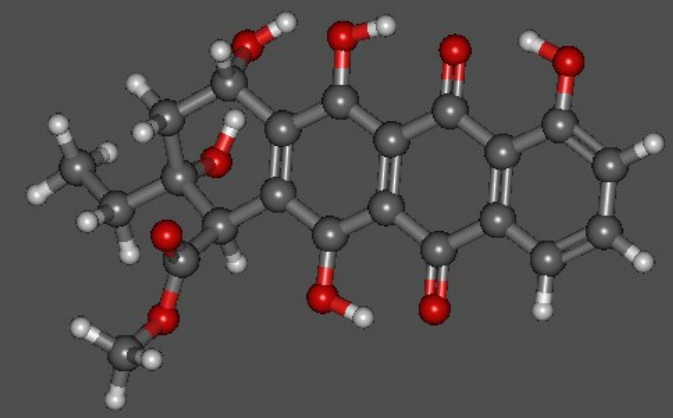
1404-15-5

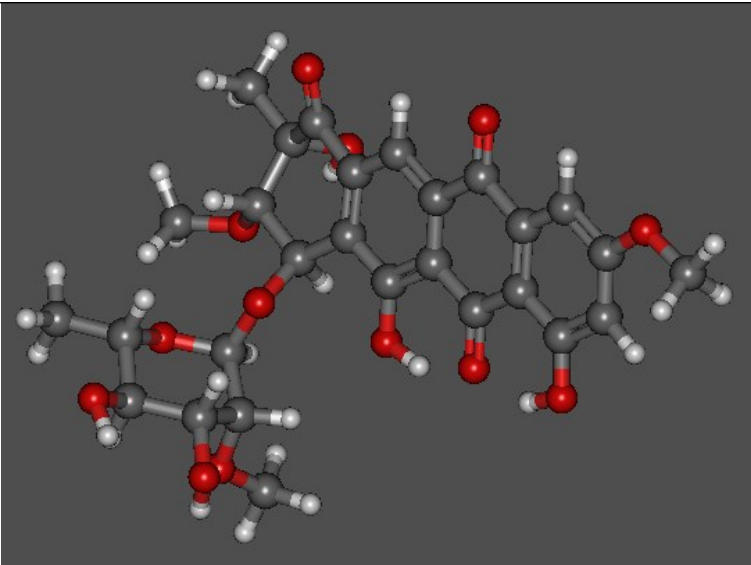
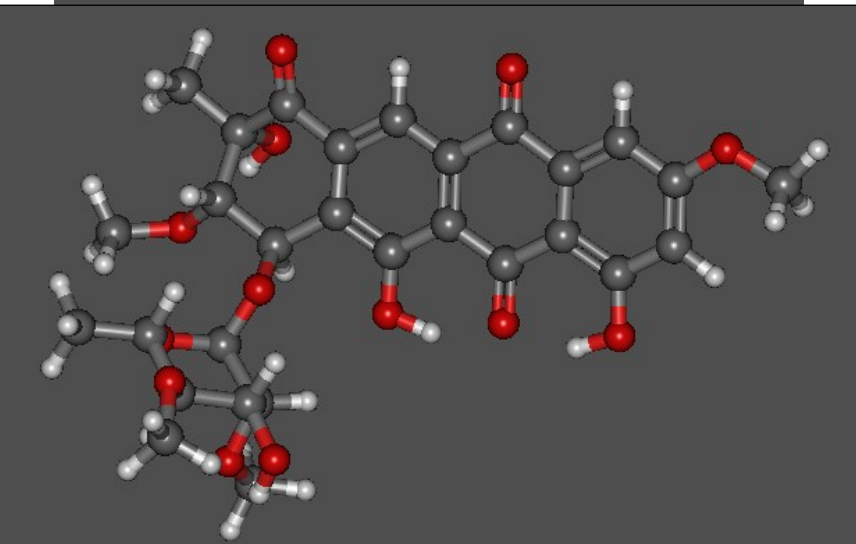


Pirarubicin

72496-41-4

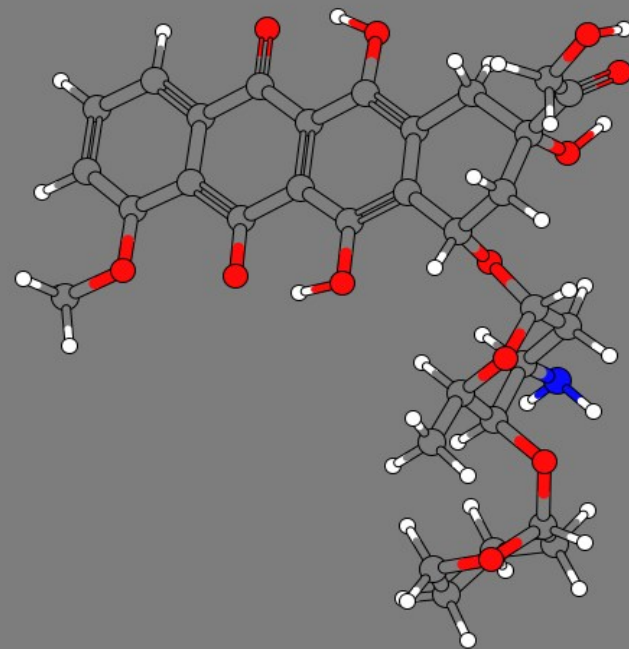


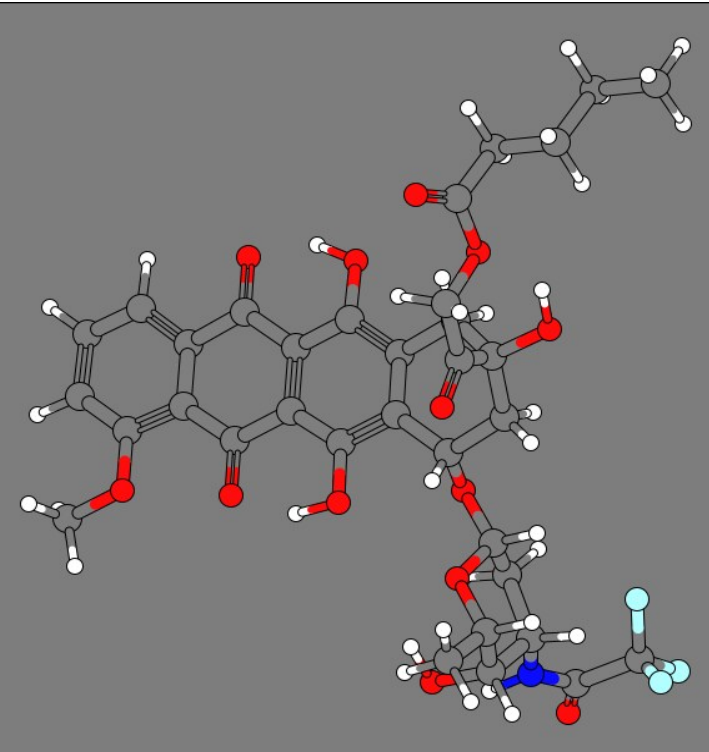
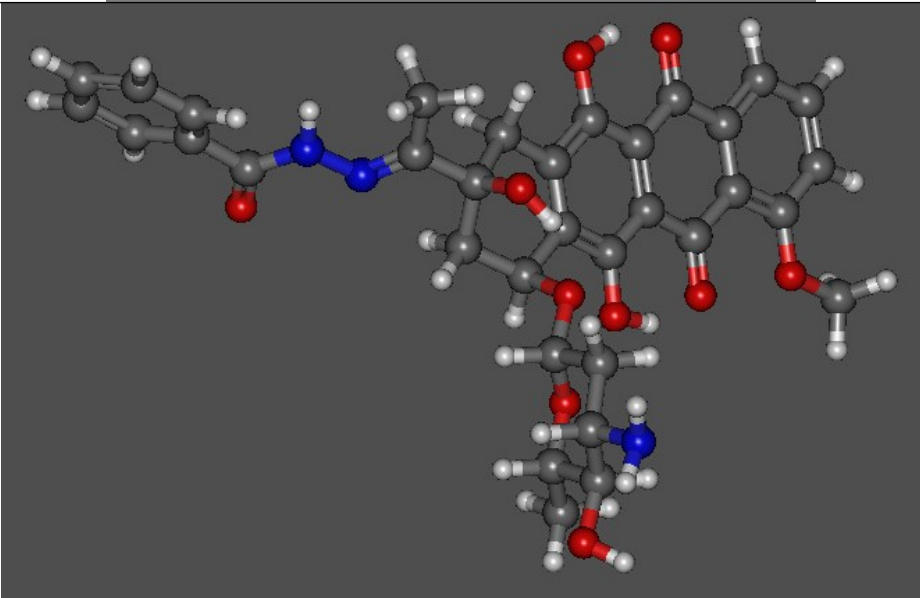
<p>Pyrrromycin</p>	<p>668-17-7</p>		 A 3D ball-and-stick model of the molecule Pyrrromycin. The structure features a complex polycyclic ring system with several hydroxyl groups (red oxygen atoms bonded to white hydrogen atoms) and a nitrogen atom (blue) bonded to two hydrogen atoms. The atoms are represented by spheres: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	
<p>Rhodomyconone</p>	<p>21288-60-8</p>		 A 3D ball-and-stick model of the molecule Rhodomyconone. The structure is a complex polycyclic ring system with multiple hydroxyl groups (red oxygen atoms bonded to white hydrogen atoms). The atoms are represented by spheres: carbon (grey), oxygen (red), and hydrogen (white).	

Steffimycin	11033-34-4	 A 3D ball-and-stick model of Steffimycin, a complex polyketide antibiotic. The molecule features a long, zig-zagging carbon backbone with several oxygen-containing functional groups, including hydroxyl and ether linkages, and a terminal methyl group. The atoms are color-coded: carbon is grey, oxygen is red, and hydrogen is white.
Steffimycin B	NCI 204856	 A 3D ball-and-stick model of Steffimycin B, another complex polyketide antibiotic. It has a similar structure to Steffimycin but with a different arrangement of oxygen-containing groups, particularly in the terminal region. The atoms are color-coded: carbon is grey, oxygen is red, and hydrogen is white.

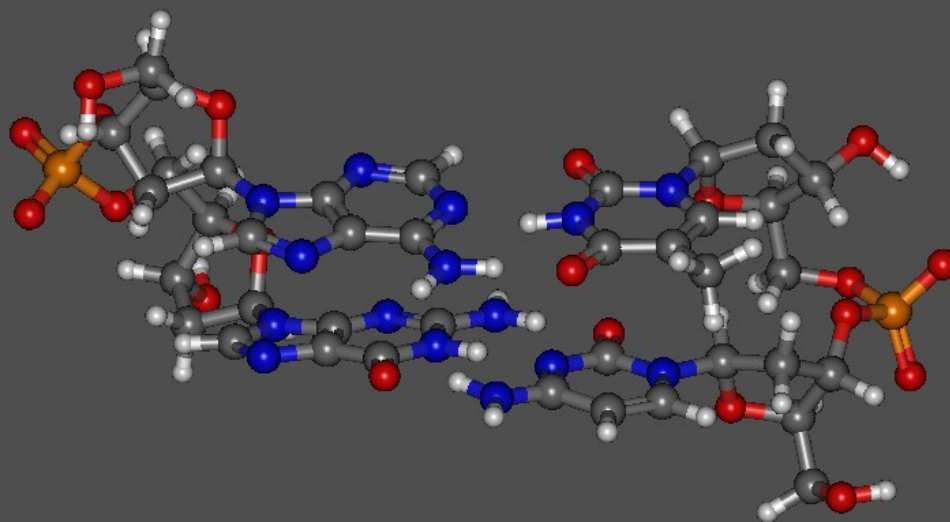
Theprubicin

95343-20-7



<p>Valrubicin</p>	<p>56124-62-0</p>	 <p>A 3D ball-and-stick model of Valrubicin, a complex polycyclic molecule. The structure features a central core with multiple fused rings, including a benzene ring and a pyridine ring. It is substituted with several hydroxyl groups (red and white), a methyl group (grey and white), and a side chain containing a carbonyl group (red and white) and a methyl group (grey and white). The model is set against a dark grey background.</p>
<p>Zorubicin / Rubidazole</p>	<p>36508-71-1</p>	 <p>A 3D ball-and-stick model of Zorubicin / Rubidazole, a complex polycyclic molecule. The structure features a central core with multiple fused rings, including a benzene ring and a pyridine ring. It is substituted with several hydroxyl groups (red and white), a methyl group (grey and white), and a side chain containing a carbonyl group (red and white) and a methyl group (grey and white). The model is set against a dark grey background.</p>

AG-TC base pairs



7. Cartesian coordinates of the optimized chemical structures of anthracycline's semi-quinone free radicals

Name	NSC No. / CAS No.	Cartesian coordinates
3'-Acetoxy-4'-O-acetylodoxorubicin	73113-92-5	H 1.0 -2.7645709770 -1.6775907201 -6.6969163819
		H 1.0 -1.0063748326 -1.9735035253 -6.7792928583
		H 1.0 -2.1374068937 -3.3478612394 -6.6513276900
		C 6.0 -1.9439526571 -2.3130087816 -6.3339661410
		H 1.0 -4.1581955812 -3.1275420452 -5.6875609320
		O 8.0 -1.7664109122 -2.2077501420 -4.9392134710
		C 6.0 -4.0067583074 -3.0353238379 -4.6193125715
		H 1.0 -5.9886535281 -3.7576585006 -4.1601506098
		C 6.0 -2.7962775189 -2.5669640244 -4.1185181602
		C 6.0 -5.0516046973 -3.3944213481 -3.7449356727
		C 6.0 -2.5839537193 -2.4415296088 -2.7048283914
		O 8.0 -0.3241388222 -1.6247403032 -2.8460173399
		H 1.0 2.1463090704 6.4391768739 -3.1277411163
		C 6.0 -4.8869032632 -3.2852891704 -2.3832421763
		H 1.0 0.9713508134 2.2666325939 -3.0696103617
		C 6.0 -1.3303982711 -1.9653469404 -2.1283643086
		H 1.0 -5.6701106464 -3.5513440539 -1.6830068971
		C 6.0 -3.6689696523 -2.8126628175 -1.8458811776
		H 1.0 3.2165384020 5.3729742658 -2.1819706342
		C 6.0 2.2064595584 5.4978855760 -2.5826648363
		H 1.0 0.6862403489 -1.3030411654 -1.8129831942
		O 8.0 4.8641964008 4.2963491049 -0.3390783724
		H 1.0 2.6633582949 3.4431497652 -1.4357958189
		H 1.0 2.0213971494 4.6686639379 -3.2724709868
		C 6.0 0.3219516052 2.0275618325 -2.2193967498
		H 1.0 -0.1038739535 1.0370725951 -2.3915868282
		C 6.0 1.1520655410 5.5410825990 -1.4886431593
		H 1.0 5.7023065762 6.5296101772 0.6194900577
		H 1.0 -0.4832171534 2.7650142863 -2.1685631882
		O 8.0 0.4333723468 6.4999660190 -1.3200087429
		C 6.0 -1.2412512189 -1.8686297445 -0.6799765950
		O 8.0 1.0356076292 -1.1279660487 -0.8594117359
C 6.0 -3.5655044622 -2.7187195849 -0.3960600037		
H 1.0 1.8605628048 1.2105353434 -0.9606056974		
C 6.0 4.2885540620 4.9274561556 0.5255950499		
C 6.0 1.8925151130 3.3320390023 -0.6734648212		
C 6.0 1.1225066209 2.0208037867 -0.9260432921		
O 8.0 0.9869549833 4.4567278858 -0.6925736352		

		C	6.0	4.7686086517	6.2410086718	1.1012886826
		C	6.0	-0.0308312405	-1.4070961815	-0.0877143420
		O	8.0	-4.5449119252	-3.0667679760	0.3549446396
		C	6.0	-2.3309377255	-2.2255463531	0.1632897336
		H	1.0	3.3493816447	2.5338036928	0.6777499194
		H	1.0	4.0102309695	7.0138643709	0.9461008587
		O	8.0	3.1273297268	4.5575549079	1.0956486775
		C	6.0	2.5492477324	3.2772121861	0.7135824263
		H	1.0	4.9179425612	6.1442999450	2.1805633666
		O	8.0	0.2040745505	1.7564667033	0.1374705721
		C	6.0	0.0686699120	-1.2426136999	1.3044466967
		C	6.0	-2.1970809823	-2.1127023948	1.5740769849
		O	8.0	1.7853719325	0.5924296609	1.4376051098
		H	1.0	2.1832462147	-1.3616510757	1.4773934437
		H	1.0	-3.9373038668	-2.7948160754	1.7454708852
		C	6.0	1.5274232270	2.9228160656	1.7862582526
		C	6.0	0.8193452547	1.6143806512	1.4048379177
		C	6.0	1.3777618747	-0.7383992161	1.8751206735
		C	6.0	-1.0134851567	-1.6236071923	2.1364212035
		H	1.0	0.7852141961	3.7236253077	1.8498000308
		O	8.0	-3.2101559012	-2.4873236439	2.3889513980
		H	1.0	2.0195907889	2.8164274571	2.7570706383
		H	1.0	1.7282034939	-5.3789887267	3.6439215886
		H	1.0	-0.0102617191	1.4037572763	2.0890609667
		O	8.0	0.8376120133	-5.6328552738	3.9465960057
		C	6.0	1.4368606069	-0.7500031601	3.4184150694
		C	6.0	-0.8921996118	-1.5812480509	3.6427834910
		H	1.0	1.0851080799	0.2144509504	3.8007415262
		O	8.0	2.2364069463	-3.4547555304	3.5296696991
		H	1.0	-1.1998609527	-0.6102828776	4.0565356335
		H	1.0	2.4789880561	-0.8694189760	3.7331453198
		C	6.0	1.0617032455	-3.2371090319	3.7959444311
		H	1.0	-1.5653928543	-2.3179767384	4.0872364726
		C	6.0	0.1264526560	-4.4209627603	3.9905486587
		C	6.0	0.5536596761	-1.8091933944	4.0729452388
		H	1.0	-0.6526096994	-4.3725781694	3.2129082197
		H	1.0	-0.3824784122	-4.3029084282	4.9576776223
		O	8.0	0.5952402832	-1.6966540908	5.5117896344
		H	1.0	1.5300372114	-1.6940805975	5.7647135867
Aclacinomycin X	NSC 670120	H	1.0	-0.4262582990	10.1567019898	3.5734493682
		H	1.0	1.0628690561	11.3294823952	1.9393872066
		C	6.0	0.2581762042	9.5993978509	2.9411497890
		C	6.0	1.0992852619	10.2451519431	2.0201067503

O	8.0	-0.5308961375	7.6147131400	3.9537472163
C	6.0	0.2871759029	8.2124166672	3.0619959091
C	6.0	1.9678818930	9.5202977880	1.2195375515
H	1.0	2.6258153610	9.9972960914	0.5016406940
H	1.0	-0.3392162191	6.6353054560	3.8670651194
C	6.0	1.1758005360	7.4398380363	2.2470800859
C	6.0	2.0212700830	8.1175626932	1.3176143664
O	8.0	0.4322796674	5.3844778829	3.2203226886
C	6.0	1.2084454860	6.0040076144	2.3703669519
C	6.0	2.9537502081	7.3780459848	0.4520116473
O	8.0	3.6994805329	7.9641405495	-0.3654855234
C	6.0	2.1170679214	5.2618804421	1.5357532951
H	1.0	0.8378611765	3.9074802253	2.9486094728
C	6.0	2.9667093052	5.9161712410	0.5966935530
O	8.0	1.3608862857	3.1785935493	2.4775846599
C	6.0	2.1721652722	3.8391613162	1.6251649866
C	6.0	3.8348053757	5.1529941796	-0.2034509869
H	1.0	4.4668756225	5.6880760747	-0.9042706945
H	1.0	-2.6536069859	1.5409816458	-0.3225312151
H	1.0	-3.4727679787	1.4188555560	-1.8774128449
H	1.0	-1.8730287074	2.1882945201	-1.7835049765
H	1.0	-0.6981435067	1.4231111080	0.4986639956
C	6.0	-2.4958270709	1.3649850092	-1.3874824147
C	6.0	3.0572349576	3.0987455089	0.8332338134
C	6.0	3.8865816631	3.7695316522	-0.0973813463
H	1.0	8.0078563629	5.1052055364	0.4488821071
H	1.0	-1.1113869919	-0.2236153104	1.0206120121
C	6.0	-0.4429150348	0.3686158192	0.3882529298
H	1.0	1.0266010348	0.3916032830	1.9836419581
H	1.0	2.9055929432	1.3029636071	1.9862529205
C	6.0	3.0131889055	1.6009926698	0.9380559194
O	8.0	1.7872563009	1.1709134771	0.2473219444
N	7.0	-1.9247964200	0.0366010827	-1.6231139370
H	1.0	4.8679256552	3.3907821553	-1.9696046601
C	6.0	4.8903840738	2.9883508691	-0.9532262134
C	6.0	0.9906896666	0.2141961714	0.9038515549
O	8.0	6.8928896176	4.2540853978	-1.0953900836
H	1.0	8.4905879162	5.4858684170	-1.2347057969
C	6.0	6.2725922008	3.2829600652	-0.3806581241
C	6.0	8.1443385093	4.7041135246	-0.5583793005
H	1.0	-2.9342157804	-0.0436463522	-3.4575573652
O	8.0	6.7811316412	2.7699881667	0.5977787162
C	6.0	-0.5640916577	-0.1073369187	-1.0667363402
H	1.0	0.1393558151	0.4955647846	-1.6729918765

H	1.0	2.6492638762	1.4174308333	-1.4458466300
H	1.0	-5.6383118609	-2.4278253546	-1.7803748970
H	1.0	-3.3856619721	-1.9188956716	-0.6783376892
C	6.0	-1.9362461638	-0.2491956158	-3.0586287275
H	1.0	-1.2154840378	0.3690263310	-3.6274087280
H	1.0	-4.9090392407	-3.3511413927	0.5636906273
C	6.0	4.2332597805	0.9104692099	0.3249536186
H	1.0	5.0940958971	1.0806978786	0.9789901596
O	8.0	3.4630531060	1.3123130168	-1.9662174517
H	1.0	-2.6585843463	-3.0742909332	1.4228708636
C	6.0	4.5732966583	1.4637447707	-1.0688340510
H	1.0	8.8661213369	3.8837483718	-0.5160077132
H	1.0	-4.3607308794	-1.9296129792	-2.9025453525
O	8.0	1.4814372579	-1.1096452135	0.7371744422
C	6.0	-4.6717431904	-2.7133619505	-2.2094572057
H	1.0	-6.6033841610	-6.6108027127	2.7781381483
C	6.0	-3.6247919507	-2.8953497343	-1.1186914172
H	1.0	-1.7230685942	-1.3030147328	-3.2445048571
C	6.0	-4.0742429578	-3.8221073950	0.0242105248
C	6.0	-0.0417327493	-1.5608992055	-1.1302716287
H	1.0	4.0389065211	-0.1644117069	0.2816840736
H	1.0	-5.8990581079	-5.2686730678	0.9652399785
O	8.0	-0.8653097011	-2.4192972843	-0.3259756633
H	1.0	-5.0140941388	-6.9899584716	3.4704507537
C	6.0	-2.9063531702	-4.0530051511	0.9982538379
O	8.0	-3.2555787135	-4.8726307740	2.0985853220
H	1.0	2.0075449308	-0.9421487317	-1.2620684663
C	6.0	-5.8438431519	-7.3920899326	2.8833675160
C	6.0	1.4103053994	-1.5942883513	-0.6078777788
H	1.0	-4.7823673244	-3.6396404071	-2.7810029988
H	1.0	-6.2967237273	-8.2283295113	3.4216434897
H	1.0	6.0013122971	1.2711933951	-2.6554231097
C	6.0	5.7533065462	0.7261153628	-1.7348428542
H	1.0	-0.0376148543	-1.9211534671	-2.1659176526
H	1.0	6.6257074925	0.7950926485	-1.0777626670
O	8.0	-2.4491813365	-3.3996360632	-1.7720860481
H	1.0	-3.4670216068	-5.7554171452	1.7468600881
O	8.0	-4.5564503310	-5.0553401750	-0.5698925451
C	6.0	-5.3950860931	-5.8678175689	0.1884272762
C	6.0	-1.3335287850	-3.6077261949	-0.9130142903
C	6.0	-1.6901173284	-4.5692386770	0.2232229101
H	1.0	-0.8393940894	-4.6782268614	0.9003449698
N	7.0	-6.8906708019	-5.6664633277	-1.7087270883
O	8.0	-4.6148006757	-6.8912861004	0.7902585085

		C 6.0 -5.3505106345 -7.8940886579 1.5225322064
		C 6.0 -6.4516428575 -6.4881781700 -0.7218387010
		H 1.0 4.6024684065 -0.8198202511 -2.7322993632
		C 6.0 2.0232674989 -2.9868591595 -0.5933354795
		C 6.0 -6.9589807682 -7.7218315034 -0.4411006647
		C 6.0 5.4813695619 -0.7386974008 -2.0886299586
		H 1.0 1.4624348793 -3.6421587417 0.0780275253
		H 1.0 -0.5729855679 -4.0398840259 -1.5749808605
		H 1.0 5.3065775549 -1.3498743885 -1.1968676418
		H 1.0 -6.2573898856 -4.9350211764 -1.9998885082
		H 1.0 3.0544765931 -2.9333099156 -0.2349954057
		H 1.0 -1.9241585955 -5.5484703225 -0.2083127917
		C 6.0 -6.5014334506 -8.4877408038 0.6965930723
		H 1.0 -7.5173028102 -6.0380599384 -2.4065507261
		H 1.0 -4.6260110524 -8.6987685526 1.6757943655
		H 1.0 -7.7496522281 -8.1566045024 -1.0466499808
		H 1.0 2.0312590046 -3.4220536279 -1.5983864274
		H 1.0 6.3388305899 -1.1705997842 -2.6165843438
		O 8.0 -6.9894250761 -9.5590912009 1.0503381374
Aclarubicin	57576-44-0	H 1.0 6.2825965797 -2.7170210918 1.1027379867
		H 1.0 5.9269260085 -2.7240940140 -1.3370344154
		H 1.0 4.5421727951 -2.8012405803 0.7621800100
		C 6.0 5.4307576621 -2.1709066393 0.6823685020
		H 1.0 -1.7543881822 -3.1983178499 1.3499956102
		C 6.0 5.6985607526 -1.8053228749 -0.7803013854
		H 1.0 -1.2848345308 -3.5968241287 -0.3297139071
		H 1.0 -6.7186700392 -1.6778388664 5.9529393724
		H 1.0 8.3997214796 -1.3308898744 -5.5619233537
		H 1.0 -2.9928730637 -3.3941005664 0.1153784620
		H 1.0 6.5817374732 -1.1627107824 -0.8484882420
		H 1.0 5.2739166895 -1.2832965856 1.3043904453
		C 6.0 -1.9839514911 -3.0129941276 0.2996454986
		H 1.0 -0.5163572680 -1.5307481157 4.0778540444
		O 8.0 3.3992198360 -1.9883417348 -1.3480538447
		H 1.0 2.0490671626 -1.6039850447 3.4164827418
		H 1.0 -0.0473742389 -2.1479018332 1.9414051661
		H 1.0 -5.5601039059 -1.5579265505 7.2827097851
		H 1.0 -4.8467795409 -2.6674567049 3.8270280507
		H 1.0 -7.8040663184 -0.9940055401 8.2347365597
		O 8.0 -2.4008838582 -1.7523984545 3.4757441765
		O 8.0 6.8172016885 -1.1658790176 -4.3139411122
		H 1.0 2.5942781438 -1.4508414059 -1.4351901095
		H 1.0 4.7799974879 -2.0000440103 -3.4392087448

C	6.0	-6.2585230944	-0.9849617724	6.6642022539
C	6.0	8.0761146948	-0.6535537696	-4.7713666209
H	1.0	-1.8408911572	-0.1590169297	5.6009182406
C	6.0	4.5247309692	-1.1109283324	-1.5016364366
H	1.0	-4.3069973869	-2.9718816959	2.1622797837
C	6.0	-1.2922868250	-0.8808762031	3.6545955534
H	1.0	8.8063771641	-0.6342957413	-3.9576362121
H	1.0	0.1052734807	-1.6565205339	-0.4760461829
C	6.0	-7.3300651582	-0.3043666580	7.5313222650
H	1.0	-8.1340090097	0.0798697122	6.8847052776
H	1.0	1.9945528574	-1.2680683572	0.9369125552
C	6.0	2.0469466533	-0.5991040767	2.9809176101
C	6.0	-4.6504998439	-2.2037697473	2.8578213380
C	6.0	-0.0445780540	-1.1116596876	1.5828780468
O	8.0	-4.4413778002	-0.5619749345	5.1872653477
H	1.0	3.0815096735	-0.2528405130	2.9127482994
C	6.0	4.8302116896	-0.9880898549	-3.0281674339
H	1.0	7.9587708483	0.3598630953	-5.1629386071
N	7.0	-1.9525188185	-1.5793389908	0.0078923473
C	6.0	-1.6357047036	0.2641154625	4.6116288346
C	6.0	6.2225158508	-0.4454497570	-3.3308172600
C	6.0	-3.5967611057	-1.1143311107	2.9943296139
H	1.0	4.0316467028	0.2352033711	0.1430573319
C	6.0	1.4141607174	-0.6067720508	1.5971375912
C	6.0	-0.5834251216	-1.0415927100	0.1354025321
H	1.0	-1.9305676681	-1.7457119533	-2.1437452675
C	6.0	-5.4430740810	0.0575623763	5.9106469456
H	1.0	1.5032885717	0.0790931063	3.6436348396
H	1.0	-0.7884077948	0.9494552292	4.6922735024
O	8.0	-0.8493908390	-0.3002392849	2.4507001672
H	1.0	-3.5213006377	-1.8146813359	-1.3529852084
C	6.0	4.2162263212	0.2842666702	-0.9332739237
H	1.0	-6.0849157123	0.6624989836	5.2487553974
H	1.0	-5.5852359862	-1.7831884951	2.4711507771
C	6.0	-2.5368246976	-1.3387337554	-1.3131079869
C	6.0	-4.0293190738	0.0271257336	3.9298933226
H	1.0	-3.3836149837	-0.6810652555	2.0087503130
H	1.0	4.3926710351	-0.8972503469	-5.7241701715
H	1.0	5.0875244998	0.9237336275	-1.1059549260
C	6.0	-6.8179848376	0.8974359731	8.3154068692
O	8.0	1.7673147968	0.2516038781	-1.1745010450
O	8.0	6.7586661542	0.5162256055	-2.8143174732
C	6.0	3.8397756908	-0.1018378105	-3.7925757823
C	6.0	-2.8740415622	1.0222003441	4.1216755992

O	8.0	-7.2992195521	1.2348014735	9.3797285584
O	8.0	-4.8192352703	0.9237056635	6.8838572200
H	1.0	-7.0140310338	2.5969530916	6.1170529595
C	6.0	3.7782726298	-0.1901003595	-5.1769872056
O	8.0	1.4963058836	0.7377418538	1.1116325302
H	1.0	-3.5150749799	1.7537320989	5.8040067858
C	6.0	3.0012097482	0.9258088792	-1.6066864828
H	1.0	-4.8910063915	0.5481307334	3.4876742637
C	6.0	-0.4508942954	0.4120842025	-0.3418147363
H	1.0	-2.6816123070	-0.2720334098	-1.4901293943
C	6.0	0.9894030715	0.9128712007	-0.2044662156
O	8.0	-3.2183738473	2.1175826809	4.9514316747
H	1.0	-0.7180799933	0.5257191285	-1.3930248969
C	6.0	3.0332625504	0.8372480562	-3.1060080761
C	6.0	-5.7075492386	1.7341706527	7.6653934282
H	1.0	-2.6548846442	1.4498494713	3.1375830813
H	1.0	-1.1055193583	1.0507688013	0.2590095050
C	6.0	-6.2894084178	2.9159595531	6.8724607622
H	1.0	2.9142554193	1.9723640810	-1.2964359520
O	8.0	3.6260325981	-0.3144309417	-7.9892477722
C	6.0	2.9229315945	0.6368524247	-5.9257150401
H	1.0	-5.0906644467	2.1249112446	8.4794996579
H	1.0	-5.4781848713	3.4413124810	6.3617825762
H	1.0	-6.7945050982	3.6040118109	7.5555797928
H	1.0	1.0347662620	1.9927109503	-0.3797268609
C	6.0	2.8998789327	0.5106561576	-7.3891843977
C	6.0	2.1607170708	1.6560174193	-3.8320393711
C	6.0	2.0962404586	1.5850965543	-5.2554627169
O	8.0	1.3713029725	2.5173842548	-3.1568314110
H	1.0	2.5597334624	0.5990295681	-10.0058545186
C	6.0	1.9818081092	1.4042122456	-8.1131589338
C	6.0	1.9192514280	1.3245114876	-9.5167306624
H	1.0	0.8539174628	3.0076371589	-3.8766552061
C	6.0	1.2015936186	2.4475221613	-5.9826643812
C	6.0	1.1591123718	2.3425080330	-7.4196938071
C	6.0	1.0636984020	2.1515121402	-10.2271618415
O	8.0	0.4468501477	3.3062390487	-5.3490045917
H	1.0	1.0200022254	2.0847849640	-11.3121928574
C	6.0	0.2838225300	3.1852191707	-8.1776087254
C	6.0	0.2451454590	3.0818633832	-9.5657435098
O	8.0	-0.5120096808	4.0867458343	-7.5646830419
H	1.0	-0.4287816395	3.7350153992	-10.1117317868
H	1.0	-0.3167495303	3.9840216298	-6.5873868960

Adriamycin 14-octanoate	51898-39-6	H	1.0	5.7078906790	1.0529375339	-2.0139084597
		O	8.0	6.3926492958	-1.3902437872	-1.7223178658
		H	1.0	4.0370766933	0.6769319692	-1.5473616181
		C	6.0	5.0844028474	0.6009485471	-1.2377297977
		H	1.0	4.9423746458	-3.3868913582	-1.2723279100
		H	1.0	5.5790923524	3.3056902381	-0.7115977451
		H	1.0	0.1757778724	-2.0621722478	-4.4814012385
		C	6.0	5.4482572597	-0.8665217966	-1.1720541592
		H	1.0	3.8018246404	5.1761671182	-0.8761307836
		H	1.0	5.6953564144	-3.1566794614	0.3093288342
		H	1.0	1.9898341384	7.0439305254	-1.0594261247
		H	1.0	3.1621974268	2.7604001523	-1.1471140678
		O	8.0	0.7174864556	-2.3638385491	-3.6772441779
		H	1.0	-2.6259567888	-0.1621805041	-6.4697894535
		O	8.0	-0.9645103919	-1.2789475593	-5.1918542601
		H	1.0	1.3963013441	4.5990500113	-1.3316961956
		C	6.0	4.7911717508	-2.9631264867	-0.2724644906
		C	6.0	4.9659346100	2.8232560155	0.0634290115
		O	8.0	4.5722449232	-1.5457556048	-0.3886347492
		C	6.0	3.1879255305	4.6573819287	-0.1248812894
		C	6.0	5.2920538354	1.3220902798	0.1095413360
		H	1.0	1.6960980201	-3.7755454729	-1.7605394737
		H	1.0	2.6798174884	-2.3316863845	-1.6607733463
		H	1.0	6.3369790927	1.1915307382	0.4186789996
		C	6.0	3.4862321707	3.1537073000	-0.1750970105
		C	6.0	1.4183629039	6.4979899886	-0.2992991760
		C	6.0	1.7103515959	4.9956789511	-0.3576072936
		H	1.0	-4.6030224802	1.3089604517	-6.9204733511
		H	1.0	0.3568933910	6.7047253355	-0.4693701871
		C	6.0	-3.1510709178	0.3481511754	-5.6706188758
		C	6.0	-1.5205217181	-0.7186699775	-4.1808034458
		H	1.0	5.2789328738	3.2714448491	1.0164415153
		C	6.0	0.1033555110	-1.7653227231	-2.6311031494
		C	6.0	1.8353887349	-2.8499279804	-1.1923678578
		H	1.0	3.5032600878	5.0579925892	0.8500753712
		C	6.0	3.6310297850	-3.7069697931	0.4067043489
H	1.0	1.6871179997	6.9168078811	0.6778771043		
C	6.0	-4.2375378374	1.1579311546	-5.9074033091		
H	1.0	4.6766513099	0.8352518103	0.8749370585		
H	1.0	2.8749347543	2.6374800014	0.5781297694		
C	6.0	-2.6757841406	0.1512987178	-4.3541379690		
H	1.0	1.0974645600	4.4742782076	0.3889604390		
C	6.0	-1.0252417420	-0.9266131305	-2.8409831012		
O	8.0	3.9355703164	-4.7106765018	1.0186435619		

C	6.0	0.6070033421	-1.9764963900	-1.3412374713
C	6.0	2.1645041292	-3.2394263750	0.2693658404
O	8.0	1.3617683755	-4.3353946005	0.6710812389
H	1.0	2.6078042469	-1.2106482875	0.9161274114
C	6.0	-4.8915111043	1.8025540006	-4.8373285711
C	6.0	-3.3166238092	0.7915347056	-3.2420285335
C	6.0	-1.6548872226	-0.2927473673	-1.7305585737
H	1.0	-5.7447510546	2.4363353670	-5.0449944414
H	1.0	0.6071848147	-3.9793853771	1.1688490944
C	6.0	1.9461044612	-2.0289688812	1.2115101010
C	6.0	-0.0100304568	-1.3422199067	-0.2441911524
C	6.0	-4.4465401431	1.6273544081	-3.5313371729
C	6.0	-2.8101741395	0.5780436590	-1.8897558821
H	1.0	2.1825878459	-2.3143098127	2.2409735738
C	6.0	-1.1335663770	-0.5209094499	-0.4286656634
C	6.0	0.4987494071	-1.5347002135	1.1572253568
H	1.0	0.4109431400	-0.5958823278	1.7116751990
O	8.0	-5.0589683907	2.2375090398	-2.4729234506
H	1.0	-5.9217023728	3.9187335595	-3.3657978103
O	8.0	-3.3349586149	1.1226905506	-0.8572362833
O	8.0	-0.3578532933	-2.5151551387	1.8395876204
O	8.0	-1.7048923827	0.0561647744	0.6503558909
H	1.0	-3.2509839944	-3.6563581129	5.0786632916
C	6.0	-6.1732015223	3.0631424492	-2.7221225242
H	1.0	-7.0039984118	2.5118096163	-3.1861931342
H	1.0	-2.4760675016	0.6026674574	0.2385067381
H	1.0	0.5376251155	-2.0195322350	5.9970114369
H	1.0	-2.8321283923	-3.0197632767	2.6229612753
C	6.0	-2.6248832205	-2.7895689328	4.7799605549
C	6.0	-0.9325176428	-2.1004014709	3.0372078892
H	1.0	-4.2133005863	-1.6187045676	4.2085440128
H	1.0	-6.4932341364	3.4342563350	-1.7459516002
N	7.0	-3.3742157822	-1.5331224411	4.7748425296
C	6.0	-2.0488757071	-3.0775869136	3.3863062099
H	1.0	-1.0317331787	-3.7164427916	5.8570664927
C	6.0	-0.3240658086	-1.7684270480	5.3666548635
H	1.0	-1.3180153020	-1.0806550897	2.9308931727
O	8.0	0.0925818368	-2.1359748875	4.0483943386
C	6.0	-1.4708086433	-2.7088569177	5.7967438240
H	1.0	0.3006680490	0.2842820549	5.2116191713
H	1.0	-1.4472309975	0.0579237383	4.9340618089
C	6.0	-0.5906203796	-0.2687878938	5.5240516414
H	1.0	-3.6498628868	-1.3020542342	5.7253028541
H	1.0	-1.6306886328	-4.0904619963	3.3569018914

		O	8.0	-1.9315552541	-2.2983790714	7.0903850742
		H	1.0	-0.7933228511	-0.0401545368	6.5745199161
		H	1.0	-2.4655885152	-3.0215060386	7.4452577289
		H	1.0	4.9461018233	0.0416232751	-5.0236848023
		H	1.0	2.5002333315	-3.3884080744	-2.1388641430
		C	6.0	4.9713713868	0.0088115830	-3.9342618041
		H	1.0	3.0659253148	-5.1756411055	-0.5318454350
		O	8.0	3.6596400597	-0.4046540101	-3.5287282638
		H	1.0	5.2052167906	0.9964830999	-3.5292278021
		H	1.0	5.7271659845	-0.7015008894	-3.5877107643
		H	1.0	3.7482690468	-2.8146084353	-1.0348446764
		C	6.0	2.6960893220	-3.1106254577	-1.0944755958
		H	1.0	1.5481133392	-1.1734362691	-2.7809704811
		C	6.0	2.4473209210	-4.3322614375	-0.2051685515
		H	1.0	1.3985629608	-4.6339813848	-0.2530382418
		C	6.0	3.4684254516	-0.4886663802	-2.1884283470
		C	6.0	2.0084022641	-0.7870759858	-1.8676145694
		H	1.0	2.6944309364	-4.1328154927	0.8427010042
		C	6.0	1.8179297638	-1.8835195222	-0.7728573966
		H	1.0	1.3621697019	1.2528319498	-3.5669779694
		O	8.0	0.4601936046	-2.3427317920	-0.8474117956
		O	8.0	4.3691811820	-0.3094012320	-1.3912121731
		H	1.0	-0.0781210133	-1.7563261430	-0.2898927051
		O	8.0	0.6286954828	3.3881819829	-4.5462824289
		C	6.0	1.1182053856	1.4763093613	-2.5337872461
		C	6.0	1.3513652422	0.5539176565	-1.5225220516
		H	1.0	-4.9073345487	-2.3242674003	0.4221404257
		H	1.0	-0.5490196969	-5.2335850871	2.9746048871
		C	6.0	2.1185416894	-1.2786439517	0.6084041647
		H	1.0	3.1497927298	-0.9123284515	0.6040990762
		H	1.0	2.0225359702	-2.0325296565	1.3943888646
		H	1.0	-0.4348404618	-3.1789174251	1.5692492238
		H	1.0	-2.6037329457	-3.8835705598	2.0856339206
		H	1.0	-4.6210734242	-3.6002727124	1.6268179474
		C	6.0	-4.9835333990	-2.5788123558	1.4946792209
		H	1.0	-2.5847819201	-1.7027177146	0.9997559499
		C	6.0	0.3334218870	3.6783104733	-3.3644404276
		H	1.0	-6.0420031601	-2.5634780458	1.7731457616
		C	6.0	0.5595638702	2.7366359239	-2.2595981578
		H	1.0	0.9336550832	-4.3170614084	3.3163406481
		H	1.0	-0.2270828760	5.6371298129	-5.0434796432
		C	6.0	-0.1570743597	-4.2998594900	3.3910536037
		C	6.0	1.0316297328	0.8755885370	-0.1816644658
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		C	6.0	-0.7108636268	-3.1027630767	2.6309029395
		C	6.0	1.1867893327	-0.1108179289	0.9412655827
		H	1.0	-4.7239350022	0.1294490771	1.2339565167
		O	8.0	-0.1625703525	-0.6075657837	1.2455499112
		C	6.0	-2.2440063580	-3.0319000222	2.6898058810
		C	6.0	-2.7816047353	-1.7088857944	2.0852080052
		H	1.0	-0.4427446347	-4.2387059114	4.4432567641
		C	6.0	-0.4941055144	5.9189872686	-4.0310220142
		N	7.0	-4.2427647314	-1.6489875357	2.3493538454
		C	6.0	-0.2563142946	4.9792569051	-3.0108939689
		C	6.0	0.2233589787	3.0810315420	-0.9178639496
		C	6.0	-4.8315908154	-0.3130489348	2.2399933658
		H	1.0	1.5431823084	0.4033530611	1.8404520446
		C	6.0	0.4599183957	2.1195508535	0.1097961868
		H	1.0	-5.9010890639	-0.3835860410	2.4627466907
		O	8.0	-0.0838484673	-1.9399772891	3.1893361493
		O	8.0	-2.7016440908	-3.1540919282	4.0273442761
		C	6.0	-0.5098031316	-0.7208682853	2.6076925033
		C	6.0	-2.0236503965	-0.5372567103	2.7229326777
		H	1.0	-2.2685257468	0.4158001700	2.2505984617
		H	1.0	-1.2308042317	7.8743983933	-4.5241312465
		H	1.0	-4.3875121214	0.3707682843	2.9637476722
		C	6.0	-1.0498755760	7.1524280303	-3.7306002987
		H	1.0	-3.5642426927	-2.6985580866	4.0147541279
		C	6.0	-0.5899004676	5.3000436232	-1.6603253979
		C	6.0	-0.3572880992	4.3582800032	-0.5941154793
		H	1.0	0.0063047835	0.0596185632	3.1770736774
		O	8.0	0.1271816483	2.3942725131	1.3885323705
		H	1.0	-2.2731510535	-0.4822150022	3.7877527177
		H	1.0	-0.2421377659	3.3366756764	1.3592364925
		C	6.0	-1.3865514249	7.4893350769	-2.4091128502
		O	8.0	-0.6655539839	4.6529440699	0.6416188992
		C	6.0	-1.1639598623	6.5811275155	-1.3773068806
		H	1.0	-1.8227259326	8.4522771700	-2.1613228397
		H	1.0	-1.2502041534	6.1342411507	0.4448130081
		O	8.0	-1.4965313962	6.9274089430	-0.1157303442
		H	1.0	7.3762858800	-1.7832195746	2.1658179681
		H	1.0	7.3087839084	-2.3262603203	-0.2386294301
		H	1.0	7.3044704959	-1.8489885084	-2.4358400136
		H	1.0	6.5595051285	-3.4247574797	-2.0535652498
		C	6.0	6.4987249401	-1.5105470402	1.5842779900
		C	6.0	6.4622500728	-1.8215851082	0.2100631381
		C	6.0	6.3761089835	-2.4352854013	-2.4970897735
2'-Bromo-4'-epi-daunorubicin	NSC 650931	H	1.0	7.3762858800	-1.7832195746	2.1658179681
		H	1.0	7.3087839084	-2.3262603203	-0.2386294301
		H	1.0	7.3044704959	-1.8489885084	-2.4358400136
		H	1.0	6.5595051285	-3.4247574797	-2.0535652498
		C	6.0	6.4987249401	-1.5105470402	1.5842779900
		C	6.0	6.4622500728	-1.8215851082	0.2100631381
		C	6.0	6.3761089835	-2.4352854013	-2.4970897735

H	1.0	6.1029724810	-2.5606144502	-3.5471130587
H	1.0	5.4313241876	-0.6165593290	3.2336607512
C	6.0	5.4366380752	-0.8705039777	2.1800190859
C	6.0	5.3539764372	-1.4848849884	-0.5603611517
O	8.0	5.2873751549	-1.7744511220	-1.8935089711
C	6.0	4.2973408143	-0.5167323016	1.4226707352
C	6.0	4.2270147309	-0.8155661850	0.0232352621
O	8.0	3.3012873582	0.4176773883	3.3728201672
C	6.0	3.2104849415	0.1578293546	2.1203148079
C	6.0	3.0417479949	-0.4373976277	-0.7417451098
O	8.0	2.9260292380	-0.6688925075	-1.9951963079
C	6.0	2.0380950416	0.5196993477	1.3606512900
H	1.0	1.9358560528	1.1077351411	3.6117030189
C	6.0	1.9590025181	0.2262762972	-0.0314081249
H	1.0	1.6019617900	-0.0840694290	-2.2922297334
O	8.0	1.0196990936	1.4496332595	3.3356610279
C	6.0	0.9537679542	1.1732726874	2.0142111170
C	6.0	0.7846758914	0.5970979295	-0.7499472132
O	8.0	0.6937916018	0.3551741247	-2.0752144508
C	6.0	-0.1908222230	1.5258191933	1.2938277386
C	6.0	-0.2791981864	1.2197200022	-0.0819326207
H	1.0	-0.8640554320	-2.8646057285	-1.1626457005
H	1.0	-0.2134157354	-1.9107102588	-2.5180608968
H	1.0	-2.9174832358	-3.1595369380	1.2213622307
H	1.0	-0.7884995154	-3.5759556837	-2.7784023259
H	1.0	-1.6646627731	-0.9035056207	-0.3307749904
C	6.0	-0.9664527057	-2.6461522027	-2.2253881197
H	1.0	-2.9176231211	-4.4020199244	0.1484137874
N	7.0	-2.8081957609	-3.3957431595	0.2379454985
H	1.0	-0.9614826702	2.7096028783	2.8811268421
O	8.0	-1.2743079036	5.3324163968	1.2168103314
C	6.0	-1.3479489783	2.1833317294	2.0025984977
H	1.0	-1.3092535676	1.6474135645	-1.9061547803
C	6.0	-1.4970399660	1.6822673749	-0.8316474494
H	1.0	-2.0251430831	1.4134004121	2.3935268661
C	6.0	-2.0950581544	4.5567735927	1.6724781713
C	6.0	-2.5772883294	-0.5016155718	-0.7839883449
H	1.0	-1.0510641392	3.7565806137	-0.5600871334
BR	35.0	-4.0763499097	-0.8646977954	1.6928571053
H	1.0	-2.6725684058	5.9053857182	3.2330691487
O	8.0	-2.6996337754	0.8578206841	-0.5718712438
C	6.0	-2.3541600854	-2.1126805583	-2.5794898263
C	6.0	-2.2530948934	3.1271056582	1.1240133697
C	6.0	-1.8900548291	3.0819021669	-0.3726106047

		C	6.0	-3.8315573101	-2.7083644574	-0.5473523478
		H	1.0	-2.9712283025	4.1755044731	3.6159550293
		O	8.0	-2.5756301076	-0.7375994410	-2.2007110131
		C	6.0	-2.9919059644	4.9409135254	2.8347794298
		C	6.0	-3.8298158142	-1.2017531553	-0.2537410135
		H	1.0	-3.4360596165	-3.9814020447	-2.2620353196
		C	6.0	-3.5711506663	-2.9094091473	-2.0697532234
		H	1.0	-2.4435309907	-2.0857475338	-3.6719050226
		H	1.0	-4.8534742388	-3.0762333966	-0.3593914165
		H	1.0	-2.7553783806	3.4463974016	-0.9367489741
		H	1.0	-3.7317487366	1.8955727986	0.9641330696
		H	1.0	-4.7020975552	-0.7305169846	-0.7062506075
		O	8.0	-3.6334310570	2.7939821882	1.3174674684
		H	1.0	-4.0273243349	4.9964056992	2.4858440093
		O	8.0	-4.7320999754	-2.5108486677	-2.7998565187
		H	1.0	-4.6319789462	-1.5559990963	-2.9359028268
Cinerubin A	NSC 243022 / 34044-10-5	H	1.0	8.6450430776	0.6769188219	-5.8562400886
		H	1.0	6.9629260196	0.5818148037	-5.2864583551
		C	6.0	7.9668361914	0.9360071367	-5.0386373335
		H	1.0	7.9365686259	2.0268549775	-4.9534035399
		H	1.0	8.4842660118	-0.8169533167	-3.9003276800
		O	8.0	10.8225466435	0.1832157178	-3.9333465878
		C	6.0	8.4422772809	0.2640707510	-3.7407612502
		C	6.0	9.8696945704	0.7103230727	-3.3932304140
		H	1.0	-8.9232922076	-1.5016477493	-2.8090605763
		O	8.0	7.5249342316	0.4437207238	-2.6541150623
		H	1.0	9.9596968435	2.7889339708	-3.0456334453
		H	1.0	7.3144244342	2.5163687210	-2.6927972651
		C	6.0	10.0176977103	1.8780259720	-2.4297917152
		H	1.0	5.2437356576	3.0385313581	-1.7044504329
		H	1.0	-8.2204718077	-3.0446957267	-2.2212043412
		C	6.0	-8.5492001140	-2.0420497526	-1.9389038801
		H	1.0	-1.0832067128	1.9725046580	-2.6615431668
		H	1.0	11.0261420369	1.8511073991	-2.0090626654
		H	1.0	2.9626341299	2.3691341306	-2.9286836875
		C	6.0	7.5518043753	1.7120437472	-1.9735720392
		H	1.0	-9.3289765478	-2.1306090206	-1.1778767916
		H	1.0	4.8346697913	2.9258077305	0.6044048421
		H	1.0	-2.6498587839	1.3183669312	-2.1404215907
		O	8.0	-7.4399228222	-1.2719511138	-1.4495695132
		C	6.0	8.9257279702	1.9194153059	-1.3510011539
		C	6.0	5.2499502561	2.0177689776	-1.2903142622
		C	6.0	-1.7629406891	1.8680134903	-1.8106574194
		H	1.0	0.8845559479	4.0409032094	-1.5262933659

O	8.0	3.1075831775	2.3661791415	-0.2390537853
H	1.0	5.0779662994	1.2986470409	-3.3173593635
C	6.0	4.4757180472	2.0544513929	0.0451026466
C	6.0	3.1103410078	1.3911644833	-2.4574551530
O	8.0	6.6046561512	1.6573245349	-0.9634448191
H	1.0	9.0714524523	1.1208522736	-0.6161339862
H	1.0	-2.0492532717	2.8677771531	-1.4825182903
O	8.0	1.1264595275	1.8756623477	-1.2693949400
H	1.0	-0.8092408168	0.0932357578	-1.0941578810
C	6.0	4.6070392464	1.0891679877	-2.3433486038
H	1.0	-5.2710073486	-0.4451213486	-0.8320434444
H	1.0	8.9441451633	2.8723190325	-0.8131596072
H	1.0	0.0426510536	5.5935486923	-1.3373367422
C	6.0	2.4331291621	1.4313144567	-1.0930769479
H	1.0	-7.4999324134	0.5904762097	-0.6718690622
H	1.0	2.6397544473	0.6324107794	-3.0889227282
O	8.0	-3.4503488289	-5.4831604999	-0.1698553557
H	1.0	-4.7437584144	-3.4237616406	-0.2410729405
C	6.0	0.5053563663	4.7569395817	-0.8023358061
H	1.0	-2.7345866468	-6.8736538545	-0.1705165451
C	6.0	-1.0726941607	1.0790535428	-0.6944687741
C	6.0	-6.8017446054	-1.8057410118	-0.3500761822
O	8.0	-2.0730007417	-7.5583537870	0.1751447643
O	8.0	-7.0415867559	1.1848996663	-0.0595013529
H	1.0	1.3681323706	5.1509369724	-0.2305435627
C	6.0	-5.6831240475	-0.8706266416	0.0927062427
C	6.0	0.2381958544	1.6904459332	-0.1528007824
C	6.0	4.6458371020	0.8194703102	0.9354090052
H	1.0	5.6879892241	0.7380859425	1.2544603506
H	1.0	4.0168591355	0.9311130890	1.8232128474
H	1.0	2.4383930907	0.4377888829	-0.6207442485
C	6.0	-4.2282712415	-2.8790205830	0.5394292783
H	1.0	-4.5485468635	1.4686101634	0.3010497588
N	7.0	-0.4986110036	4.1282934730	0.0581658811
O	8.0	-7.1745821517	-2.8377599984	0.1524989850
O	8.0	4.7659456152	-0.2806430933	-2.0182456619
C	6.0	-2.8650479142	-4.9236405956	0.8204284653
H	1.0	0.6784619777	0.9302961270	0.5057488265
H	1.0	5.7229956526	-0.4404827560	-2.0034526395
O	8.0	-1.9421726880	0.7795956921	0.4008953710
C	6.0	-4.5704015364	-1.5739827475	0.8685054992
C	6.0	-6.2804718252	0.3751487504	0.8455803775
C	6.0	-1.4742337454	-6.9371318150	1.2132256920
H	1.0	-8.7204325162	-1.2932306718	1.3528329150

		H	1.0	4.3829397816	-0.1045696942	0.4196102370
		H	1.0	-1.3422165070	6.0095100328	0.3657619320
		C	6.0	0.0273183238	2.9304913670	0.7567375529
		C	6.0	-3.2115458648	-3.5659060459	1.2214692713
		H	1.0	-2.7892505927	2.6260127177	0.7664897845
		H	1.0	-0.2257397198	-8.6167520553	1.6436324825
		C	6.0	-5.0793164102	1.2417106820	1.2294644520
		C	6.0	-1.8381658040	-5.6087894362	1.5772775468
		H	1.0	-9.0859579452	0.4458989538	1.2584694684
		C	6.0	-1.0442206263	5.1396432384	0.9597152526
		C	6.0	-0.4863994625	-7.6048678708	1.9392383766
		H	1.0	1.0045316409	3.1683254223	1.2158155158
		C	6.0	-2.2180264193	1.8493494112	1.3032092006
		C	6.0	-8.5994755576	-0.3310539015	1.8555835577
		H	1.0	-5.4436385532	2.1902707532	1.6393553479
		C	6.0	-3.8569515550	-0.8859148559	1.8869002282
		C	6.0	-7.1272629207	0.0232459564	2.1011793612
		H	1.0	-1.9353162454	4.7792589871	1.4769003032
		H	1.0	-0.3195773089	5.4903747281	1.7214021284
		C	6.0	-0.9176828545	2.4248871942	1.8658350070
		C	6.0	-2.5484255140	-2.9353733929	2.3110769050
		C	6.0	-4.1266287968	0.5720903880	2.2209865146
		C	6.0	-1.1849310532	-4.9741453585	2.6849355196
		H	1.0	-6.6332153157	-0.7868857509	2.6482767943
		H	1.0	-9.1286388717	-0.4012161714	2.8119122953
		C	6.0	-2.9028963556	-1.5905421814	2.6396112206
		H	1.0	-0.4324088510	1.6082820117	2.4092770921
		C	6.0	0.1507507333	-6.9856061762	3.0207477882
		O	8.0	-2.9262671024	1.3660735924	2.3993858865
		H	1.0	-7.1017287077	0.9039129545	2.7556103013
		C	6.0	-1.5350395158	-3.6300028876	3.0673557980
		H	1.0	-1.1422998236	3.1969376566	2.6036788905
		C	6.0	-0.1809686639	-5.6866760995	3.4042601891
		H	1.0	0.9190778542	-7.5049721011	3.5859426028
		H	1.0	-4.5560179181	0.6200490096	3.2289752712
		O	8.0	-0.9449938577	-3.0486813174	4.0756704874
		O	8.0	-2.3174889942	-0.9844481279	3.6873173941
		H	1.0	-1.6715542636	-1.6675900764	4.0543876627
		O	8.0	0.4627545588	-5.1285350467	4.4579474734
		H	1.0	0.0651802427	-4.2148978376	4.5426920784
N-(1-Cyano-2-methoxyethyl) doxorubicin	NSC 639659	H	1.0	1.8698951923	-3.5044337255	-7.0095746463
		O	8.0	1.5747809429	-4.3790750852	-6.6944325443
		H	1.0	-0.0073336651	-4.3843828560	-5.3358517552

C	6.0	1.0596997109	-4.1264532317	-5.4115618637
O	8.0	1.7205518692	-1.9004849651	-5.8655499655
C	6.0	1.2152429181	-2.6583062537	-5.0486105861
H	1.0	1.5636235889	-4.7285826232	-4.6413557834
H	1.0	0.1561268652	-0.3637648743	-4.6547191242
H	1.0	2.5056763143	-0.9429754853	-3.4265328629
C	6.0	0.7598101003	-2.1865141402	-3.6673491239
H	1.0	-1.1796802832	-1.3598315587	-4.1140468428
C	6.0	-0.1942621969	-0.9843788056	-3.8199214607
H	1.0	2.7128202479	-2.5827395204	-2.7788426618
C	6.0	2.0109579419	-1.7475402275	-2.8735878886
O	8.0	-2.1567680312	0.9291200689	-3.6649632024
H	1.0	-2.7870007307	1.6918200889	-3.4418591359
O	8.0	0.1130586929	-3.2993082611	-3.0559061194
C	6.0	-0.3284454528	-0.1172023607	-2.5866452028
C	6.0	-1.3372124690	0.8553633515	-2.5960789918
C	6.0	1.6432828248	-1.2568282015	-1.4738929192
H	1.0	0.2668770517	-3.2418805212	-2.0969004328
H	1.0	2.5366938842	-0.8585090769	-0.9823330386
C	6.0	0.5513409149	-0.2063476999	-1.4846133442
O	8.0	-3.3231912927	2.8486618313	-2.5464606832
C	6.0	-1.4826528974	1.7614157049	-1.5124903717
O	8.0	1.2316349485	-2.4535220320	-0.7303729014
C	6.0	-2.5188306315	2.7651503754	-1.5560351681
C	6.0	0.4147795168	0.6800575341	-0.4012023323
C	6.0	-0.5985292878	1.6798385229	-0.3999177107
H	1.0	-4.2542620244	4.6922710490	-1.3817438694
H	1.0	-0.5794985315	-2.3660671024	1.2096662141
O	8.0	1.2637997150	0.6055560179	0.6583309808
H	1.0	0.1434969429	-3.9855563306	1.1941967973
C	6.0	-2.6131498936	3.6976934009	-0.4395529303
C	6.0	1.5103816952	-2.4362539507	0.6408170646
C	6.0	-3.6115894959	4.6928927051	-0.5091410582
C	6.0	0.3226709117	-2.9352606218	1.4519637815
H	1.0	1.7604602023	-1.4137092232	0.9236867553
H	1.0	0.9511957596	1.4114316678	1.2572865671
C	6.0	-0.7000923114	2.5927264578	0.7250005210
C	6.0	-1.7228433260	3.6255017886	0.6822730310
O	8.0	2.6385632300	-3.2831398398	0.8799506787
N	7.0	-2.7825882913	-1.5089450957	3.2071171626
O	8.0	0.1194750163	2.4653820232	1.7154239764
C	6.0	-3.7425838631	5.6214206718	0.4975855610
H	1.0	-4.5106578935	6.3888951385	0.4459086162
H	1.0	0.7784729280	-0.7513339500	2.6068979721

		C	6.0	-1.7580624762	-1.2277167044	3.6761234401
		C	6.0	0.6645822989	-2.7994127336	2.9442411152
		C	6.0	-1.8885972806	4.6167422887	1.7078379104
		H	1.0	-0.0896628193	-3.3194542216	3.5448970059
		C	6.0	-2.8771521567	5.5884374466	1.6091084474
		N	7.0	0.6947732020	-1.3873207726	3.4004862045
		C	6.0	3.1455897694	-3.1588022674	2.2178590277
		H	1.0	3.2435239797	-0.9578043971	2.3946205051
		H	1.0	1.8604583047	-4.5577096595	3.2210429518
		H	1.0	4.6722003165	-1.7303620341	1.6915465498
		O	8.0	-1.0336482353	4.5679757565	2.7769084822
		C	6.0	2.0262404471	-3.4738881932	3.2549149782
		H	1.0	3.8870884233	-3.9621943776	2.2969312418
		C	6.0	-0.4131391236	-0.9529767398	4.2498265912
		C	6.0	3.8896529983	-1.8369049491	2.4485886582
		H	1.0	-2.9959499826	6.3291045000	2.3899903890
		H	1.0	-0.3160539303	1.1380443783	3.6486264187
		H	1.0	-0.8957492962	6.6012692228	3.2273487923
		H	1.0	-0.3659845901	-1.5089220671	5.1946355442
		C	6.0	-1.0634055273	5.6284807173	3.7093442383
		C	6.0	-0.2515241556	0.5400147675	4.5699472635
		O	8.0	2.4311217098	-3.1569195895	4.5766668839
		H	1.0	4.3596118250	-1.8505489724	3.4355476168
		H	1.0	-0.2506146557	5.4304659298	4.4113375442
		H	1.0	2.2182743040	-2.2084637487	4.6513400071
		H	1.0	-2.0117783273	5.6710060103	4.2637949583
		O	8.0	-1.2630995943	0.8974119688	5.4891004178
		H	1.0	0.7536212845	0.6846564536	4.9981120263
		H	1.0	-1.4883880894	2.8169975890	4.7048248188
		C	6.0	-1.3587235102	2.2996465708	5.6642202212
		H	1.0	-2.2263583928	2.4833883809	6.3031327735
		H	1.0	-0.4619029867	2.7074052356	6.1594148092
		H	1.0	-3.7177354209	4.2946088464	4.8202662384
		H	1.0	-5.2041346875	4.3681922662	3.8331846754
		C	6.0	-4.1096082711	4.2728609927	3.7941138426
		H	1.0	-3.6965598893	5.1154931850	3.2365121818
		H	1.0	-5.1873119762	2.6342616713	5.2643789110
		O	8.0	-3.7021152346	3.1142848719	3.0970150464
		C	6.0	-4.8297631274	1.7575497654	4.7391004344
		C	6.0	-4.0495249414	1.8941011871	3.5959169306
		H	1.0	-5.7745851666	0.3995539275	6.1248336099
		C	6.0	-5.1633022179	0.4795717746	5.2292989326
		O	8.0	-2.4261770617	1.9431499533	1.1418773367
Cyanomorpholino doxorubicin	88254-07-3	H	1.0	-3.7177354209	4.2946088464	4.8202662384
		H	1.0	-5.2041346875	4.3681922662	3.8331846754
		C	6.0	-4.1096082711	4.2728609927	3.7941138426
		H	1.0	-3.6965598893	5.1154931850	3.2365121818
		H	1.0	-5.1873119762	2.6342616713	5.2643789110
		O	8.0	-3.7021152346	3.1142848719	3.0970150464
		C	6.0	-4.8297631274	1.7575497654	4.7391004344
		C	6.0	-4.0495249414	1.8941011871	3.5959169306
		H	1.0	-5.7745851666	0.3995539275	6.1248336099
		C	6.0	-5.1633022179	0.4795717746	5.2292989326
		O	8.0	-2.4261770617	1.9431499533	1.1418773367

C	6.0	-3.5718884596	0.7383169416	2.8907802395
C	6.0	-2.7627820568	0.8226825660	1.6856163657
H	1.0	-1.7084066782	1.5006794539	-0.0018847587
C	6.0	-4.7166001825	-0.6518894959	4.5850041797
C	6.0	-3.9221607427	-0.5462895247	3.4227262478
O	8.0	-1.1925906837	0.8370310924	-0.6310656010
H	1.0	-4.9505323528	-1.6490461863	4.9392374413
H	1.0	5.8912605787	-0.2139004289	-0.7802579373
C	6.0	-2.3162419824	-0.4166747757	1.0778009847
C	6.0	-1.5029441845	-0.3612216103	-0.0859456274
C	6.0	-3.4735958464	-1.7872304346	2.8000373766
H	1.0	5.4503951062	-0.6002750498	0.8919490600
O	8.0	4.5370589732	1.9665748948	-1.1180183886
H	1.0	4.5024691649	1.4474808698	-1.9363754085
H	1.0	-0.4003210174	-0.5744760127	-2.4737969777
C	6.0	5.1667795722	-0.7422474578	-0.1555367703
C	6.0	-2.6505844976	-1.6905625940	1.6186177380
H	1.0	1.9774663253	-0.5062448403	-3.1538508139
H	1.0	5.2073575691	-1.8096276287	-0.3873063155
O	8.0	-3.7969750960	-2.9225837181	3.2937445720
C	6.0	-1.0168019669	-1.5368388469	-0.6732331635
C	6.0	-0.0805304006	-1.4088285854	-1.8409275851
C	6.0	-2.1694760707	-2.8742228220	0.9938133226
H	1.0	-0.9052403173	-2.8496084770	-3.2221394964
C	6.0	3.6297936539	1.3134913398	-0.2210577532
C	6.0	2.0733608175	-0.2350446435	-2.0931178163
C	6.0	3.7626422250	-0.2092738256	-0.3889592616
H	1.0	2.2625893007	1.8352714900	-2.6382786089
H	1.0	3.9216322934	1.6184347996	0.7892823667
C	6.0	-1.3480523728	-2.8002653164	-0.1385135309
H	1.0	1.7171348980	5.7607602261	-2.2891387957
H	1.0	-3.0709927569	-3.8797728076	2.2951966738
O	8.0	1.2457120865	-1.0756557986	-1.2974066014
O	8.0	3.4173233561	-0.5295865982	-1.7623168752
C	6.0	0.0270720509	-2.6914108086	-2.6705301090
O	8.0	-2.4971404864	-4.0884499081	1.4851027829
O	8.0	0.2251244538	5.2765319191	-1.0059168944
C	6.0	1.7367395769	1.2491688937	-1.8745012497
N	7.0	1.8856732908	3.1065495823	-0.1250460294
H	1.0	0.8342308627	-2.5937397080	-3.4070222424
H	1.0	-1.7297797817	-4.5533582931	-1.3150701923
H	1.0	3.0567590953	-0.7135638120	0.2806153962
C	6.0	2.1530445143	1.7110864327	-0.4593743316
C	6.0	0.6499799152	3.4495635954	0.5741371245

		C	6.0	1.3308569077	4.8585589493	-1.8022902009
		H	1.0	-1.2096193273	4.5486334049	0.2430155375
		C	6.0	-0.8899751782	-4.0907374384	-0.7800087331
		C	6.0	-0.3667985472	4.1702783047	-0.3391340318
		H	1.0	2.8191115806	4.9760793772	-0.2670793995
		C	6.0	2.4103303174	4.2048738503	-0.9371574040
		H	1.0	0.6631600557	1.3968885925	-2.0049368755
		C	6.0	0.2822602060	-3.9225480778	-1.7706430515
		H	1.0	0.9854817915	4.1599070994	-2.5831898559
		H	1.0	0.1614124306	2.5434601550	0.9442119992
		H	1.0	1.5635200335	1.1180093906	0.2467170290
		O	8.0	-0.5753231849	-5.5564037100	-3.3280368146
		H	1.0	-0.5926685171	-4.8022250320	-0.0031867678
		H	1.0	1.7157394241	-2.8642314568	-0.9779232682
		H	1.0	-0.7420056763	3.4365830518	-1.0670445989
		C	6.0	0.3734751337	-5.1577285835	-2.6661792485
		O	8.0	1.5323799306	-3.8132244310	-1.0954316324
		H	1.0	3.2383699043	3.8326383648	-1.5411424056
		C	6.0	1.6943239782	-5.9053552060	-2.7566528834
		H	1.0	0.6675035578	-6.9588219739	-3.9529718205
		H	1.0	2.4768481651	-5.1912739340	-3.0522210630
		O	8.0	1.5971459638	-6.9783994069	-3.6582716784
		H	1.0	1.9668807420	-6.2382763580	-1.7435806145
		C	6.0	0.9732895379	4.2962917855	1.7535563830
		N	7.0	1.2446264525	4.9594913256	2.6674742779
		H	1.0	5.2135421315	2.6011266145	-1.0249977026
		H	1.0	4.3719461263	3.2980358699	0.3525850056
		H	1.0	3.5967589980	3.2893081348	-1.2441538979
		C	6.0	4.2281777107	2.7140079959	-0.5550527460
		H	1.0	4.4466239129	1.4916283984	-2.5785386417
		O	8.0	4.8874735107	0.0004650347	-4.2937771764
		N	7.0	4.0457566345	0.5945319465	-2.3186426997
		C	6.0	3.6172058130	1.3676806002	-0.2300202344
		C	6.0	4.2607732303	-0.3588749036	-3.2977032477
		H	1.0	4.8747457307	0.4869205996	1.8446793496
		O	8.0	4.3280492838	1.2626332212	2.0365395285
		H	1.0	2.6522479005	3.2221595389	1.6524494495
		N	7.0	3.5645503409	0.3834087926	-1.0583084225
		C	6.0	3.1466481776	1.1384407513	1.2093864439
		H	1.0	2.2355530065	-1.4987476339	-1.6470971525
		C	6.0	2.1962815173	2.2298375189	1.7127709349
		C	6.0	3.7545688644	-1.7624332559	-3.1648463555
		H	1.0	0.8614129067	2.8820417045	0.1245250745
Daunomycin 3,4-dichlorobenzoyl hydrazone	66996-54-1	H	1.0	5.2135421315	2.6011266145	-1.0249977026
		H	1.0	4.3719461263	3.2980358699	0.3525850056
		H	1.0	3.5967589980	3.2893081348	-1.2441538979
		C	6.0	4.2281777107	2.7140079959	-0.5550527460
		H	1.0	4.4466239129	1.4916283984	-2.5785386417
		O	8.0	4.8874735107	0.0004650347	-4.2937771764
		N	7.0	4.0457566345	0.5945319465	-2.3186426997
		C	6.0	3.6172058130	1.3676806002	-0.2300202344
		C	6.0	4.2607732303	-0.3588749036	-3.2977032477
		H	1.0	4.8747457307	0.4869205996	1.8446793496
		O	8.0	4.3280492838	1.2626332212	2.0365395285
		H	1.0	2.6522479005	3.2221595389	1.6524494495
		N	7.0	3.5645503409	0.3834087926	-1.0583084225
		C	6.0	3.1466481776	1.1384407513	1.2093864439
		H	1.0	2.2355530065	-1.4987476339	-1.6470971525
		C	6.0	2.1962815173	2.2298375189	1.7127709349
		C	6.0	3.7545688644	-1.7624332559	-3.1648463555
		H	1.0	0.8614129067	2.8820417045	0.1245250745

C	6.0	2.7183784620	-2.1894695689	-2.3235557824
H	1.0	2.0590781070	2.0246334376	2.7797615303
H	1.0	5.1363500439	-2.3432875965	-4.7024164045
C	6.0	0.8200683087	2.2553700468	1.0225218014
C	6.0	4.3541881178	-2.6839335332	-4.0356232910
H	1.0	3.0619602095	-1.0316442338	1.0350655685
C	6.0	2.4668571368	-0.2138467048	1.4513826460
H	1.0	0.3203878477	3.8368293334	4.2895470349
O	8.0	-0.0681699820	3.0306006416	1.8783692023
H	1.0	-1.0203795905	5.7135347241	5.4167283091
H	1.0	2.4558834024	-0.3595254256	2.5406811120
C	6.0	2.2894553950	-3.5161383506	-2.3570081207
H	1.0	-1.3831886247	5.1245286351	3.0431056878
H	1.0	1.4736593364	-3.8407385746	-1.7180908708
C	6.0	0.3124837824	0.8864052107	0.6272892789
C	6.0	3.9442512563	-4.0100143311	-4.0538224212
C	6.0	1.0709556433	-0.2816559578	0.8728083658
C	6.0	-0.6786695562	3.4097027483	4.1465895426
N	7.0	-1.9220863459	5.4296738204	5.0373560735
C	6.0	2.9027154999	-4.4306768771	-3.2133692905
C	6.0	-1.7154944976	4.5254875176	3.9002709847
O	8.0	-1.5545771507	1.9278753221	-0.3997659689
C	6.0	-0.6408519697	2.3940638973	2.9942327975
H	1.0	-0.0747210272	1.4969153022	3.2701664990
CL	17.0	4.7479025267	-5.1236055285	-5.1487827977
C	6.0	-0.9049996615	0.7975345397	-0.0709189615
H	1.0	-2.4352022358	3.4882887895	1.4871027355
H	1.0	-0.9464695230	2.8790328046	5.0690407986
C	6.0	0.5610834454	-1.5338349970	0.5179738477
H	1.0	-2.3978321118	1.5845179521	-0.8767105308
H	1.0	-2.3873643416	4.8900388856	5.7666677021
CL	17.0	2.3502955987	-6.0898814283	-3.2181991775
O	8.0	1.2938528107	-2.6423433951	0.7881674876
O	8.0	-1.9548927893	1.9061710162	2.7338774696
C	6.0	-3.0638550866	3.8852971881	3.5236418870
C	6.0	-1.4380368226	-0.4697382402	-0.4401799477
C	6.0	-2.8776499653	2.9426708258	2.3264575826
H	1.0	-3.7836367639	4.6774501168	3.2882574952
C	6.0	-0.6923555623	-1.6454350091	-0.1423466068
H	1.0	0.7135009064	-3.4041871272	0.4439044018
O	8.0	-3.3547855840	0.5537662821	-1.3697905595
C	6.0	-2.7215808343	-0.5304377210	-1.1212584270
O	8.0	-3.6016829856	3.1703304248	4.6454767291
H	1.0	-3.2055811125	2.2863678574	4.5866838331

		C 6.0 -1.1782650088 -2.9433062934 -0.5334420736 H 1.0 -3.9533815947 1.6105069815 1.0151327715 C 6.0 -4.1558073549 2.2565752380 1.8711957131 H 1.0 -4.8919311325 3.0100529096 1.5698438819 O 8.0 -0.4851032707 -4.0079803983 -0.3125077467 C 6.0 -3.2372929055 -1.8470201095 -1.4883315849 C 6.0 -2.4656854221 -3.0206511332 -1.2034089591 H 1.0 -4.5927111398 1.6626620444 2.6789760540 O 8.0 -5.2384029320 -0.9199812801 -2.4084015920 C 6.0 -4.4989414506 -2.0355364108 -2.1439846483 C 6.0 -2.9377268262 -4.3017245043 -1.5686090873 H 1.0 -6.8901635099 -0.0613454758 -3.1521810161 H 1.0 -2.3092693642 -5.1520139453 -1.3312410828 H 1.0 -6.3886572062 -1.5224400333 -4.0459297014 C 6.0 -6.4861354872 -1.0704847406 -3.0484712907 C 6.0 -4.9395456481 -3.3095763935 -2.4894924296 C 6.0 -4.1522504020 -4.4411869234 -2.1998586982 H 1.0 -5.8929411784 -3.4435133757 -2.9850321372 H 1.0 -7.1852300382 -1.6781551605 -2.4562777288 H 1.0 -4.5171668595 -5.4260053905 -2.4812381521
Daunomycin 4-nitrobenzoylhydrazone	66996-56-3	H 1.0 5.3940111968 2.3052135118 -0.8156190012 H 1.0 3.8507808468 3.1736752007 -0.8608143372 H 1.0 4.7137145835 2.9617109620 0.6763872494 C 6.0 4.4602765907 2.4793203047 -0.2674720931 H 1.0 4.3064591862 1.3579980684 -2.4743072149 O 8.0 3.8950986372 -0.0728921213 -4.3353407777 H 1.0 2.6653358967 3.0260573459 1.7972690919 N 7.0 4.0509835106 0.4305612290 -2.1430531910 H 1.0 -4.8303759850 2.8885383563 0.9721740967 H 1.0 -2.3750084020 3.3313978035 1.1614343705 C 6.0 3.7546721952 -0.4483642187 -3.1766864762 H 1.0 1.0104651669 2.6845040246 0.1232811604 H 1.0 -3.8584958285 1.4789605677 0.5058847291 C 6.0 3.7346736121 1.1783069937 -0.0064047708 H 1.0 -3.8883016209 4.5135500527 2.8321812751 N 7.0 3.5770439894 0.2450068146 -0.8723686625 H 1.0 -1.4656283986 4.9215424738 2.8382381483 C 6.0 -4.1429346566 2.1199791785 1.3423479252 C 6.0 2.1989392877 2.0363265677 1.8255129806 C 6.0 -2.9103672320 2.7794261777 1.9404591854 H 1.0 1.9773305884 -1.8839852208 -4.5171737204 O 8.0 -0.0740719762 2.8331256340 1.7871467348 C 6.0 0.8889612133 2.0596889464 1.0153134574

O	8.0	4.2959817628	1.0553617835	2.3182718012
C	6.0	3.2928947966	-1.8242685634	-2.8220163659
C	6.0	3.1838547306	0.9403025513	1.4035548515
C	6.0	-3.2070347786	3.7073450068	3.1271016179
H	1.0	1.9677885259	1.8356420366	2.8771251588
C	6.0	2.3431456876	-2.4336128008	-3.6567553682
H	1.0	4.8337195083	0.2598654134	2.1937510789
N	7.0	-2.2055058061	5.2182730291	4.7689182034
C	6.0	-1.8956646502	4.3212524776	3.6498374149
H	1.0	-4.6732637705	1.5247882763	2.0910702546
O	8.0	-1.3228190229	1.7487555632	-0.6448085916
H	1.0	4.5367795114	-2.0965214897	-1.0668479769
H	1.0	-1.3438466664	5.4840637722	5.2427928453
H	1.0	-2.7516235917	4.6793625144	5.4404448235
H	1.0	-2.1026156417	1.4154390802	-1.2227309549
O	8.0	-2.0506816892	1.7232185007	2.4259279190
C	6.0	3.7962767391	-2.5242481901	-1.7252109532
C	6.0	-0.7635356974	2.1877803855	2.8289726908
C	6.0	0.4174154053	0.6911041305	0.5711422321
O	8.0	-3.8665195888	2.9838114777	4.1759928441
C	6.0	1.8575556681	-3.7057859898	-3.3605261072
C	6.0	-0.7178387191	0.6116718945	-0.2572040541
C	6.0	-0.9074615841	3.1854832890	3.9882747127
H	1.0	0.0771415718	3.5944262817	4.2419181120
H	1.0	1.0850116961	-4.1492071537	-3.9797233726
C	6.0	2.4790793585	-0.4103553246	1.5910696230
H	1.0	-3.4790561615	2.0946427116	4.1423912067
O	8.0	3.4302128336	-5.6643098693	-0.0945595750
C	6.0	3.3185800356	-3.8042928058	-1.4660404935
H	1.0	-0.2404298705	1.2781519066	3.1454204628
H	1.0	3.1042974709	-1.2361650964	1.2396158652
C	6.0	1.1421719508	-0.4780748001	0.8859221121
O	8.0	-2.9939663389	0.3901317720	-1.8432139728
C	6.0	2.3343181875	-4.4041249615	-2.2525125180
H	1.0	2.3669120221	-0.5453789863	2.6760862184
H	1.0	-1.2787329055	2.6459226199	4.8686834335
N	7.0	3.8622702826	-4.5301257773	-0.3182138962
C	6.0	-1.2052592173	-0.6492360031	-0.6989432722
C	6.0	-2.3960638276	-0.6970920951	-1.5335898695
H	1.0	1.9490235298	-5.3763458761	-1.9786097943
H	1.0	-6.2543463423	-0.1863588973	-4.1016355733
C	6.0	0.6687461507	-1.7295284956	0.4712623444
O	8.0	4.7435965476	-3.9810588248	0.3533733902
C	6.0	-0.5033049060	-1.8302526597	-0.3230825252

		O	8.0	-4.7195425347	-1.0604694750	-3.1533222871
		H	1.0	-5.6408155373	-1.6388609324	-4.9377825603
		C	6.0	-5.8704097119	-1.1982850833	-3.9570108974
		O	8.0	1.3570194773	-2.8401304579	0.8233908023
		C	6.0	-2.8618228528	-2.0071090820	-1.9854921951
		C	6.0	-4.0248189326	-2.1819767336	-2.8059406607
		C	6.0	-0.9449251518	-3.1246435314	-0.7816421223
		H	1.0	0.8334895061	-3.5989177239	0.3986193291
		H	1.0	-6.6441724655	-1.8100855912	-3.4716216908
		C	6.0	-2.1376567166	-3.1864720111	-1.6161720626
		O	8.0	-0.3021805508	-4.1936384702	-0.4817363855
		C	6.0	-4.4184739483	-3.4500894987	-3.2244256767
		H	1.0	-5.2974954490	-3.5734316402	-3.8445989009
		C	6.0	-2.5612127929	-4.4605728451	-2.0548775579
		C	6.0	-3.6808867438	-4.5883442642	-2.8452584867
		H	1.0	-1.9748008705	-5.3163852134	-1.7412702839
		H	1.0	-4.0088666667	-5.5686257997	-3.1827127506
Daunomycin 3-oxime	34610-60-1	H	1.0	-7.4831192452	2.2151344243	-3.6613992939
		H	1.0	-6.7335821264	3.5961605713	-2.8150517256
		C	6.0	-7.0481491308	2.5555030871	-2.7105498001
		H	1.0	-8.0964530340	0.3501000830	-2.5613980861
		O	8.0	-5.8856919710	1.8352764975	-2.3688295173
		C	6.0	-7.1928216700	-0.1885955958	-2.3048394896
		C	6.0	-5.9833212769	0.4864047003	-2.1780770630
		H	1.0	-8.2147277095	-2.0883177926	-2.2048813044
		C	6.0	-7.2581341562	-1.5817198388	-2.1010797261
		O	8.0	-3.3261369834	1.7051176232	-1.8566341071
		H	1.0	-7.8213180893	2.4914832591	-1.9311954837
		C	6.0	-4.7790400887	-0.2161832397	-1.8394275262
		H	1.0	2.6682096491	-1.0815004344	-1.8661768170
		H	1.0	-1.8803382421	1.8722965961	-1.5995549481
		C	6.0	-3.4863366285	0.4453989340	-1.6948498084
		C	6.0	-6.1247225727	-2.2905523703	-1.7754440939
		H	1.0	1.4631901033	0.9685187410	-1.4595219992
		C	6.0	-4.8816142008	-1.6324555102	-1.6409306070
		O	8.0	-0.9217073372	1.5662112995	-1.3607773425
		H	1.0	-6.1406854092	-3.3619706652	-1.6127602537
		C	6.0	-2.3387497372	-0.3810651561	-1.3525853537
		C	6.0	-1.0661158314	0.2330241986	-1.2030054607
		H	1.0	1.4066044861	-3.4039385309	-1.2369799147
		C	6.0	-3.7241325266	-2.4484993753	-1.2971356141
		C	6.0	-2.4480515043	-1.7883649022	-1.1586131210
		O	8.0	-3.8421627367	-3.7130898538	-1.1246464811

C	6.0	0.0609082785	-0.5408185058	-0.8897788135
C	6.0	1.3720343992	0.1690991523	-0.7181919050
C	6.0	-1.2946133854	-2.5523625672	-0.8256702874
C	6.0	2.5800854016	-0.7669896508	-0.8208496796
C	6.0	-0.0476385372	-1.9320540832	-0.6851755692
H	1.0	-2.3685625448	-4.0894534495	-0.7922633316
O	8.0	-1.3840703005	-3.8884855058	-0.6463815458
H	1.0	3.4901189746	-0.2189184426	-0.5585636261
C	6.0	1.1543880196	-2.7926482148	-0.3580025029
H	1.0	3.7478882205	-3.2877383063	-2.1258864006
H	1.0	1.1996893220	2.6670343112	-0.2467002511
C	6.0	3.6240356711	-2.9571559240	0.0123577408
H	1.0	5.5146644513	1.6624714492	0.3407918733
C	6.0	2.4167277451	-2.0089824966	0.0760934634
H	1.0	5.1509447419	-3.8371443627	-1.1822890796
H	1.0	0.9035547138	-3.5129388930	0.4268391347
C	6.0	4.4026521056	-3.0487494777	-1.2782953055
O	8.0	1.3563013078	0.8154656640	0.6049193606
O	8.0	3.0455143506	2.4555862034	0.5309060061
C	6.0	1.6393745372	2.1907744727	0.6347162544
N	7.0	4.0141559483	-3.7811197253	0.9215159148
H	1.0	5.5239662464	3.2018611798	1.2305388004
C	6.0	5.2823512907	2.1379021370	1.2974217805
H	1.0	4.9105718387	-2.1078875919	-1.5202608716
H	1.0	1.7436813870	-0.7763700762	1.4778296003
C	6.0	3.8141186590	1.9393107232	1.6413811880
H	1.0	3.6024849905	0.8691216024	1.7597639088
O	8.0	2.3095413818	-1.5689239945	1.4491838804
H	1.0	5.9139148649	1.6902294801	2.0712597360
C	6.0	1.0616490049	2.7784379262	1.9251612114
H	1.0	1.0560382289	3.8710610665	1.8252663153
H	1.0	3.3825099342	4.2854151306	1.8387240607
H	1.0	0.0209323328	2.4547842625	2.0206637382
O	8.0	3.3486632276	-3.8262510296	2.1370231705
H	1.0	2.7583643823	-3.0419203039	2.1873093580
C	6.0	3.3699460600	2.6835462009	2.9089494559
O	8.0	3.6026010916	4.0904220443	2.7633002510
C	6.0	1.8807899734	2.4046811452	3.1784904002
H	1.0	1.7775753290	1.3270642224	3.3604674696
H	1.0	3.9584496880	2.3620213463	3.7750291054
H	1.0	1.7072415492	4.0901579315	4.2793958445
N	7.0	1.4824462600	3.1038169954	4.4024386725
H	1.0	0.4726559195	3.0447864484	4.5183343980

Daunorubicin / Daunomycin	20830-81-3 / 23541-50-6	H	1.0	-4.5631121078	5.2690230186	1.9915039681
		O	8.0	-2.3767776036	5.3769536212	0.7473120973
		H	1.0	-4.7538336434	3.5307919279	1.5599654734
		C	6.0	-4.0947563930	4.2832359106	2.0030620384
		H	1.0	-1.5012884918	3.4604626064	-0.9535336075
		C	6.0	-2.7844134604	4.3407330499	1.2452966383
		H	1.0	-3.9156209825	3.9520083162	3.0307511246
		H	1.0	-2.9912229662	2.5131826202	-0.7728579356
		C	6.0	-1.9718719637	2.6440527820	-0.3959320118
		C	6.0	-1.9881509118	3.0305026590	1.0992554525
		O	8.0	2.9398109940	-1.5590704158	-1.1210566368
		H	1.0	-1.0566242352	1.1855296649	-1.7036297148
		H	1.0	1.5716507669	-1.0823482574	-1.4525581931
		O	8.0	-2.6516343675	2.0344883135	1.8779081508
		C	6.0	3.2661744348	-0.7842556742	-0.1556402378
		C	6.0	-1.1936337260	1.3483292352	-0.6300149468
		O	8.0	0.7285232252	-0.4975981046	-1.3503149124
		C	6.0	1.0630842724	0.3386305811	-0.3437438720
		C	6.0	2.3288580717	0.2348475696	0.2927039511
		C	6.0	0.1387481874	1.3125026416	0.0650632520
		H	1.0	7.1782101818	-3.1931554282	-1.5386699920
		O	8.0	4.1979629425	1.8472929602	3.0011108404
		C	6.0	2.6337171973	1.1298153252	1.3595165560
		H	1.0	-2.5312218330	1.1818447410	1.4269204658
		C	6.0	0.4352908468	2.1919806915	1.1256388302
		C	6.0	3.9048381201	1.0511249492	2.0390910664
		C	6.0	1.6794988670	2.1040024549	1.7637622110
		C	6.0	4.5518270055	-0.8707111559	0.5298255281
		H	1.0	-0.2084834421	4.2403261936	1.2345144178
		C	6.0	-0.5395417130	3.2540122349	1.5842400642
		H	1.0	2.8938403545	2.6923213999	3.0658792383
		C	6.0	4.8518396301	0.0347513398	1.6011082708
		O	8.0	1.9603821682	2.9609096980	2.7713590469
		O	8.0	5.2744512282	-2.6993854794	-0.8320232620
		C	6.0	5.5591269190	-1.8333315882	0.1866121543
		H	1.0	5.8043599897	-4.2284008155	-2.0148708747
		C	6.0	6.2425337764	-3.6569294722	-1.1935465403
		C	6.0	6.0926284095	-0.0318923429	2.2749987023
		H	1.0	6.2612651645	0.6798442984	3.0749046599
		C	6.0	6.7707832028	-1.8753309734	0.8678237530
O	8.0	-1.9940971799	0.2216953311	-0.1245394491		
C	6.0	7.0337659869	-0.9680636878	1.9150506190		
H	1.0	7.5247715872	-2.6052596965	0.6005681506		
H	1.0	-0.5376019599	3.3011233405	2.6781591624		

		H 1.0 7.9885873064 -1.0195044439 2.4332215503 O 8.0 -3.7428556725 -0.0075530757 -1.5775513663 H 1.0 6.4796265226 -4.3420167866 -0.3663825403 H 1.0 -5.4093472919 -0.2085619228 -2.6614000402 C 6.0 -2.5405275860 -0.6299268866 -1.0763223856 H 1.0 -3.6057334695 0.2064328064 -4.2599181498 H 1.0 -1.8282052219 -0.7798614282 -1.8949852513 C 6.0 -4.4690788643 -0.7689837928 -2.5436520762 H 1.0 -3.4777182844 -1.7391888692 0.4895504596 C 6.0 -3.7869970289 -0.8160968630 -3.9146597730 C 6.0 -2.8725953328 -1.9542658216 -0.3986724257 H 1.0 -5.5117309561 -1.9229417550 -1.0775745668 H 1.0 -1.9407161965 -2.4199918278 -0.0610217726 H 1.0 -2.8468622254 -1.3664865448 -3.8781361655 C 6.0 -4.8400335795 -2.1392475297 -1.9239126553 H 1.0 -4.4358799255 -1.3165162205 -4.6411312158 C 6.0 -3.6397528705 -2.8958680209 -1.3381347529 H 1.0 -6.2319819653 -2.5317600309 -3.2403170456 O 8.0 -5.4893117960 -3.0125075057 -2.8524554765 H 1.0 -4.0558188927 -3.7265552490 -0.7390187852 N 7.0 -2.7628729176 -3.3657430724 -2.4147702976 H 1.0 -2.0009307065 -3.9155707397 -2.0267034823 H 1.0 -3.2955266091 -3.9661255943 -3.0383310251
4-Demethoxyadriamycin / Medorubicin	64363-63-9	H 1.0 2.2726585267 4.1968709828 -7.2481741887 H 1.0 0.8563059445 2.1905212846 -6.7950245156 C 6.0 2.2570165008 3.7445189705 -6.2593026130 C 6.0 1.4700728056 2.6342607332 -6.0178588889 O 8.0 -0.1117094587 0.3675260166 -5.4610619430 H 1.0 3.6620686514 5.1675648039 -5.4149751488 C 6.0 3.0435450344 4.2942540655 -5.2214966152 H 1.0 -0.7771485109 -0.8262898927 -4.7077913005 C 6.0 1.4358072419 2.0318809080 -4.7405448019 C 6.0 0.5973457582 0.8615471979 -4.5161869214 O 8.0 -0.9514347767 -1.4153006005 -3.9002641195 C 6.0 3.0261595231 3.7219429596 -3.9636739178 C 6.0 2.2293303565 2.5871327596 -3.6936900033 C 6.0 0.5984237551 0.2842267104 -3.1885527420 H 1.0 3.6194816577 4.1212071112 -3.1474502938 C 6.0 -0.2023561018 -0.8607801748 -2.9216118190 C 6.0 2.2286086198 2.0032493472 -2.3611828057 H 1.0 -2.0270522795 -2.5632927738 -1.9354896478 C 6.0 1.3943108102 0.8432406157 -2.1412941496 H 1.0 -0.5698316532 -3.5379526996 -1.9235730870

C	6.0	-0.2239573409	-1.4377712485	-1.6455513611
C	6.0	-1.0585774059	-2.6822645617	-1.4392480662
O	8.0	2.9422134496	2.5010401079	-1.4183093104
C	6.0	1.3610322972	0.2461803237	-0.8533926121
O	8.0	-1.1092264431	-5.4192913172	-0.3145724014
C	6.0	0.5629132140	-0.8798004753	-0.6131172645
C	6.0	-1.3028316880	-3.0388951717	0.0427645458
C	6.0	-1.7609571876	-4.4923450616	0.1478428034
O	8.0	-2.3367217758	-2.2436251250	0.6165141314
O	8.0	2.1034667943	0.7609963058	0.1530136860
H	1.0	2.5932240458	1.5488949283	-0.2820275038
H	1.0	-1.9125482691	-1.4636693636	1.0183508226
H	1.0	0.7658753242	-3.5563669628	0.3967927571
C	6.0	0.5308920219	-1.4429676964	0.7797017103
C	6.0	0.0176377488	-2.8861723532	0.8317749724
H	1.0	-3.8722957282	-4.2561295580	0.3665672005
H	1.0	1.5323561414	-1.3837603227	1.2178321375
C	6.0	-3.0620065871	-4.8039488083	0.8708902452
O	8.0	-0.3569111327	-0.5806050714	1.5711906183
H	1.0	-2.5450882073	-6.5661024544	0.4013802767
H	1.0	-3.0049110013	-4.3778674277	1.8832924526
H	1.0	-0.1331099448	-3.1961429448	1.8730452360
H	1.0	-1.7082726136	1.3198346312	2.0576727011
O	8.0	-3.2959591007	-6.1892661384	0.8972725758
H	1.0	0.7394420330	2.0338814698	2.0015572509
H	1.0	-3.7791003982	0.7644054180	3.3525413859
C	6.0	-0.1225519599	-0.5159589719	2.9729720077
C	6.0	-1.6941369488	1.2789393023	3.1526746950
H	1.0	0.0273668961	-1.5263253101	3.3790237013
H	1.0	1.9504871876	0.1158004591	2.7643439919
O	8.0	-1.3238038287	-0.0599849985	3.5671936912
H	1.0	-3.4519490235	2.5108866325	3.3561403836
C	6.0	0.7630058497	1.8801404320	3.0851125991
C	6.0	-3.0886789173	1.5372172682	3.7002562607
H	1.0	-0.8794143186	3.2735030051	3.4047686477
C	6.0	1.0598711311	0.3916636385	3.3323943511
C	6.0	-0.6203610873	2.2417820956	3.6747713043
H	1.0	1.8261588110	3.6197006286	3.2339907854
N	7.0	1.8539947257	2.6872019065	3.6412073332
H	1.0	-3.0809819044	1.5420876610	4.7932109620
H	1.0	1.2892991104	0.2361935669	4.3954346507
H	1.0	1.6664977620	2.8056642615	4.6367949868
O	8.0	-0.5805345487	2.2099514176	5.1088604249
H	1.0	-0.6516334456	1.2711917740	5.3412502867

N,N-dibenzyl-daunorubicin	70878-51-2	H 1.0 5.7427127730 -0.6633936726 -7.4940678168 H 1.0 5.3883866417 2.4845687444 -1.4817360000 C 6.0 4.8592979537 -0.7483036441 -6.8669390570 H 1.0 4.5303598074 1.3813616278 -6.7608147026 H 1.0 4.9277110770 -2.9009876098 -6.7787554565 C 6.0 4.1780209513 0.4006711533 -6.4519354022 C 6.0 4.7129125193 1.7633426381 -1.0275932245 C 6.0 4.4011046474 -2.0026928561 -6.4674229567 H 1.0 5.2980634240 2.2505680328 0.9923104556 H 1.0 3.9171714897 1.0944565834 -2.9190548004 C 6.0 4.6653889686 1.6293173225 0.3633389230 C 6.0 3.8912919648 0.9811270395 -1.8393932069 C 6.0 3.0482729764 0.2947890005 -5.6433975372 C 6.0 3.2667746870 -2.1071532033 -5.6568919853 H 1.0 2.5108665758 1.1776565138 -5.3084685241 C 6.0 3.7912459606 0.7071061547 0.9395001085 H 1.0 2.8464980079 -1.5413254611 -2.6626692906 H 1.0 2.9135276922 -3.0871746692 -5.3438895278 C 6.0 3.0141550780 0.0474366247 -1.2718647774 C 6.0 2.5794535887 -0.9643634524 -5.2385732166 H 1.0 3.6968273741 0.6015699652 2.0159361677 C 6.0 2.9792481155 -0.0806736287 0.1211311425 C 6.0 2.1623540989 -0.8548427172 -2.1508799215 N 7.0 1.3744612887 -0.1899758143 -3.2115173507 H 1.0 0.8494633260 1.9439689616 -1.6530448745 H 1.0 5.1576890249 -0.2349204955 4.5718982943 C 6.0 1.3193673615 -1.0549609968 -4.3974758270 H 1.0 2.2868064374 -0.7732770642 0.5913505776 H 1.0 0.5183308174 0.5479750833 -0.6430732057 H 1.0 1.5200430769 -1.4861784383 -1.5130193895 H 1.0 0.0599981010 2.8898609449 -3.5276553435 C 6.0 0.1450936386 1.1214140554 -1.4871490474 H 1.0 0.4829867448 -0.7393160302 -5.0248880555 H 1.0 1.1181896428 -2.1109363663 -4.1380509541 O 8.0 0.0846902410 2.2612437228 -4.2643699339 C 6.0 4.6048925412 -0.9807653756 5.1468924335 C 6.0 0.0437397729 0.2805469392 -2.7680075114 H 1.0 4.6770776550 -0.7358387696 6.2162645184 H 1.0 5.0597697173 -1.9680691571 4.9831010101 C 6.0 -0.6833223203 1.1387145866 -3.8397074793 O 8.0 3.2760925110 -0.9225584821 4.6767239646

H	1.0	-1.0515138311	2.4399647128	-0.2669863776
H	1.0	0.5278090244	0.7976929844	2.2011547071
H	1.0	-0.6173605950	-0.5809456132	-2.5505030299
H	1.0	-0.8726906443	0.5556975569	-4.7471093310
C	6.0	-1.2013100576	1.6953099039	-1.0526379190
O	8.0	1.4102412107	0.0805967055	3.1413042006
O	8.0	-1.8336994941	2.4127488807	-2.1242958182
H	1.0	-2.2696221910	3.2805530110	-4.6139424606
O	8.0	-0.3467042194	0.9857603623	1.6858579958
C	6.0	-2.0482014484	1.5925905356	-3.2827731125
H	1.0	3.7020028406	-2.7184013817	6.6028254808
C	6.0	2.3507651745	-1.7662962676	5.2259078114
O	8.0	-2.0064832621	0.6464872508	-0.5875801905
C	6.0	-2.8521891271	2.4206378301	-4.2744029170
C	6.0	0.5996489570	-0.7567987139	3.6811573239
C	6.0	2.6868596522	-2.6678351223	6.2297212959
H	1.0	-2.6223243048	0.7032432386	-2.9902658105
H	1.0	-2.7184506419	1.9691572520	0.8225201461
H	1.0	-3.1179482968	1.8185316765	-5.1497801123
C	6.0	-1.2087628150	0.0842099335	2.2021173452
C	6.0	1.0080004545	-1.6896350455	4.7236069062
C	6.0	-2.8826253544	0.9210591188	0.5345664846
H	1.0	-3.7722200767	2.7777175364	-3.8040457113
H	1.0	-4.5172348676	3.3038579499	1.3332223935
C	6.0	-0.7853137208	-0.7937967100	3.2384866469
H	1.0	-5.9359307948	3.7008204078	2.3388468203
C	6.0	-2.5206859152	0.0255834713	1.7023046581
H	1.0	-4.6256481351	1.5853967624	-0.5700749407
C	6.0	1.7126259070	-3.5290776167	6.7743552262
C	6.0	-5.5429193013	3.0155836682	1.5863137554
C	6.0	-4.3204541617	0.7254927955	0.0335575561
H	1.0	1.9999404990	-4.2250677678	7.5588464118
C	6.0	0.0445002939	-2.5846818862	5.2961486010
H	1.0	-6.1364765535	3.0820295240	0.6691284612
H	1.0	-4.3238047615	-0.1443965186	-0.6314356877
C	6.0	-1.7318460207	-1.6961852502	3.8025837000
C	6.0	0.4162576864	-3.4890004771	6.3157686592
C	6.0	-5.5896978820	1.5994091394	2.1307294488
C	6.0	-3.4650284945	-0.8402518359	2.2961867317
C	6.0	-1.3439842018	-2.6039950159	4.8550993087
C	6.0	-5.3251456951	0.4298199680	1.1426137457
C	6.0	-3.0731004089	-1.6959959616	3.3331452709
O	8.0	-5.9596146411	1.3751539984	3.2688490024
H	1.0	-0.3567032864	-4.1384910822	6.7099877343

		C	6.0	-4.9132154821	-0.8545375893	1.8606421947
		O	8.0	-6.6078161376	0.2724722904	0.4893847422
		O	8.0	-2.1887552909	-3.4079655839	5.3864264400
		H	1.0	-5.1081205800	-1.6855053832	1.1679028106
		H	1.0	-5.5451349784	-1.0154560750	2.7390192156
		H	1.0	-7.2062484216	-0.0858823371	1.1614712334
		H	1.0	-3.4671042740	-3.0365269775	4.5838556430
		O	8.0	-3.9877582453	-2.5312569724	3.8732842778
N,N-diethyladriamycin	70844-09-6	H	1.0	-2.0288479399	-6.8570070548	-3.8382645968
		H	1.0	-2.3036796897	-4.6569990410	-4.4386483957
		H	1.0	3.3025841996	2.0925977745	-4.1253072949
		H	1.0	-1.7462472862	-7.8523096546	-2.4073310528
		H	1.0	-4.6930883025	-3.9311082879	-4.5915826417
		H	1.0	-0.5287532597	-6.6790087760	-2.9242552655
		C	6.0	-1.6061678858	-6.8500276772	-2.8280861974
		O	8.0	2.7082766104	2.7936865499	-3.8204275021
		H	1.0	-4.5685678588	-5.3488908609	-3.5504045837
		C	6.0	-4.2860590892	-4.2954972658	-3.6421937625
		C	6.0	-2.7697458405	-4.0877180860	-3.6099666277
		H	1.0	-0.2346334292	-3.8966153903	-3.0795906554
		H	1.0	0.9761261067	0.9603964116	-3.1464979099
		H	1.0	-2.5732417510	-3.0354475012	-3.8300034970
		H	1.0	2.5762424544	0.3229904788	-2.7163075604
		H	1.0	0.4076695282	3.3203748889	-2.7979802721
		H	1.0	0.9712206947	-1.5835135097	-2.5492134511
		H	1.0	-1.4881021540	-1.7419166687	-2.7326937447
		C	6.0	-2.2830980071	-5.8009547433	-1.9229836410
		H	1.0	-3.3526078347	-6.0332048272	-1.8690787438
		C	6.0	2.3182364664	2.4494809049	-2.4730730233
		C	6.0	1.7866066588	1.0188985071	-2.4120836423
		N	7.0	-2.1627302765	-4.3933500954	-2.3130561603
		H	1.0	-4.7613381690	-3.7438270648	-2.8256826745
		C	6.0	-0.8367138763	-3.7626115289	-2.1569396769
		C	6.0	1.2133845697	3.4140757010	-2.0564844915
		H	1.0	1.8403472459	-3.6069928724	-1.9563716670
		H	1.0	1.5490516280	4.4524330153	-2.1060223820
		C	6.0	-0.9979014242	-2.2487562261	-1.8974195400
		H	1.0	-1.9154873982	-5.8932473090	-0.8993351730
		C	6.0	3.6178106562	2.6136636938	-1.6599382916
		O	8.0	4.3560690182	1.6616475717	-1.4422066436
		C	6.0	0.3374385056	-1.5533921763	-1.6386843022
		H	1.0	3.3676786587	4.3954428221	-0.5023998661
		H	1.0	4.0134529375	4.6597873504	-2.1257127582

H	1.0	0.2474468208	-5.4099425553	-1.2202983639
C	6.0	4.0786073842	4.0029222745	-1.2462824987
O	8.0	0.0639933416	-0.2582036118	-1.2447746233
C	6.0	0.0320487329	-4.3553595580	-1.0196673767
C	6.0	1.2200744320	0.6089822806	-1.0326667042
C	6.0	1.3652472220	-3.5801159051	-0.9592306164
H	1.0	-1.6320165934	-2.1029586806	-1.0178383971
O	8.0	1.0670578827	-2.2320895851	-0.6043187455
C	6.0	0.7368844204	3.0940560463	-0.6589425788
H	1.0	1.9595655101	0.0286827730	-0.4745987883
O	8.0	0.3107344526	5.4050238931	-0.3157871585
H	1.0	2.6572244724	-5.1370131058	-0.1928073410
C	6.0	0.7666071554	1.7663721360	-0.1730251685
C	6.0	2.3345275520	-4.1263290539	0.0789575312
H	1.0	3.2133858867	-3.4802553225	0.1443530424
O	8.0	-0.6066388211	-4.3110698629	0.2489269036
O	8.0	5.3927836713	3.9657444313	-0.7471360616
C	6.0	0.3163589972	4.1401563760	0.1676980602
H	1.0	-0.0258285417	5.9611402775	0.4694232977
H	1.0	5.5966460937	3.0154728248	-0.6784217139
H	1.0	-0.5166393789	-3.3966783952	0.5639926452
H	1.0	1.8549107564	-4.1676024127	1.0591180824
C	6.0	0.3970236047	1.4957270329	1.1571240420
C	6.0	-0.0898067303	3.8793895940	1.5051251008
O	8.0	0.4783977923	0.2360874555	1.6153978069
C	6.0	-0.0454200907	2.5488606640	2.0110119158
O	8.0	-0.5480817612	6.1789551681	1.8989709114
C	6.0	-0.5220509954	4.9734278306	2.3399831662
H	1.0	0.1633821414	0.3164100209	2.5865909852
C	6.0	-0.4322649424	2.2366174643	3.3805784522
C	6.0	-0.9302010225	4.6722204788	3.7040639582
O	8.0	-0.3572978002	1.0330808254	3.8000994295
H	1.0	-1.3670368554	6.7365291799	4.0581310330
C	6.0	-0.8946209595	3.3377725060	4.2247602240
C	6.0	-1.3652936642	5.7503920889	4.5077989400
C	6.0	-1.3222770481	3.1544960175	5.5817837197
C	6.0	-1.7663044211	5.5345591688	5.8057386090
O	8.0	-1.2949452249	1.8832331353	6.0803139937
C	6.0	-1.7477270496	4.2343328360	6.3492842604
H	1.0	-2.1019714443	6.3630003051	6.4252266545
C	6.0	-1.7103449778	1.6695609663	7.4099297971
H	1.0	-2.7599085156	1.9568364183	7.5690896229
H	1.0	-1.6041913554	0.5968793159	7.5859142010
H	1.0	-2.0690531526	4.0860370100	7.3726839834

		H	1.0	-1.0864932272	2.2148846458	8.1329639551
N,N-dimethyladriamycin	67106-76-7	H	1.0	3.3224218970	0.5002502122	-5.9981446382
		H	1.0	5.5462643699	1.6471696560	-5.8699761985
		C	6.0	3.8022559212	0.7097215811	-5.0491766761
		O	8.0	1.3458776376	-0.5543612672	-5.2081974520
		C	6.0	5.0229810906	1.3391389870	-4.9678978895
		H	1.0	0.0114643070	-1.2592200622	-4.8326775952
		O	8.0	-0.6724957776	-1.6400028748	-4.1858007429
		C	6.0	1.8329133389	-0.3488534163	-4.0406540983
		C	6.0	3.1224985772	0.3098889646	-3.8769414685
		H	1.0	6.5712339627	2.0916084424	-3.6705375949
		C	6.0	5.6105244977	1.5937245681	-3.7122143315
		C	6.0	-0.1391898664	-1.3964052562	-2.9684296143
		C	6.0	1.1256108210	-0.7561795042	-2.8504505903
		H	1.0	-5.8113103422	-2.5571230063	-1.4068502277
		C	6.0	3.6921313361	0.5503790198	-2.5831293399
		H	1.0	-2.7500339996	-2.0111234626	-2.7961760754
		C	6.0	4.9652123990	1.2112211143	-2.5410091566
		H	1.0	-5.6547696993	-2.9095305599	0.3020412795
		H	1.0	-1.9768076535	-3.5277042652	-2.3753162855
		C	6.0	-5.5430267940	-3.3545620387	-0.6974639548
		C	6.0	-2.1659082108	-2.5079591316	-2.0149946932
		H	1.0	6.7234130097	3.1051083825	-1.6683469319
		O	8.0	-6.3470451592	-4.4962011471	-0.8561138170
		H	1.0	7.5518057890	1.5259099595	-1.7278612487
		C	6.0	-0.8489427671	-1.7876533302	-1.8267037914
		C	6.0	1.6884581037	-0.5263563543	-1.5624491431
		O	8.0	5.5059864264	1.4450536923	-1.3090033094
		C	6.0	2.9771763178	0.1238999268	-1.3857894403
		C	6.0	6.7536815406	2.0965278765	-1.2313055010
		H	1.0	-5.7149622586	-5.2006416404	-1.0925196335
		C	6.0	-4.0762456869	-3.6966943542	-0.9074184456
		C	6.0	-3.0293111673	-2.5966309631	-0.7376074382
		C	6.0	-0.2952906478	-1.5512193945	-0.5504907856
O	8.0	-3.7432252548	-1.3870304008	-0.4979694638		
O	8.0	3.4364543303	0.2976048226	-0.2011381142		
C	6.0	0.9589921360	-0.9378484151	-0.4140915808		
H	1.0	6.9822305240	2.1760835099	-0.1663478391		
H	1.0	-3.2000234555	-0.8485236304	0.1058346728		
O	8.0	-3.7762096226	-4.8492742986	-1.1889940681		
H	1.0	-1.6609005845	-3.9292251376	0.2748134240		
C	6.0	-2.1336708795	-2.9610295288	0.4687595072		

		C	6.0	-1.0543857679	-1.8981011837	0.6982555628
		H	1.0	2.3868317628	-0.2980054574	0.6206883718
		O	8.0	1.4721567132	-0.7474927768	0.8202514876
		H	1.0	-2.5356520581	1.6088342365	1.3181068301
		O	8.0	-1.6933172804	-0.6658585594	1.1835775805
		H	1.0	-2.7498781718	-3.0689940630	1.3699407750
		H	1.0	-0.3512915627	-2.2342668545	1.4674528445
		H	1.0	-4.9387992903	1.7370009408	2.0136139322
		H	1.0	-4.1324577348	3.3158356968	2.1374672778
		H	1.0	-0.1604024895	1.6225413113	1.8585580368
		C	6.0	-2.8172788840	1.6227157138	2.3777404994
		C	6.0	-4.1676874354	2.3004477809	2.5451802641
		H	1.0	0.8757098201	4.0066555931	2.8262399348
		C	6.0	-1.8425396584	-0.5428555533	2.5955190176
		O	8.0	-2.9769339962	0.2611966327	2.8382161593
		H	1.0	-1.5957039459	3.3222487434	2.8538170300
		H	1.0	2.2761005437	1.8221242936	2.2088459698
		H	1.0	-2.0887640122	-1.5214412050	3.0308786367
		C	6.0	-0.3684489318	1.5253667206	2.9404634755
		C	6.0	-1.6921131275	2.2848153766	3.1892768931
		H	1.0	-4.4344091294	2.3643151966	3.6027942339
		H	1.0	0.2756809564	-0.5509621556	2.8977954080
		C	6.0	-0.5796025306	0.0283748193	3.2479134522
		C	6.0	0.8094650360	3.5026997741	3.8113199151
		H	1.0	-0.0628336134	3.8840955159	4.3461884024
		N	7.0	0.7618910770	2.0476594609	3.7317710585
		C	6.0	2.0440017925	1.5306840080	3.2483590557
		H	1.0	1.6982816239	3.7907419223	4.3823059788
		H	1.0	2.0657189157	0.4408594156	3.2909149333
		H	1.0	-2.3294105734	1.4635340422	4.8158097002
		O	8.0	-2.0489867709	2.3567503633	4.5689061627
		H	1.0	-0.6530572229	-0.0979317817	4.3354221550
		H	1.0	2.8438562700	1.9045828679	3.8964383105
		H	1.0	5.3395360926	-2.4020310356	-1.8254288497
		H	1.0	1.5263214802	-1.1815925652	-3.5947756440
		H	1.0	0.5547181227	0.7388414063	-2.3867122026
		H	1.0	5.3955844679	-3.8584856091	-2.8801334551
		C	6.0	4.8024511894	-3.2953922834	-2.1577838120
		H	1.0	2.8457335586	-0.2482331291	-2.9013483367
		H	1.0	3.0679963334	1.5103998872	-1.7425053513
		C	6.0	1.9865064234	-0.8803408759	-2.6489691596
		H	1.0	1.0285751392	-3.6055133254	-2.5932787256
		C	6.0	0.9678005056	-0.0962866483	-1.8149247231
N,N-dimethyl-daunomycin	70095-84-0					

C	6.0	3.4852369141	-2.8976271939	-2.7900110250
H	1.0	4.6232905629	-3.8882625680	-1.2553382509
O	8.0	-1.4918878848	0.9812079993	-1.0452141950
O	8.0	3.2222088859	-3.1643617539	-3.9504879494
H	1.0	-2.4540868019	1.1487341345	-0.6994800005
C	6.0	-0.1467917726	-0.9640481949	-1.2950188636
H	1.0	3.7627812944	1.0063379310	0.6568163496
C	6.0	2.4692338716	-2.1472167357	-1.9120972866
C	6.0	1.2612721837	-3.0764665107	-1.6594492718
C	6.0	-1.3492267688	-0.3534964898	-0.9027962133
C	6.0	2.4107346294	1.6497437749	-0.8742074362
H	1.0	4.0015295289	2.6751926779	0.1469777548
C	6.0	0.0189423690	-2.3614491088	-1.1727518398
C	6.0	3.2386477888	1.9256343388	0.3832840944
O	8.0	1.6412334532	0.4904582863	-0.6359930962
O	8.0	-3.7553152254	0.8003146160	-0.1191253500
H	1.0	4.1768092322	0.9188893490	2.7324131691
C	6.0	-2.4123411523	-1.1302394561	-0.3643141198
C	6.0	-1.0178848345	-3.1397903430	-0.6442794084
C	6.0	-3.6453163702	-0.4664148865	0.0322928086
H	1.0	1.5495617436	-3.8460123628	-0.9358751208
H	1.0	-8.2264493874	0.7542404204	0.7552940600
O	8.0	1.6087924726	2.7672436276	-1.2252564577
C	6.0	-2.2365138753	-2.5371579386	-0.2291480834
O	8.0	-0.8457047150	-4.4770944944	-0.5437031619
H	1.0	-7.2899012584	2.2277830619	1.1264696062
O	8.0	-6.1480176989	0.5954317077	0.9033839954
H	1.0	2.6035671747	-1.1086109712	-0.2772755377
O	8.0	3.1353807653	-1.8089925829	-0.6935913039
C	6.0	-4.7113313607	-1.2904381107	0.5928406557
H	1.0	-1.7149938575	-4.8039265173	-0.1325091207
C	6.0	-7.3722946341	1.1560036056	1.3195630944
C	6.0	-3.2888799926	-3.3597724120	0.3179441853
C	6.0	-5.9687460558	-0.7528942872	1.0279713524
C	6.0	-4.5243559966	-2.7055700939	0.7265051413
H	1.0	2.6443217184	4.5771243190	-0.2496504827
C	6.0	3.6970011635	1.6336654167	3.4054463180
O	8.0	-3.1464968694	-4.6279390109	0.4438800197
H	1.0	2.8640324176	1.1078702422	3.9127525697
H	1.0	4.4322379331	1.9140132880	4.1676378281
C	6.0	2.3874098709	2.4725060006	1.5474571748
C	6.0	-6.9559757161	-1.5796868856	1.5536694728
C	6.0	-5.5459723845	-3.5203924876	1.2644815554
H	1.0	-7.9018813070	-1.1647869889	1.8790209950

		H 1.0 1.6630543308 1.6945813193 1.8531216246 C 6.0 0.6924862012 3.1573322107 -0.1714407916 C 6.0 -6.7386777776 -2.9676880422 1.6699964766 H 1.0 -5.3462426887 -4.5829778909 1.3402315874 N 7.0 3.2692189577 2.8233066157 2.6796949909 H 1.0 -7.5590014280 0.9978027458 2.3917334488 O 8.0 2.3228742463 4.7766119528 0.6426526132 H 1.0 0.0961302546 2.2869371003 0.1145041851 H 1.0 -0.7556235731 3.7966613605 -1.6167303122 H 1.0 0.3346187261 5.1007166055 -1.0683207861 H 1.0 -7.5250218924 -3.5944370760 2.0840431908 C 6.0 1.5318519056 3.6482190261 1.0182248238 C 6.0 -0.2266625729 4.2148558084 -0.7579135381 H 1.0 0.8526701571 3.9961205473 1.8032637292 C 6.0 2.7258221559 3.8098057298 3.6045669576 H 1.0 -0.9681857710 4.5195871942 -0.0125402757 H 1.0 3.4683654974 3.9972209117 4.3880771803 H 1.0 1.7911623388 3.4906920422 4.1075172368 H 1.0 2.5446549293 4.7526424456 3.0862360562
Doxorubicin / Adriamycin	25316-40-9 / 23214-92-8	H 1.0 -2.7202958187 -4.6947561437 -0.6773970421 H 1.0 -2.6770208139 -3.9289650280 0.7754357082 H 1.0 7.2640481612 -0.9073455788 2.4420069025 H 1.0 6.5132738062 -3.2677929902 -1.4305172735 N 7.0 -2.7048039261 -3.7820138597 -0.2300983696 H 1.0 7.2014365972 -1.8384350843 0.1600821880 O 8.0 -4.0263222136 -4.3819192232 -2.5855499953 C 6.0 6.3599636154 -0.7966141730 1.8479083402 H 1.0 -1.6281132396 -3.4885506687 -3.6139774789 C 6.0 6.3266131055 -1.3286953956 0.5438951201 H 1.0 -4.0008696347 -4.3613581077 -3.5508699676 H 1.0 -1.2319548069 -2.8779834602 -2.0050245612 H 1.0 -4.8359235514 -3.5407959157 -0.1925380042 H 1.0 5.2536745045 0.2728759093 3.3611686520 C 6.0 6.2481266760 -2.3810904767 -2.0243296275 C 6.0 -3.9261785465 -3.0568067785 -0.5945064608 C 6.0 5.2617315800 -0.1469137752 2.3620442806 C 6.0 -1.6548148049 -2.6017908236 -2.9706043691 H 1.0 5.9690471689 -2.6970259443 -3.0317450734 H 1.0 7.1292319878 -1.7260729958 -2.0851757919 C 6.0 5.1844432326 -1.2024258884 -0.2417064701 C 6.0 -4.0918483689 -3.0290283771 -2.1228900360 O 8.0 5.1210005450 -1.7109594388 -1.5066731349 H 1.0 -1.0366192910 -1.8196795212 -3.4171555197

C	6.0	4.0879056053	-0.0056718369	1.5874976915
H	1.0	-3.6041441091	-1.6151464172	1.0006065343
C	6.0	4.0197865572	-0.5298704011	0.2558080264
H	1.0	-1.8413178976	-1.1323311143	-0.6970403072
C	6.0	-3.0928789838	-2.0887732077	-2.8419155758
C	6.0	-3.8672841074	-1.6154297691	-0.0634434849
H	1.0	-5.0950481960	-2.6154627676	-2.3165273871
C	6.0	2.9613892118	0.6856241865	2.1908898936
O	8.0	3.0409598165	1.1633253561	3.3837996766
H	1.0	-3.4813096224	-1.9292732595	-3.8598563573
C	6.0	-2.8646204154	-0.7655885873	-0.8386420739
H	1.0	-4.8484323664	-1.1365947032	-0.1607844125
C	6.0	2.7998301954	-0.3611079999	-0.5360317912
H	1.0	1.6837628121	1.7697848198	3.5375159515
C	6.0	1.7513507688	0.8168482229	1.4203061712
O	8.0	0.7224148453	2.0161367011	3.2475613028
O	8.0	-3.1921262087	-0.7988104994	-2.2400579574
C	6.0	1.6713788058	0.3147913271	0.0894805385
C	6.0	0.6265503885	1.4669707687	1.9977809648
O	8.0	2.6995697164	-0.7767473762	-1.7378645517
H	1.0	-2.6458306710	1.6832987609	1.7774327829
H	1.0	1.3043524961	-0.3477810791	-2.1022353913
C	6.0	0.4662031797	0.5010994487	-0.6595103109
C	6.0	-0.5550244030	1.5753997588	1.2757607353
O	8.0	-2.9940220902	0.5495297051	-0.4101857170
O	8.0	0.3855264259	0.0721179177	-1.9335469930
H	1.0	-1.6069814329	2.6746991547	2.8075831340
C	6.0	-0.6292412601	1.1402629507	-0.0662598120
C	6.0	-1.7536643675	2.3185110418	1.7922864486
C	6.0	-1.9089898859	1.4484764327	-0.8160772845
H	1.0	-1.7515205016	1.3109593012	-1.8872317476
C	6.0	-1.9918164264	3.4752370660	0.8056500050
O	8.0	-0.4355315788	4.6402810287	3.0977341242
H	1.0	1.0652297933	4.8056610452	1.6509264787
C	6.0	-2.4473986319	2.8788486391	-0.5381818330
H	1.0	-0.0076226427	3.7836385084	3.3095151968
H	1.0	-2.7070488311	4.6297071910	2.1804516686
H	1.0	-3.5390217104	2.8234718680	-0.5252412922
O	8.0	-2.9959800938	4.3871808145	1.2859268135
C	6.0	-0.0051351459	5.0016978499	1.8007140447
C	6.0	-0.7267939377	4.3643854419	0.5965332593
H	1.0	-2.1412832038	3.5457702686	-1.3463023968
O	8.0	-0.3355875103	4.6904039501	-0.5087652422
H	1.0	-0.1418771864	6.0851482908	1.6930576092

Duborimycin	NSC 180510	H 1.0 0.0876837715 4.1440533871 -7.4706420919 H 1.0 -1.1282462431 2.0889047092 -6.7088118222 C 6.0 0.2839631013 3.7068490090 -6.4944371578 H 1.0 1.7546054253 5.2006059475 -5.9896392781 C 6.0 -0.3887590862 2.5786970268 -6.0858825757 C 6.0 1.2372047998 4.3120193076 -5.6498701221 H 1.0 3.7038173235 5.3267220582 -4.8809759563 O 8.0 -1.7410451201 0.3100913878 -5.2587051524 C 6.0 -0.1339388329 2.0118236801 -4.8166662499 H 1.0 2.4169900245 6.3366481892 -4.1690558965 C 6.0 1.5097900229 3.7758777061 -4.3959833267 C 6.0 3.1048099744 5.5008071357 -3.9752281151 C 6.0 -0.8861044109 0.8197851859 -4.4502662324 C 6.0 0.8309735615 2.5991293830 -3.9331143700 H 1.0 -2.2316587044 -0.8995362560 -4.4143369589 O 8.0 2.4261302756 4.3396427022 -3.5540894290 H 1.0 3.7715357981 5.7707083775 -3.1533765346 O 8.0 -2.2479067995 -1.4987920281 -3.5948791318 C 6.0 -0.6389147142 0.2359978623 -3.1534636253 C 6.0 1.0824509941 1.9966425622 -2.6292184724 C 6.0 -1.3510185750 -0.9285938999 -2.7590013548 C 6.0 0.3186398105 0.8116547737 -2.2700352036 O 8.0 1.9412445032 2.4665410847 -1.8013278389 C 6.0 -1.1284482058 -1.5141812102 -1.5061819656 H 1.0 -2.9471914339 -2.6502499087 -1.4098152952 H 1.0 -1.5377378707 -3.5746274626 -1.8587670127 C 6.0 0.5327648002 0.2065300786 -1.0011944103 H 1.0 1.8154099831 1.5457236020 -0.6872731230 C 6.0 -1.8854494442 -2.7845042196 -1.1778227541 C 6.0 -0.1815579391 -0.9441448470 -0.6272239194 H 1.0 -1.1567491735 -5.6657600445 -1.2244863731 O 8.0 1.4389805196 0.7386834997 -0.1474541736 C 6.0 -1.3066435031 -5.8018518826 -0.1498501127 C 6.0 -1.7629089344 -3.2610766150 0.2770413225 H 1.0 -3.2058632798 -4.7983732562 -0.0770464018 H 1.0 -1.7509269921 -6.7889235232 0.0110387663 H 1.0 -0.3328024160 -5.7912830561 0.3478917793 C 6.0 0.0773515709 -1.5612155601 0.7256754096 H 1.0 0.3664188682 -3.5991454428 0.1626830846 C 6.0 -2.2281979342 -4.7375647312 0.4346901306 H 1.0 1.1328901718 -1.4582142223 0.9888073473

		C	6.0	-0.3322818207	-3.0333052204	0.7895025859
		O	8.0	-2.7087030456	-2.5478754534	1.1084369779
		H	1.0	-2.2586560436	-1.7630391844	1.4659747281
		O	8.0	-0.6940468398	-0.8551605909	1.7652422774
		H	1.0	-0.2377891232	-3.3990097227	1.8160034366
		O	8.0	-2.3911565698	-5.0324343327	1.8173315965
		H	1.0	-2.7594485900	-4.2025079582	2.1697759315
		O	8.0	0.7152107620	-0.7540049832	3.5595428033
		C	6.0	0.0265979047	0.0274112065	2.5658407298
		H	1.0	0.7587118640	0.5532999207	1.9452530691
		H	1.0	-1.6872911942	0.3864675745	3.7783792137
		C	6.0	-0.9448687089	0.9886745935	3.2425888314
		H	1.0	3.3693784654	-0.3026884135	3.3221900681
		H	1.0	-1.4686485936	1.5846640826	2.4888235503
		H	1.0	1.8729412003	-0.7195769897	5.1949813878
		C	6.0	1.5523382495	0.0045248702	4.4365258758
		C	6.0	2.8212873432	0.5364799445	3.7602216503
		H	1.0	-0.0084627141	0.4778431084	5.8028743262
		H	1.0	2.6181139275	1.2546776975	2.9646865577
		C	6.0	0.6798091154	1.0510421219	5.1602162120
		C	6.0	-0.2028623591	1.9112026247	4.2220364013
		H	1.0	0.8592272420	2.6621183469	2.6174181507
		H	1.0	3.4575425894	1.0247460323	4.5031949216
		H	1.0	-0.9532363385	2.3951467819	4.8711193058
		N	7.0	0.5024103255	2.9836376764	3.5127331148
		O	8.0	1.5382759173	1.8638462251	5.9680482946
		H	1.0	1.3032702837	3.2785692533	4.0668784308
		H	1.0	0.9703906187	2.4296223572	6.5088615871
		H	1.0	-0.6820815571	4.7792495056	0.7355405074
		H	1.0	-2.2614896851	5.0968679552	-1.5836436430
		O	8.0	-1.5058991282	5.0891295991	0.3062039779
		H	1.0	7.5127102519	-0.7856244056	-2.6393470313
		C	6.0	-1.5923956299	4.4823299757	-0.9683218324
		H	1.0	-0.6241112351	4.4609120609	-1.4867351888
		O	8.0	-2.2439289441	2.5374797811	-2.1428915779
		H	1.0	7.8870640425	0.6460643083	-0.9498610838
		H	1.0	7.8088335491	2.8337028582	0.1859864483
		C	6.0	6.9295554349	1.0402307914	-0.6331705908
		C	6.0	6.8828192917	2.2892816204	0.0170631378
		C	6.0	7.0116716254	-1.4287194458	-1.9016335701
		C	6.0	-2.1505694558	3.0467153547	-1.0410065292
		H	1.0	6.7797204294	-2.3896985227	-2.3655421654
		O	8.0	5.7747931213	-0.8956744827	-1.4842896029
Epirubicin	56390-09-1	H	1.0	-0.6820815571	4.7792495056	0.7355405074
		H	1.0	-2.2614896851	5.0968679552	-1.5836436430
		O	8.0	-1.5058991282	5.0891295991	0.3062039779
		H	1.0	7.5127102519	-0.7856244056	-2.6393470313
		C	6.0	-1.5923956299	4.4823299757	-0.9683218324
		H	1.0	-0.6241112351	4.4609120609	-1.4867351888
		O	8.0	-2.2439289441	2.5374797811	-2.1428915779
		H	1.0	7.8870640425	0.6460643083	-0.9498610838
		H	1.0	7.8088335491	2.8337028582	0.1859864483
		C	6.0	6.9295554349	1.0402307914	-0.6331705908
		C	6.0	6.8828192917	2.2892816204	0.0170631378
		C	6.0	7.0116716254	-1.4287194458	-1.9016335701
		C	6.0	-2.1505694558	3.0467153547	-1.0410065292
		H	1.0	6.7797204294	-2.3896985227	-2.3655421654
		O	8.0	5.7747931213	-0.8956744827	-1.4842896029

H	1.0	5.6105557043	3.7664929191	0.9419014068
C	6.0	5.7611359756	0.3202366677	-0.8644466103
C	6.0	5.6804876690	2.8107340503	0.4356760343
H	1.0	7.6987240313	-1.5928761084	-1.0589178750
C	6.0	4.4782394389	2.1009145066	0.2163604606
C	6.0	4.4869760156	0.8312049902	-0.4496435454
H	1.0	1.7020560915	-1.2615934129	-1.3316097083
C	6.0	3.2440158634	2.7025307041	0.6920779469
H	1.0	-1.5527935107	3.3310491665	1.8218719975
C	6.0	3.2303485629	0.1205450307	-0.6868446402
O	8.0	0.7164937730	-1.0900064048	-1.0966633539
O	8.0	3.2462912018	3.8500209289	1.2739707144
C	6.0	2.0173260941	1.9711395607	0.5037047678
C	6.0	2.0062776968	0.7173722168	-0.1717640802
H	1.0	-5.9338835117	-2.0798478290	-1.1747783138
H	1.0	-3.6069291831	3.9077573358	0.8960935697
H	1.0	1.7821545557	4.0239584162	1.5621902396
C	6.0	0.7595404703	0.0596264831	-0.3947847670
C	6.0	0.8011181402	2.5114159793	0.9947469474
C	6.0	-2.6889845174	2.3432135057	0.2342606244
O	8.0	0.7868856438	3.7499165025	1.5742796295
O	8.0	3.1720923155	-0.9847209760	-1.3239216323
H	1.0	-1.6959640780	-0.2077880681	-1.3871836799
C	6.0	-0.3882421626	1.8011680419	0.8546841818
C	6.0	-1.6828691855	2.3426910625	1.3905872594
C	6.0	-0.4333718502	0.6122633569	0.0947413282
O	8.0	-3.8980005509	3.0393502296	0.5748504837
H	1.0	-3.6972373944	0.8003651167	-0.9093851130
C	6.0	-1.7605712320	-0.0046930254	-0.3136473442
C	6.0	-5.6926261320	-3.0007818291	-0.6366029083
C	6.0	-3.0163518059	0.8781047779	-0.0590791634
H	1.0	-6.4774186167	-3.2063451581	0.0957448021
H	1.0	-5.6616854471	-3.8225652091	-1.3603666854
H	1.0	-2.0844400779	1.6949014174	2.1813245732
O	8.0	-3.3670360453	-2.6172413839	-0.9502872509
H	1.0	-4.3815994690	-2.0172353054	0.7632314306
C	6.0	-4.3500479099	-2.8640662360	0.0638962576
H	1.0	-3.5327991078	0.4907862529	0.8240638503
O	8.0	-1.9430680229	-1.2780174691	0.3635933046
H	1.0	-1.4293327791	-2.2792296084	-1.3574070212
C	6.0	-2.0403258527	-2.4089331973	-0.4607051612
C	6.0	-3.9611580769	-4.1155120180	0.8624151187
H	1.0	-3.9297760722	-4.9682173457	0.1552435695
O	8.0	-4.9163472759	-4.3534162314	1.8843152203

		C	6.0	-1.5618690788	-3.6145159597	0.3551981316
		H	1.0	-2.6123957475	-3.0921623915	2.1588982641
		H	1.0	-1.4705481764	-4.4756228185	-0.3206921253
		C	6.0	-2.5627462175	-3.9413471282	1.4676095162
		H	1.0	-4.4278802022	-4.8922383218	2.5309488725
		H	1.0	-0.5684399248	-3.3919401207	0.7559287087
		N	7.0	-2.2706539305	-5.1347596261	2.2850375037
		H	1.0	-2.0057077161	-5.9057289637	1.6721187114
		H	1.0	-1.4634635926	-4.9574844815	2.8784515504
		H	1.0	3.2289213262	2.3199864348	-5.6787783154
		O	8.0	2.9090951825	1.5969930967	-5.1255937500
		H	1.0	3.1967298006	2.7655778055	-3.4031378428
		H	1.0	-0.5286622965	6.5619242990	-1.1439559130
		C	6.0	3.4574062783	1.7882632725	-3.8380179107
		H	1.0	4.5580707106	1.7423203195	-3.8361078379
		H	1.0	-2.8533164942	3.4224556449	0.6943411040
		H	1.0	-1.5301706620	2.1692826047	-0.9162136692
		O	8.0	-0.6116790027	3.9524520285	-0.7728210810
		H	1.0	1.0108881517	5.8100554151	-1.5969569456
		H	1.0	-1.7581073031	5.7431682674	0.9514202988
		C	6.0	0.3833427250	6.1015360266	-0.7495969481
		C	6.0	-1.0005406590	2.7276493653	-0.1407028894
		H	1.0	0.2982056186	1.3460479460	-1.6403801935
		C	6.0	-1.9147954608	2.9860489509	1.0561257690
		C	6.0	2.9504239696	0.6851219399	-2.9027669331
		O	8.0	2.3503462533	-0.2771137057	-3.3273781389
		C	6.0	0.0388095469	4.8847013913	0.0994121814
		H	1.0	2.1848076773	2.7796473181	-1.2567191825
		H	1.0	0.9227011992	6.8482322654	-0.1568118737
		H	1.0	-2.1416704885	2.0208645680	1.5185378133
		C	6.0	-0.8543261287	5.2258489095	1.2990458133
		H	1.0	-2.3048468416	-0.8659258933	0.0754469808
		C	6.0	0.8124419952	1.2128776476	-0.6785808209
		C	6.0	-1.2759125034	3.9574646972	2.0506629030
		O	8.0	0.1081042620	1.9968959061	0.3139555339
		C	6.0	2.2249009301	1.8081958974	-0.7533214173
		N	7.0	-2.2457015355	4.2998176051	3.1057938662
		H	1.0	-0.3186909195	5.9136002602	1.9692440652
		H	1.0	0.9678286193	4.4287950687	0.4733848303
		O	8.0	4.5246236249	1.6019324276	-1.3130273160
		C	6.0	3.2674406646	0.8935800848	-1.4045811238
		H	1.0	5.2220447682	0.9360458182	-1.3919243117
		O	8.0	-1.5766709447	-0.1795682064	-0.1766632164
Esorubicin	63950-06-1					

		H	1.0	-2.5409593659	3.4402468004	3.5673952791
		H	1.0	-1.7748227107	4.8481394500	3.8249739909
		C	6.0	0.7996165866	-0.2552126466	-0.3009613605
		H	1.0	-0.3673489658	3.4774992584	2.4511168233
		H	1.0	2.5680571521	1.9891682140	0.2711007561
		C	6.0	-0.4324086139	-0.8817865406	-0.0426103423
		H	1.0	3.9073056958	-1.1736601936	-1.1799113158
		C	6.0	3.3358343346	-0.4221430469	-0.6223556895
		H	1.0	-6.1600070313	-4.2030274779	1.4753086225
		C	6.0	1.9910941114	-1.0096730399	-0.2582885329
		H	1.0	-5.5531825619	-5.7959597621	0.9462021976
		O	8.0	-2.8413279053	-2.1660731417	0.5220041818
		C	6.0	-0.4830992171	-2.2507369928	0.3476941372
		O	8.0	-4.1648322494	-4.2747156507	1.2995211237
		C	6.0	-5.3661272670	-4.9407219506	1.6119513014
		C	6.0	-1.7731564041	-2.8614980206	0.6367695225
		H	1.0	3.9133607892	-0.2079835589	0.2889331306
		C	6.0	1.9609779599	-2.3552727744	0.1220201068
		C	6.0	0.7312703043	-2.9880163755	0.4411495449
		H	1.0	2.8381809759	-3.9754838359	0.4733196656
		C	6.0	-2.9902550135	-4.9684623797	1.3820354089
		C	6.0	-1.7857985160	-4.2611549951	1.0528952630
		H	1.0	-5.3853280682	-5.2995216468	2.6515619279
		O	8.0	3.1252069175	-3.0440614829	0.1819879128
		H	1.0	-3.8682976529	-6.8280062257	2.0167431910
		C	6.0	-2.9533594947	-6.3036735715	1.7701857382
		C	6.0	-0.5551309050	-4.9920543653	1.1443054911
		C	6.0	0.7261688497	-4.3763181746	0.8342081990
		C	6.0	-1.7249849639	-6.9920587543	1.8477380496
		C	6.0	-0.5487108221	-6.3488420385	1.5405862875
		O	8.0	1.8151235137	-5.0518182160	0.9098915316
		H	1.0	-1.7206611491	-8.0359517658	2.1530122005
		H	1.0	0.4124840868	-6.8475095042	1.5889107122
11-Hydroxy aclacinomycin A	NSC 670121	H	1.0	-8.0609413708	-6.9240960627	0.0228441060
		H	1.0	-6.6333813119	-5.9863603973	-1.7207062385
		H	1.0	-7.7163266731	-8.2727894507	-1.0480492332
		H	1.0	-5.4707330122	-7.3120535471	-1.5914985360
		H	1.0	-5.5163533117	-2.5039666025	-1.8141765006
		C	6.0	-7.2511788806	-7.5677923262	-0.3540030759
		H	1.0	-4.7613749355	-3.8550273234	-2.6916930358
		C	6.0	-6.1765979862	-6.6965496928	-1.0245057162
		H	1.0	-4.2288501391	-2.1869846626	-2.9907743865
		C	6.0	-4.5753302377	-2.8847586768	-2.2260455108

H	1.0	-2.9313225148	-0.1274631496	-3.3883695491
O	8.0	-7.2289581099	-9.4162813158	1.1850632859
C	6.0	-6.7476778701	-8.3505627155	0.8522960939
H	1.0	-3.4830561971	1.3290715627	-1.8038499566
H	1.0	-6.0235921415	-5.2827595770	0.6264658726
C	6.0	-5.3736196473	-5.9408920231	0.0261644984
O	8.0	-4.3694180379	-5.2124731724	-0.5832142687
H	1.0	-4.8367785617	-3.5155306039	0.5240005052
C	6.0	-3.5309711989	-3.0151743930	-1.1268906128
H	1.0	-6.9624948204	-6.1539005796	2.5537294024
C	6.0	-1.9226111930	-0.3018844741	-3.0020171995
H	1.0	-1.6796968830	-1.3483883293	-3.1921902607
H	1.0	-1.2273221451	0.3389687798	-3.5777909865
H	1.0	-3.3266875464	-2.0284865286	-0.6919034900
C	6.0	-3.9684793599	-3.9535280023	0.0104417237
C	6.0	-2.5009332326	1.2960381071	-1.3223880687
C	6.0	-5.6459998919	-7.6981508901	1.6986750204
O	8.0	-2.3263329010	-3.4891096455	-1.7544745494
O	8.0	-4.7535799929	-6.9130722138	0.8962671288
H	1.0	-1.9005446439	2.1344148202	-1.7220942532
C	6.0	-6.2391341206	-6.9086532372	2.8771238917
H	1.0	-6.7482733829	-7.5940811634	3.5598705311
N	7.0	-1.9034430396	-0.0182444562	-1.5666197602
H	1.0	-2.6539660668	1.4659383540	-0.2557202470
H	1.0	-5.0296637539	-8.5109030358	2.0931361176
H	1.0	-5.4331705963	-6.3972718257	3.4098423260
C	6.0	-2.8211951683	-4.1413548763	1.0154672302
H	1.0	-3.4587838178	-5.8292929253	1.7378210586
C	6.0	-1.2253431338	-3.6624767893	-0.8727386777
H	1.0	-1.7707155861	-5.6128210463	-0.1588322136
H	1.0	-2.6107252624	-3.1574546952	1.4478673605
H	1.0	0.0189609343	-1.9382187693	-2.1254893465
O	8.0	-3.1712698670	-4.9753951911	2.1057924033
H	1.0	-0.4400102317	-4.0795733431	-1.5152040945
C	6.0	-0.5370200651	-0.1380710252	-1.0200711030
C	6.0	-1.5735587528	-4.6232316152	0.2674899038
H	1.0	0.1512858521	0.4776389778	-1.6310230810
O	8.0	-0.7954063355	-2.4566935642	-0.2856043016
C	6.0	0.0108321364	-1.5822205864	-1.0884073072
H	1.0	-0.6918395023	1.3871920990	0.5493859300
H	1.0	-1.0699647982	-0.2689621261	1.0682248516
C	6.0	-0.4161413170	0.3383040875	0.4347671212
H	1.0	-0.7317095804	-4.7012120184	0.9597891380
C	6.0	1.4660227090	-1.5898969804	-0.5727813854

H	1.0	2.0491361530	-0.9282126046	-1.2301467861
H	1.0	2.1151436345	-3.4090175806	-1.5619319177
C	6.0	1.0221736382	0.2104736629	0.9421012448
H	1.0	2.6176616946	1.4597574330	-1.4221630990
H	1.0	-0.5585657092	10.0934051961	3.6946615716
H	1.0	1.5590863445	-3.6345352110	0.1181623456
O	8.0	-0.6344030584	7.5451381955	4.0380883151
C	6.0	2.1043114272	-2.9711797293	-0.5581478471
C	6.0	0.1388505346	9.5534453834	3.0617405786
O	8.0	1.7975552430	1.1821285830	0.2789289267
H	1.0	0.9320904717	11.3070015140	2.0926386460
H	1.0	-0.4283207224	6.5683324521	3.9390750523
C	6.0	0.1836009283	8.1648086539	3.1640022019
O	8.0	3.4252248507	1.3729981767	-1.9553043472
O	8.0	1.5383442102	-1.1021104117	0.7719640633
C	6.0	0.9810287660	10.2223153025	2.1584367161
H	1.0	1.0625358640	0.3915131898	2.0209278319
O	8.0	0.3620738304	5.3419106425	3.2853631518
C	6.0	1.0888607454	7.4146434297	2.3474007985
C	6.0	1.8670590527	9.5219736290	1.3560501996
C	6.0	1.1369484247	5.9768503392	2.4506571874
H	1.0	2.5241622699	10.0218760610	0.6537134244
C	6.0	1.9352786255	8.1170610325	1.4362218136
H	1.0	0.7968818536	3.8439597924	3.0047129486
H	1.0	4.5870410883	-0.7073861551	-2.7857498694
O	8.0	1.3333070992	3.1406022252	2.5248989928
C	6.0	2.0584823231	5.2549093652	1.6124494609
C	6.0	2.8710101255	7.3919889045	0.5855479958
C	6.0	2.1318275566	3.8385442368	1.6798439821
H	1.0	3.1361116957	-2.8978341108	-0.2047044746
C	6.0	2.9077687990	5.9492091593	0.6958250922
O	8.0	3.6327263800	8.0143622417	-0.2334159823
H	1.0	4.7665009011	3.4997631742	-1.9590047438
C	6.0	3.0298435621	3.1318987672	0.8702510050
C	6.0	3.8050537660	5.2103076484	-0.1223248229
C	6.0	3.0196014738	1.6308348649	0.9567121296
C	6.0	3.8592026630	3.8115544388	-0.0447301319
O	8.0	4.6258488931	5.8471247100	-0.9829456078
C	6.0	4.5462913659	1.5464046714	-1.0788645812
H	1.0	4.3951007991	6.8320857597	-0.8592415108
C	6.0	5.4643623979	-0.6319160057	-2.1395152163
C	6.0	4.8400886327	3.0825262666	-0.9518261502
H	1.0	5.9739114457	1.3912981312	-2.6753359302
H	1.0	2.9358949628	1.3220327744	2.0039616994

		H	1.0	4.0887206611	-0.1008804005	0.2811052456
		C	6.0	4.2484856286	0.9798355469	0.3196914951
		C	6.0	5.7281110809	0.8294835864	-1.7662070765
		H	1.0	5.2899418486	-1.2571610946	-1.2573931627
		H	1.0	6.3249758924	-1.0517997475	-2.6721146418
		H	1.0	5.1124754015	1.1786439388	0.9629892998
		H	1.0	6.6053556756	0.8904207911	-1.1120376180
		C	6.0	6.2662162309	3.3378055416	-0.4706760489
		O	8.0	7.0573075603	3.7925915779	-1.4732334049
		O	8.0	6.6879730198	3.1376838446	0.6514343348
		H	1.0	8.8929754922	4.4587164404	-1.9963883530
		C	6.0	8.4047449139	4.0910131720	-1.0930225607
		H	1.0	8.4231065813	4.8555235320	-0.3121542961
		H	1.0	8.9145814359	3.1980437516	-0.7192543549
11-Hydroxy aclacinomycin X	NSC 670122	H	1.0	-7.4931213764	-6.0651302272	-2.4143617960
		H	1.0	-7.7263123895	-8.1855599990	-1.0571351703
		N	7.0	-6.8733415769	-5.6913344126	-1.7116070050
		H	1.0	-6.2416799407	-4.9563368251	-1.9972662786
		C	6.0	-6.9410168725	-7.7482528328	-0.4464391402
		C	6.0	-6.4371867420	-6.5121281146	-0.7227208184
		H	1.0	-5.6386434804	-2.4483442582	-1.7711646080
		H	1.0	-4.7693421844	-3.6540211194	-2.7676916198
		O	8.0	-6.9731673846	-9.5869118005	1.0432515423
		H	1.0	-4.3569507263	-1.9416023662	-2.8849572562
		C	6.0	-4.6677420064	-2.7277276632	-2.1944803314
		C	6.0	-6.4868386580	-8.5136799790	0.6929075287
		C	6.0	-5.3889318698	-5.8884454864	0.1949523492
		H	1.0	-5.9001029051	-5.2938726462	0.9705233796
		H	1.0	-2.9446780076	-0.0419335310	-3.4153043520
		O	8.0	-4.5499590449	-5.0702272305	-0.5567632030
		H	1.0	-6.6064572413	-6.6412707127	2.7774741116
		H	1.0	-4.9186175027	-3.3690023742	0.5761687269
		H	1.0	-3.4958209248	1.4121082188	-1.8297630245
		C	6.0	-3.6265002150	-2.9048709198	-1.0974308281
		C	6.0	-5.3422291726	-7.9169171624	1.5254129834
		O	8.0	-4.6071247017	-6.9098117368	0.7984873846
		H	1.0	-6.2958859848	-8.2586411010	3.4194447742
		C	6.0	-4.0778454212	-3.8351519489	0.0418202042
		C	6.0	-5.8440692422	-7.4194925344	2.8848273980
		C	6.0	-1.9456352384	-0.2404220256	-3.0154399676
		H	1.0	-1.7227808787	-1.2914770795	-3.2055793868
		H	1.0	-3.3952256541	-1.9274750819	-0.6549493146
		O	8.0	-2.4439112301	-3.4014647604	-1.7442893369

H	1.0	-1.2292558912	0.3865080073	-3.5801843804
H	1.0	-4.6151416697	-8.7188968587	1.6806159859
C	6.0	-2.5191467538	1.3628638106	-1.3387472040
N	7.0	-1.9392635169	0.0392232865	-1.5787465014
H	1.0	-1.9013993357	2.1917971841	-1.7309968319
H	1.0	-5.0187943747	-7.0148127280	3.4764377379
H	1.0	-2.6794070693	1.5337346003	-0.2733494797
H	1.0	-3.4697199145	-5.7698104628	1.7630260256
C	6.0	-2.9149416861	-4.0617364921	1.0228010890
H	1.0	-1.9182503766	-5.5495321873	-0.1803879705
C	6.0	-1.3328949508	-3.6048318030	-0.8783049186
O	8.0	-3.2670775773	-4.8864655764	2.1184831591
H	1.0	-0.5653318285	-4.0315615497	-1.5356082593
H	1.0	-2.6751014604	-3.0831205029	1.4521078434
C	6.0	-1.6913555513	-4.5699317231	0.2541862152
H	1.0	-0.0403642195	-1.9082252096	-2.1208256396
C	6.0	-0.5791042287	-0.0994867212	-1.0195208623
O	8.0	-0.8749890683	-2.4146487928	-0.2862924957
H	1.0	0.1226929624	0.5072173656	-1.6237430954
C	6.0	-0.0507204281	-1.5508783738	-1.0842068215
H	1.0	-1.1306561518	-0.2222873416	1.0658811829
H	1.0	-0.8439733339	-4.6763950528	0.9358676920
H	1.0	-0.7233364944	1.4275958614	0.5492156087
C	6.0	-0.4634288092	0.3744956172	0.4364516440
H	1.0	2.0278816219	-3.4077027360	-1.5441080226
C	6.0	1.3993787424	-1.5810082907	-0.5560591993
H	1.0	1.9978213583	-0.9272292998	-1.2074225453
H	1.0	1.4546960990	-3.6285452777	0.1308293982
C	6.0	2.0156839532	-2.9721139684	-0.5393064288
C	6.0	0.9694568868	0.2252175631	0.9542478440
H	1.0	2.6162658892	1.4494433897	-1.4002626849
O	8.0	1.4654579143	-1.0963738223	0.7896428439
O	8.0	1.7641112556	1.1825354491	0.2952109590
O	8.0	3.4299175181	1.3341711277	-1.9180536386
H	1.0	1.0042472353	0.4066070188	2.0332283400
H	1.0	4.5730884445	-0.7740048893	-2.7092055471
H	1.0	3.0456268830	-2.9157604793	-0.1777295045
O	8.0	-0.6467788315	7.6130177069	3.9429519200
H	1.0	-0.4520651683	6.6326298025	3.8571328548
H	1.0	-0.5313098316	10.1565046149	3.5768184721
O	8.0	0.3336660207	5.3900019820	3.2287161771
C	6.0	0.1941343322	8.2132776270	3.0771797338
H	1.0	0.7533935800	3.8830122388	2.9711314557
C	6.0	0.1694049731	9.6014048270	2.9608891440

		O	8.0	1.2884018637	3.1685955884	2.5062497863
		C	6.0	1.1308940559	6.0064014690	2.4013255117
		C	6.0	1.1031175817	7.4437525954	2.2833358881
		C	6.0	1.0350461975	10.2502447601	2.0654459069
		H	1.0	1.0015906279	11.3347411601	1.9883074769
		C	6.0	2.1107357037	3.8481448819	1.6689478126
		C	6.0	2.0568723544	5.2644993850	1.5863840784
		C	6.0	1.9735404656	8.1259546273	1.3795793948
		C	6.0	2.9829893711	1.6223975936	0.9849025911
		C	6.0	1.9249707100	9.5305530123	1.2845251004
		H	1.0	4.8087300923	3.4413493516	-1.9178608166
		C	6.0	3.0135744929	3.1219601383	0.8823764575
		C	6.0	4.5401964283	1.4981885366	-1.0259424063
		C	6.0	5.4422819154	-0.7036878698	-2.0514359963
		C	6.0	2.9304075254	5.9385545848	0.6770494422
		H	1.0	2.5999444520	10.0152277145	0.5884746630
		C	6.0	2.9140437150	7.3801808800	0.5518488849
		H	1.0	4.0376916147	-0.1301835009	0.3393926909
		C	6.0	3.8668448846	3.7814715409	-0.0256917036
		C	6.0	3.8318679046	5.1798630245	-0.1180607466
		O	8.0	3.6970777021	7.9848164663	-0.2603626029
		H	1.0	5.9876756112	1.3069551612	-2.5998185255
		H	1.0	5.2472312691	-1.3175912199	-1.1656924523
		H	1.0	2.8801478481	1.3253777264	2.0339051477
		H	1.0	6.3043225562	-1.1405758892	-2.5677084825
		O	8.0	4.6750069354	5.7977601413	-0.9709035309
		C	6.0	4.2119691350	0.9484781701	0.3726593203
		C	6.0	4.8551825280	3.0308222725	-0.9063224792
		C	6.0	5.7209636391	0.7577152646	-1.6889424412
		H	1.0	4.4543557166	6.7866641713	-0.8600490361
		H	1.0	5.0680070077	1.1402962763	1.0284519022
		H	1.0	6.5894788719	0.8128785363	-1.0227992784
		C	6.0	6.2751576154	3.2672987620	-0.3982043786
		O	8.0	7.0930574086	3.7019937754	-1.3880295629
		O	8.0	6.6711311318	3.0693110017	0.7336325166
		H	1.0	8.9496644942	4.3331449776	-1.8798487853
		C	6.0	8.4382402901	3.9787310902	-0.9840497325
		H	1.0	8.9251889786	3.0788387066	-0.5966023176
		H	1.0	8.4556845003	4.7467043380	-0.2065823957
3'-Hydroxy daunorubicin	64842-75-7	O	8.0	5.4537819555	-0.5718944611	-2.4173968244
		H	1.0	0.3210545717	3.1610979786	-3.5581392654
		H	1.0	2.2434407710	0.2290388340	-3.5297957521
		O	8.0	0.9920619408	2.4112963745	-3.4179478125

O	8.0	-0.8367366051	4.1034187519	-3.1328127636
H	1.0	5.5956137719	-2.4648959254	-4.0761096763
C	6.0	4.4944800108	-1.2800689278	-2.6742533997
O	8.0	2.2662179334	-2.0956354354	-2.3761504184
H	1.0	-2.5834945783	5.6468195496	-2.6817444640
C	6.0	2.5950768157	0.3397685792	-2.4989026233
H	1.0	3.8413313498	-2.3125493969	-4.4453635478
C	6.0	4.5894967736	-2.4294622768	-3.6550309402
H	1.0	3.4338616800	1.0477676215	-2.5349371100
C	6.0	0.7336295452	1.9761059457	-2.1643449383
C	6.0	3.1313848306	-1.0237336201	-2.0049166099
H	1.0	1.6131861235	-2.1972543690	-1.6616703303
C	6.0	-1.0496833049	3.6802026033	-1.9409136027
C	6.0	-2.8249370221	5.3505699895	-1.6675080179
C	6.0	1.4890543461	0.9187431390	-1.6443298188
H	1.0	-4.3880607212	6.7863340698	-1.3668440522
C	6.0	-0.2834659908	2.5917821059	-1.3831997967
H	1.0	-0.4405241248	-5.3059431850	-1.4149663017
H	1.0	4.3434280068	-3.3688798263	-3.1512722247
C	6.0	-2.0790198103	4.2883250587	-1.1085540344
C	6.0	-3.8132039366	5.9691790699	-0.9372954663
C	6.0	3.3204721437	-0.9709722442	-0.4757511590
C	6.0	1.2370489837	0.4648498123	-0.3320642915
H	1.0	3.7524660993	-1.9156822008	-0.1235431359
C	6.0	-1.0215342600	-5.2613296584	-0.4903671242
C	6.0	-0.5347495142	2.1359392297	-0.0570705212
H	1.0	4.0391227166	-0.1802072588	-0.2403315183
O	8.0	1.1231599583	-1.8732433909	0.1410863962
H	1.0	-2.0852590783	-5.2257311112	-0.7460220138
H	1.0	-0.8641173925	-3.1217490397	-0.2655221236
O	8.0	0.7938790847	-4.0974809483	0.5277054529
C	6.0	-2.3370670372	3.8373316260	0.2276600600
C	6.0	1.9982488382	-0.6938408352	0.2467238239
H	1.0	-0.8391259556	-6.1707715158	0.0880927581
C	6.0	-4.0938968997	5.5504034249	0.3791349037
H	1.0	2.4071719642	-3.1156207344	1.1933091415
C	6.0	0.2389423902	1.0590425883	0.4552028315
C	6.0	-0.6359744488	-4.0266419291	0.3086990393
C	6.0	-1.5547029640	2.7391622563	0.7875562480
C	6.0	1.3329223961	-2.9104528295	1.0849174862
H	1.0	-4.8762566672	6.0501488850	0.9365006057
C	6.0	-3.3755551399	4.5079766052	0.9557690926
H	1.0	2.1788315927	-0.5115086100	1.3109756921
O	8.0	0.0254047923	0.5966764295	1.7061113669

		H 1.0 -0.7272349984 1.2137366308 2.0561124689
		O 8.0 -1.7299464620 2.2962117835 1.9747979892
		O 8.0 -3.6229320015 4.0783530242 2.2280470044
		H 1.0 -0.0737595822 -5.2833618664 2.2926645064
		H 1.0 -5.6257597791 4.6118824537 2.4953589059
		C 6.0 -1.3087410916 -3.9300525777 1.6809672170
		C 6.0 0.7027232994 -2.6041147662 2.4516940260
		H 1.0 -1.2176674351 -1.7772891656 1.9332776496
		H 1.0 -2.3992928843 -3.9074373388 1.5802192557
		H 1.0 1.0043839594 -1.6158263294 2.8051272063
		C 6.0 -4.6392043616 4.7130054046 2.9705366873
		O 8.0 -1.0087641354 -5.0947901039 2.4713566934
		H 1.0 1.0827416021 -3.3444700181 3.1684213059
		C 6.0 -0.8355786093 -2.6734978055 2.4303166970
		H 1.0 -4.4348865509 5.7825211064 3.1246802609
		H 1.0 -4.6572763056 4.2101385214 3.9398039523
		O 8.0 -1.3660562794 -2.6779588624 3.7491749528
		H 1.0 -1.2724275904 -3.5987266900 4.0418308314
		H 1.0 -3.0532741480 -2.3250588243 -2.6107648984
		H 1.0 -4.5134995272 -1.6159210038 -2.3522369279
		N 7.0 -3.6052916888 -1.8026096738 -1.9358394612
		H 1.0 -4.2099000111 -3.6017031712 -0.9355470180
		C 6.0 -3.7963450874 -2.5986372077 -0.7199282750
		H 1.0 -1.6892954055 -3.1342928623 -0.6753166057
		O 8.0 -5.9929186364 -1.6596623582 -0.5459264740
		H 1.0 -3.5846768078 0.4318911839 -0.8859127672
		C 6.0 -2.4582280388 -2.7733134747 0.0173296891
		H 1.0 -6.5561430094 -1.0707736802 -0.0275598239
		H 1.0 -5.1431948787 0.9678151460 -0.2506543230
		C 6.0 -4.8049829177 -1.9070047243 0.2129576565
		H 1.0 -1.7857985987 -0.7064155370 -0.0953641784
		C 6.0 -4.1432968311 0.6180657892 0.0308704066
		H 1.0 -2.5604524970 -3.5175798070 0.8153223304
		H 1.0 1.4751853012 -2.6906203007 0.6126645134
		H 1.0 -5.0208075397 -2.6254370981 1.0205787781
		C 6.0 -1.9971751210 -1.4706668126 0.6620257383
		H 1.0 3.1797259345 -2.1850362180 0.7186210202
		C 6.0 -4.2475231982 -0.6375531690 0.9037169962
		H 1.0 -3.6403103548 1.4047931125 0.5982765433
		H 1.0 2.2450023466 -3.8303413182 2.4477464591
		C 6.0 2.1546845629 -1.9089112732 0.9765074638
		O 8.0 4.0759319650 1.0524073516 -2.8368188898
		O 8.0 3.6629109732 -0.7732316327 -1.1633161114
Idarubicin	57852-57-0	

		H	1.0	4.0498383132	-0.1887787227	-1.8960710519
		O	8.0	-0.8740808974	-1.7368468346	1.4353486701
		C	6.0	2.5804160018	-0.0890850279	-0.7336175884
		O	8.0	-3.0245234781	-0.9886860818	1.5494557212
		C	6.0	1.8051231642	-0.6032496667	0.3079678929
		C	6.0	3.0342905048	1.6708803513	-2.4199434067
		H	1.0	-4.9244616568	-0.4066911224	1.7410263846
		C	6.0	2.2165214184	1.1459021373	-1.3468835477
		O	8.0	1.7159025975	-3.2323799392	2.9936968709
		H	1.0	4.2737792915	2.9411259111	-4.3888743464
		C	6.0	2.6319884515	2.9378706868	-3.0158983248
		C	6.0	0.6433670444	0.0737776977	0.7376346837
		C	6.0	3.3980377298	3.4939750412	-4.0645299897
		C	6.0	1.0538003397	1.8455865949	-0.8928739270
		C	6.0	1.9804333305	-1.8953083502	2.5124804648
		C	6.0	0.6524222167	3.1030565124	-1.4838187115
		C	6.0	0.2679718114	1.2896722459	0.1586357456
		C	6.0	1.4745340780	3.6345078321	-2.5612023981
		O	8.0	-0.3891716637	3.7333840352	-1.0794956286
		C	6.0	-0.1430712957	-0.5493060459	1.8625155097
		C	6.0	3.0393347042	4.6946384588	-4.6476063947
		H	1.0	3.6393251596	5.1105829312	-5.4539077929
		C	6.0	1.1265717941	4.8597941777	-3.1721335277
		C	6.0	1.8911358189	5.3851505274	-4.1966975343
		O	8.0	4.1800638522	-0.8688377217	2.6410746417
		O	8.0	-0.8363607033	1.9380140599	0.5966096496
		H	1.0	0.2399582891	5.3659891459	-2.8041314315
		C	6.0	0.7915803920	-1.0097112178	2.9825561323
		C	6.0	3.2648289777	-1.4109438553	3.2283257864
		H	1.0	-0.8714442148	2.7770541622	0.0171661365
		H	1.0	0.2268108709	-1.5778102045	3.7280000769
		H	1.0	1.6114074622	6.3298390027	-4.6575699266
		H	1.0	-0.8644679741	0.1686784002	2.2596838829
		H	1.0	3.4743426043	-2.7531820850	4.8942391776
		H	1.0	1.1698678732	-0.1021723066	3.4675920828
		C	6.0	3.3405073781	-1.6804412902	4.7265674979
		H	1.0	4.1843214519	-1.1317057665	5.1481880436
		H	1.0	2.4126935224	-1.4003399702	5.2339542677
5-Imino daunorubicin	67324-99-6	H	1.0	3.5162269263	1.3991395343	-7.0478656548
		H	1.0	1.3780148533	2.3029472810	-6.1006239950
		C	6.0	3.1569596654	1.0854215084	-6.0708392062
		H	1.0	4.8350811579	-0.2304251763	-5.7389326006
		C	6.0	1.9844338564	1.5856604964	-5.5597363937

C	6.0	3.9111694312	0.1536566488	-5.3251464036
H	1.0	5.2368032069	-2.2284709630	-4.7979591204
O	8.0	-0.3757338952	2.5937723266	-4.5566100400
C	6.0	1.5156377556	1.1799951306	-4.2874101414
C	6.0	3.4694030940	-0.2597273265	-4.0767155242
H	1.0	6.1403903943	-0.8895826966	-4.0369878472
C	6.0	5.4011565590	-1.6822176387	-3.8594086773
C	6.0	0.2706195019	1.7596486350	-3.8219597250
H	1.0	-1.5706123659	2.8895349984	-3.6502785934
C	6.0	2.2524176240	0.2316920825	-3.4999139162
O	8.0	4.1962863442	-1.1687994327	-3.3320248885
H	1.0	5.7898370552	-2.3719501054	-3.1070315991
O	8.0	-2.1315136753	2.8062327726	-2.8031043602
C	6.0	-0.2139557942	1.3730597544	-2.5170890477
C	6.0	1.7390909293	-0.1762540837	-2.1916672163
H	1.0	-4.0351536288	0.2471358857	-2.2579704071
C	6.0	-1.4317838810	1.9313378964	-2.0406612875
C	6.0	0.4967403310	0.4308164248	-1.7193427787
N	7.0	2.3024556270	-1.0637504093	-1.3781008592
H	1.0	-5.3206274720	-0.9611771551	-1.9522841011
H	1.0	3.1606597602	-1.4571829599	-1.7363443839
H	1.0	-5.6269096942	0.7916524750	-1.7343015242
C	6.0	-4.8913416505	-0.0122873093	-1.6269407559
H	1.0	-3.8473206452	2.4308827982	-1.2108813804
C	6.0	-1.9277180013	1.5797927317	-0.7812758583
C	6.0	-0.0300147723	0.0714949947	-0.4384955037
C	6.0	-3.2545340206	2.1527458486	-0.3372569127
H	1.0	1.4579477305	-1.1231174025	-0.2667731579
C	6.0	-1.2233915352	0.6637389096	0.0280844001
C	6.0	-4.4642742205	-0.1254552540	-0.1801031064
H	1.0	-3.1245692389	3.0754146603	0.2454719648
O	8.0	0.5921882439	-0.8375950745	0.3257497664
C	6.0	-3.9962022580	1.1604547201	0.5503460894
O	8.0	-4.5853889191	-1.1672849232	0.4447389203
O	8.0	-5.2278695696	1.7944341777	0.9648430870
H	1.0	-1.8064256830	-0.8552022894	1.3890838744
C	6.0	-1.7437483136	0.2389312708	1.3878441735
H	1.0	-5.6292041478	1.2039268218	1.6190677610
C	6.0	-3.1205926355	0.8345168367	1.7576618024
H	1.0	-2.9542016889	1.7759789187	2.2919645541
O	8.0	-0.7714674278	0.6492869954	2.3729589623
H	1.0	0.3180742342	-2.0621664020	2.2962719440
H	1.0	-3.6526856204	0.1482195073	2.4262949755
H	1.0	1.4775272091	0.1301531884	2.6530757725

		H 1.0 -1.9048028888 -1.7372914661 3.2775715351
		C 6.0 0.2188161419 -2.1564806047 3.3823349083
		H 1.0 0.7551051680 -4.1189381537 3.2333711563
		C 6.0 -0.8591193756 0.1483763573 3.6888252490
		H 1.0 2.3749047085 -2.0164730670 3.6403143064
		N 7.0 0.0446680640 -3.5758589421 3.7218914192
		C 6.0 -1.0296553265 -1.3743652072 3.8224715786
		C 6.0 1.5185934635 -0.0207485445 3.7362446615
		H 1.0 -1.6635983952 0.6604184199 4.2406033969
		C 6.0 1.4739125029 -1.5254896533 4.0301857574
		O 8.0 0.3345388082 0.5612661121 4.3401063754
		H 1.0 2.6326570755 1.7750775799 4.1588749833
		H 1.0 3.6400705337 0.3424857556 3.8628884759
		C 6.0 2.7174985060 0.6991070736 4.3325520371
		H 1.0 0.2622916954 -3.6713664417 4.7146163355
		H 1.0 -1.2265742570 -1.5777562832 4.8839091019
		O 8.0 1.4783955504 -1.7548103797 5.4491462046
		H 1.0 2.7892348180 0.5173105212 5.4087750347
		H 1.0 0.9045290738 -1.0581490452 5.8055875597
Marcellomycin	63710-10-1	H 1.0 -3.5798127508 -2.7389638094 3.3939182702
		H 1.0 -1.8748050815 -3.2338977143 3.4249145850
		C 6.0 -2.7969420880 -3.2645947574 2.8388618183
		H 1.0 -3.0926092578 -4.2973137155 2.6493432323
		O 8.0 -2.0565545199 -0.7581546991 2.6055707731
		H 1.0 -2.8886217522 1.3186386867 1.5255925900
		O 8.0 -2.5961312717 -2.6748384199 1.5506353375
		C 6.0 -2.1907857012 -1.3800130962 1.5696042178
		H 1.0 -4.6118036661 -0.5961928562 1.1234576172
		H 1.0 -1.3421857851 2.9461967049 0.7445570495
		H 1.0 -3.7201580174 2.1863656412 0.2176003004
		C 6.0 -2.9058682955 1.4916376391 0.4455560203
		H 1.0 -5.7931202017 1.3048065724 -0.0120663651
		H 1.0 -6.6275271825 -0.2115174773 -0.3598200462
		C 6.0 -1.5941815059 2.1530297855 0.0283243952
		C 6.0 -4.5050641448 -0.4684677883 0.0393977126
		C 6.0 -5.6889627326 0.3340897881 -0.5084313772
		O 8.0 0.9248703582 3.0736652417 -0.5012136265
		H 1.0 1.9083730765 3.2373090173 -0.6573187969
		C 6.0 -0.4327199935 1.1871723144 -0.0572345067
		C 6.0 -1.9791663339 -0.8386457912 0.1607855788
		C 6.0 -3.1229246388 0.1479727525 -0.2672647430
		C 6.0 0.8321011465 1.7253077944 -0.3097468666
		C 6.0 -0.6033183356 -0.2075904192 0.0330542401

		O	8.0	3.4086615507	2.7596617653	-0.7993845797
		H	1.0	1.2778218991	-2.7636458729	0.0020700969
		H	1.0	-4.5210790208	-1.4741709579	-0.3979094593
		C	6.0	1.9776645936	0.8972025442	-0.3977722390
		C	6.0	0.5164354997	-1.0494569720	-0.0369026843
		C	6.0	3.2740442913	1.4705717377	-0.6462626322
		C	6.0	1.8169359700	-0.5146291412	-0.2448716941
		O	8.0	0.3394671070	-2.3802353454	0.0916706406
		O	8.0	-1.8220886798	2.7793521454	-1.2637455842
		H	1.0	-5.5549835645	0.5152447109	-1.5773354404
		H	1.0	-2.0307921348	-1.6930117961	-0.5184596347
		H	1.0	4.9930614899	2.8555758240	-1.0276004434
		O	8.0	2.8110161141	-2.6733310689	-0.1957398167
		H	1.0	-0.9564657930	3.1481547771	-1.5075673681
		C	6.0	2.9524744582	-1.4084832637	-0.3241357866
		C	6.0	4.4138677111	0.5915877744	-0.7195762462
		H	1.0	-2.5527586574	1.1185580527	-1.8720859705
		O	8.0	-3.0575422574	0.3061436609	-1.6852833532
		O	8.0	5.9067653467	2.4516788163	-1.1139241416
		C	6.0	4.2662576641	-0.8208845356	-0.5608818021
		C	6.0	5.7206491679	1.1255141233	-0.9562150315
		C	6.0	5.3978438080	-1.6564679479	-0.6378473946
		H	1.0	5.2488931344	-2.7230233829	-0.5139030601
		C	6.0	6.8202751015	0.2734634075	-1.0258000768
		C	6.0	6.6511382248	-1.1119541527	-0.8658550514
		H	1.0	7.7982759531	0.7090922468	-1.2055980803
		H	1.0	7.5216965220	-1.7615983239	-0.9236447805
Menogaril	71628-96-1	H	1.0	7.4598779898	0.6023520980	-0.4179872041
		H	1.0	6.6351098929	2.1510605594	-0.1781070352
		H	1.0	4.3154677539	4.8240583789	2.7218577179
		H	1.0	5.3444299661	2.8634793014	1.6171391456
		C	6.0	6.4792214932	1.0882313636	-0.3524391736
		H	1.0	3.6411658800	5.1874209974	1.1228749959
		H	1.0	6.7495327193	-1.3495303196	0.4373550154
		C	6.0	3.4479181007	4.6821509974	2.0701387750
		O	8.0	4.5350525017	3.1569535448	-0.2126109532
		N	7.0	5.7408583555	0.4578294713	0.7415564803
		H	1.0	5.9859249319	0.9838656009	-1.3371584656
		C	6.0	4.4356852340	2.5656723619	1.0810168464
		H	1.0	2.5723576451	5.1271571324	2.5491311742
		C	6.0	5.7166861721	-0.9884294163	0.5045799929
		H	1.0	4.7518222647	0.2711614202	2.9878966819
		H	1.0	3.7048124789	2.9583108107	-0.6747272806

C	6.0	3.2283952897	3.1876263804	1.8497925273
C	6.0	4.3920509031	1.0128061731	1.0185312756
H	1.0	5.2043743008	-1.5122122495	1.3082832450
O	8.0	3.2176775569	2.6093248266	3.1706520207
H	1.0	5.2035291096	-1.2553559397	-0.4400068066
C	6.0	3.8638209470	0.3790097959	2.3518915222
H	1.0	1.9513272754	4.5341040579	-0.2798339217
H	1.0	3.6790348067	0.7375543782	0.2181365755
C	6.0	2.8655659483	1.2521300401	3.1374774727
H	1.0	2.8289480527	0.9118300014	4.1749308984
C	6.0	1.9363059621	2.8558541865	1.1117205741
C	6.0	1.4804697128	3.5985456132	0.0006878179
O	8.0	3.3054714948	-0.9103820727	2.1979681932
O	8.0	1.5559153145	1.0502160643	2.6443446945
H	1.0	2.3452569858	-0.8411423363	1.9882578318
C	6.0	1.2610185774	1.6897377793	1.4629935317
C	6.0	0.3614556394	3.1914473443	-0.7210928759
O	8.0	-0.0907275052	3.9807052664	-1.7166493166
C	6.0	0.2417030793	1.1402603296	0.6501188649
H	1.0	-0.8711661092	3.4866316493	-2.1066292056
C	6.0	-0.2644570640	1.9398620831	-0.4264012093
O	8.0	0.4250683979	-1.0865928617	1.5229143386
C	6.0	-0.1920615231	-0.2511294882	0.8131069064
C	6.0	-1.3772250282	1.4885906997	-1.2200909808
O	8.0	-1.8627316557	2.2343709458	-2.1745828005
C	6.0	-1.3748403553	-0.6612211881	0.0418664896
C	6.0	-1.9476438458	0.1955124208	-0.9382076491
H	1.0	-3.0512589989	1.3419820646	-2.6490553012
H	1.0	-1.4216349718	-2.5854773774	0.9614739295
C	6.0	-1.9152538496	-1.9415062804	0.2407272996
C	6.0	-3.0863264779	-0.2645755239	-1.6665389512
O	8.0	-3.6341628432	0.5168811070	-2.6216138882
C	6.0	-3.0270990075	-2.3808132267	-0.4669066435
C	6.0	-3.6471416694	-1.5250244516	-1.4114746168
H	1.0	-5.5824430220	0.2569155515	-0.6017804580
H	1.0	-2.6938316467	-4.4614202713	-0.7311481643
H	1.0	-3.5276458604	-4.0806722952	0.7659062366
C	6.0	-3.4778269154	-3.8227772171	-0.2978362826
H	1.0	-4.9062345289	-1.4825319380	-3.1431538847
C	6.0	-4.8921838153	-1.9554339967	-2.1533017386
C	6.0	-6.3237628657	-0.1762434710	-1.2833440744
H	1.0	-6.2724069799	0.3675767481	-2.2339896559
O	8.0	-6.1256759408	-1.5682211801	-1.4740055723
H	1.0	-4.1967376607	-3.8124624929	-2.9720098898

		H	1.0	-7.3210928040	-0.0642918236	-0.8478868214
		C	6.0	-4.8328055358	-4.2031348467	-0.9343005209
		C	6.0	-4.9857959909	-3.4777310356	-2.2875851796
		O	8.0	-5.9117263147	-3.8654802919	-0.0565227689
		H	1.0	-6.1391937809	-2.9368052710	-0.2418827884
		H	1.0	-4.1362530893	-6.0955519445	-1.7824099908
		H	1.0	-4.8210025392	-6.2192652170	-0.1472655203
		C	6.0	-4.9214106807	-5.7211728798	-1.1172993183
		H	1.0	-5.9519322390	-3.7395684510	-2.7337420378
		H	1.0	-5.8972235096	-5.9889427795	-1.5341904014
		H	1.0	-1.6755893210	-1.2335150052	-4.6571956844
		O	8.0	-0.7078652215	-1.2512157815	-4.3405062849
		O	8.0	-3.1862040126	-0.9573261527	-4.5127698946
		H	1.0	-5.5386010933	-0.6119987362	-4.4985598968
		H	1.0	1.3145849942	1.4455080051	-4.3382834449
		H	1.0	1.6442077170	-0.9208021180	-4.0712522247
		H	1.0	2.9056612184	0.9998004057	-4.9647756388
		C	6.0	2.3918536303	1.6613741919	-4.2532065460
		C	6.0	-5.6463799850	-0.1770575960	-3.5116871959
		H	1.0	-7.7692871145	0.1022945542	-3.6082590312
		H	1.0	1.9543853775	-2.0701680059	-2.7921748239
		C	6.0	-3.2173760378	-0.4639767937	-3.3290053909
		C	6.0	1.7174205525	-1.0145066227	-2.9850104774
		C	6.0	-0.7693581552	-0.7361467440	-3.0909635572
		O	8.0	4.0867485159	-0.6916304216	-3.0305114403
		O	8.0	2.6797029539	3.0098156829	-4.5280507976
		C	6.0	-6.8662383453	0.2186353285	-3.0136791573
		H	1.0	4.8235850260	-0.2838750404	-2.5523983037
		C	6.0	-4.4737317541	-0.0254484679	-2.7379882733
		C	6.0	-2.0151018270	-0.3239485674	-2.5440217492
		C	6.0	2.8742906211	-0.1925298258	-2.4254781888
		C	6.0	0.4084825286	-0.6084699358	-2.3465351889
		C	6.0	2.8353042393	1.2892091521	-2.8460145470
		H	1.0	2.9534487790	3.3767504699	-3.6677778619
		O	8.0	3.2575137983	2.1735496001	-2.1125904349
		C	6.0	-6.9603077149	0.7805694061	-1.7245586816
		C	6.0	-4.5318785925	0.5430938567	-1.4235525693
		H	1.0	3.0528463175	-1.4246810955	-0.7107677119
		C	6.0	-2.0604774187	0.2394128120	-1.2374416638
		C	6.0	2.9119946328	-0.3570161103	-0.9083464872
		C	6.0	0.3701754275	-0.0720182483	-1.0382181663
		H	1.0	-7.9301957995	1.0853525648	-1.3517707980
		C	6.0	-5.8227258070	0.9421742577	-0.9403813886
4'-O-methyldoxorubicin	77121-90-5					

		H	1.0	3.7637986573	0.1830945239	-0.4811547540
		C	6.0	-3.3081827466	0.6959648078	-0.6416527325
		C	6.0	-0.8502609807	0.3668793150	-0.4978189920
		C	6.0	1.6229134400	0.0950217798	-0.2006820406
		H	1.0	1.7184682247	1.1498521185	0.0822661561
		O	8.0	-5.8817777593	1.4810292015	0.3131289564
		O	8.0	-3.2959119682	1.2101986105	0.5299872688
		O	8.0	1.5100028736	-0.6801341191	1.0215053353
		H	1.0	-7.5943421893	2.6735041772	0.2024876217
		O	8.0	-0.8662359007	0.9237698492	0.7303539427
		H	1.0	-7.8420136535	1.0467835455	0.8932091155
		H	1.0	1.1234646781	1.0232805299	2.1031411163
		C	6.0	-7.1348348016	1.8853853483	0.8163802311
		H	1.0	-1.8645330806	1.1499700519	0.8720128331
		C	6.0	1.5823154309	0.0394646290	2.2220377386
		H	1.0	-0.1245714411	-1.0388466503	2.9179787855
		H	1.0	-6.9406001122	2.2803825339	1.8159154768
		C	6.0	0.8655025415	-0.7744856121	3.3017919465
		H	1.0	3.7027130526	-1.4893372999	1.9475958890
		O	8.0	2.9397358827	0.3136180441	2.6019710803
		H	1.0	1.6662163333	-2.6826349279	2.7922511894
		H	1.0	0.7174116015	-0.1356482268	4.1778133232
		C	6.0	3.7239130006	-0.8628052326	2.8514962789
		C	6.0	1.6546525798	-2.0423602154	3.6842232834
		H	1.0	5.5095727696	0.1873718044	2.2591478424
		H	1.0	0.0876710564	-2.8925802970	4.6862263804
		N	7.0	1.0990109587	-2.8353029995	4.7853199907
		C	6.0	5.1561607458	-0.4111965745	3.1031688667
		C	6.0	3.1369922951	-1.7312458789	3.9810827385
		H	1.0	3.6754276513	-2.6864631240	3.9754308953
		H	1.0	5.8127049109	-1.2799778540	3.2168751999
		H	1.0	1.8900308494	0.0258827475	6.0234341188
		H	1.0	3.0503715330	0.7828896586	4.9070154444
		H	1.0	1.2864432623	-2.3531650180	5.6616176704
		H	1.0	5.2326056374	0.1906305669	4.0116536854
		C	6.0	2.9408749126	0.0393459548	5.6999936822
		O	8.0	3.3958549336	-1.2522084370	5.3095498380
		H	1.0	3.5527040874	0.3318441497	6.5600041304
Morpholino adriamycin	89196-04-3	H	1.0	-4.0120526910	4.2520919112	4.8486899958
		H	1.0	-5.4737236594	4.2122017823	3.8255808927
		C	6.0	-4.3746352783	4.1855222960	3.8129047379
		H	1.0	-4.0036700621	5.0440562701	3.2492274723
		H	1.0	-5.3720709759	2.5138861720	5.2962299626

O	8.0	-3.8776438592	3.0453796409	3.1480007084
C	6.0	-4.9783356439	1.6497842206	4.7757719106
C	6.0	-4.1878317551	1.8116906766	3.6430138521
H	1.0	-5.8964753661	0.2588719160	6.1484559156
C	6.0	-5.2765592841	0.3606809860	5.2609651177
O	8.0	-2.5161903019	1.9171032269	1.2243670558
C	6.0	-3.6611964801	0.6743022881	2.9439048183
C	6.0	-2.8342388196	0.7879572786	1.7503205465
H	1.0	-1.7465110402	1.5022688426	0.0769396070
C	6.0	-4.7875578230	-0.7542300302	4.6193761584
C	6.0	-3.9822635228	-0.6218788599	3.4666076073
O	8.0	-1.2307468466	0.8464379546	-0.5496003304
H	1.0	-4.9969243518	-1.7589585643	4.9676733149
H	1.0	5.9018205985	-0.3076339452	-0.8337111204
C	6.0	-2.3538770864	-0.4392978694	1.1386882794
C	6.0	-1.5333753814	-0.3582858844	-0.0190102560
C	6.0	-3.4975413399	-1.8468902933	2.8418905534
H	1.0	5.4840311117	-0.6753870341	0.8490331133
O	8.0	4.6098237079	1.9055426837	-1.1591662596
H	1.0	4.5159532890	1.3996295010	-1.9811817685
H	1.0	-0.4296303341	-0.5260438299	-2.4054673596
C	6.0	5.1750670866	-0.8121123252	-0.1921109683
C	6.0	-2.6689573325	-1.7237169692	1.6664634032
H	1.0	1.9331431216	-0.4902256254	-3.1237906820
H	1.0	5.1784970798	-1.8811180081	-0.4202935247
O	8.0	-3.7982483735	-2.9931423808	3.3273839233
C	6.0	-1.0318826388	-1.5221325587	-0.6188638554
C	6.0	-0.1043394832	-1.3717392706	-1.7906787037
C	6.0	-2.1687840090	-2.8937778042	1.0308530796
H	1.0	-0.9480282986	-2.7923908886	-3.1805985835
C	6.0	3.6994231171	1.2896322559	-0.2373257041
C	6.0	2.0574971306	-0.2224205406	-2.0651328833
C	6.0	3.7835023324	-0.2367300608	-0.3996785139
H	1.0	2.2719794046	1.8428737906	-2.6200958597
H	1.0	4.0267028145	1.5918410105	0.7629659454
H	1.0	0.9077935959	4.2365854931	1.3173915536
C	6.0	-1.3499452763	-2.7957386343	-0.1009613573
H	1.0	1.9237171218	5.7056807056	-2.3404527196
H	1.0	-3.0563512230	-3.9265634327	2.3205590855
O	8.0	1.2261280941	-1.0461380844	-1.2542987717
O	8.0	3.4011014888	-0.5512148440	-1.7640045539
C	6.0	-0.0059742289	-2.6399291761	-2.6440684117
O	8.0	-2.4793077341	-4.1186847695	1.5086222923
O	8.0	0.3498576296	5.2298175090	-1.1548547126

		C	6.0	1.7599438006	1.2685051634	-1.8381047268
		N	7.0	2.0092236596	3.1259161077	-0.0693156796
		H	1.0	0.7862197590	-2.5276718073	-3.3946616886
		H	1.0	-1.7277453170	-4.5392754832	-1.2911813803
		H	1.0	3.0764003756	-0.7167499244	0.2863026154
		C	6.0	2.2288073369	1.7301752591	-0.4356974912
		C	6.0	0.7214420089	3.4955723707	0.5239840141
		C	6.0	1.5169344386	4.8118341041	-1.8520534905
		H	1.0	-1.1358928424	4.5109040573	0.0396615942
		C	6.0	-0.8854872441	-4.0739291930	-0.7624831939
		C	6.0	-0.2533600148	4.1227605936	-0.4767215981
		H	1.0	2.8890451605	5.0123820967	-0.2254009413
		C	6.0	2.5506963454	4.2052228133	-0.8948766442
		H	1.0	0.6859203972	1.4356562332	-1.9386547374
		C	6.0	0.2707658233	-3.8837475713	-1.7678772074
		H	1.0	1.2450964063	4.0857075638	-2.6376417644
		H	1.0	0.2513710996	2.6240372831	0.9852135609
		H	1.0	1.6468502576	1.1479945818	0.2867596081
		O	8.0	-0.6028856127	-5.5081463659	-3.3279831621
		H	1.0	-0.5694150915	-4.7922344611	0.0006184848
		H	1.0	1.7080989872	-2.8283707880	-0.9806355651
		H	1.0	-0.5874470648	3.3730983617	-1.2097670321
		C	6.0	0.3563760581	-5.1032134809	-2.6850854463
		O	8.0	1.5308017403	-3.7773005205	-1.1114652481
		H	1.0	3.4260843507	3.8442108402	-1.4371880026
		C	6.0	1.6867779797	-5.8263686991	-2.8235885974
		H	1.0	0.6476001340	-6.8745394709	-4.0139417969
		H	1.0	2.4502670423	-5.0936092557	-3.1230837379
		O	8.0	1.5850790665	-6.8827766022	-3.7444748046
		H	1.0	1.9898692072	-6.1747150177	-1.8244895535
MX2	NCI 619003	H	1.0	-2.8175053836	3.0967007919	-4.6363037685
		H	1.0	-3.8750516140	1.7207762399	-5.0191686619
		H	1.0	-1.5673356438	0.8972964969	-4.6663311010
		C	6.0	-3.2534834388	2.1757922833	-4.2401755603
		H	1.0	-0.0615070746	2.8228912294	-3.9621346556
		O	8.0	0.7515995001	0.8082854932	-3.8479140014
		O	8.0	-0.6746084304	3.0671636546	-3.2495472013
		C	6.0	-2.1524795011	1.2094826204	-3.7939842140
		H	1.0	0.8428072451	-0.1342498811	-4.0847341288
		H	1.0	-3.9187268065	2.4555974901	-3.4151244798
		H	1.0	0.6888016618	-2.8528668244	-3.8038416456
		H	1.0	-2.5961298011	0.2989334514	-3.3747474726
		O	8.0	0.6396137581	-1.8267215905	-3.6494581594

C	6.0	-1.1629987699	1.8063458869	-2.7655330474
C	6.0	0.0745461165	0.8764681889	-2.5982763231
O	8.0	0.4369615699	-4.2656536999	-3.4991780013
H	1.0	0.7359011326	1.3953447015	-1.8897251128
C	6.0	-0.0780574566	-1.6975245118	-2.5016658152
H	1.0	0.1235324415	-6.6843739003	-3.1678472642
C	6.0	-0.3548391886	-0.4357918858	-1.9760350244
C	6.0	-0.2461973110	-4.1633529685	-2.4159608103
H	1.0	-2.9137721723	2.0016447863	-1.4856000952
C	6.0	-1.8249116155	2.0520311778	-1.3877156417
C	6.0	-0.5498384278	-2.8706385302	-1.8467129104
C	6.0	-0.4566262558	-6.6255618792	-2.2542561545
H	1.0	-1.5751996910	3.0653124687	-1.0622065827
C	6.0	-0.7359532180	-5.3487888439	-1.7291044727
H	1.0	-0.7019440930	-8.7432552614	-2.0140170766
C	6.0	-1.1226414498	-0.3172510362	-0.7903480806
C	6.0	-0.9198671167	-7.7591517831	-1.6053787603
C	6.0	-1.3156050198	-2.7514174063	-0.6471620243
C	6.0	-1.4085137755	1.0735047552	-0.2717454894
H	1.0	5.7250565539	2.5315345778	0.2761821201
C	6.0	-1.4970871800	-5.2233057133	-0.5277574386
C	6.0	-1.5934882809	-1.4529488946	-0.1272748728
H	1.0	3.5074875728	3.7857150378	0.3732483025
C	6.0	-1.7986539968	-3.9260339201	0.0308543349
C	6.0	-1.6697385254	-7.6611740119	-0.4233240391
O	8.0	-0.2125990714	1.6404978282	0.3569469735
H	1.0	4.3599239222	1.4646849422	0.6824104981
H	1.0	-2.1894842445	1.0313917679	0.4905787322
C	6.0	-1.9618327562	-6.4109523485	0.1198762933
H	1.0	-2.0363964991	-8.5435870697	0.0915557188
O	8.0	-2.3101699794	-1.3070091739	1.0124205256
C	6.0	4.9632087638	2.3177826170	1.0339292892
H	1.0	1.5460378192	3.4367123117	1.1549665837
C	6.0	4.0773596340	3.5457326023	1.2772028991
O	8.0	-2.4946249875	-3.8219826082	1.1254131464
H	1.0	-2.5374111428	-2.2436894241	1.2969122444
H	1.0	-0.7455398217	3.6990174374	1.5833136731
H	1.0	4.7461391162	4.3968943144	1.4826105485
O	8.0	-2.6833693264	-6.3449282640	1.2555049080
H	1.0	-2.7690850423	-5.3661984369	1.4544309968
H	1.0	2.1034071813	1.0146543594	1.2097150749
O	8.0	5.6669681169	1.9627022100	2.2218268279
C	6.0	0.0176438587	1.2118019423	1.6712046900
C	6.0	1.7872630728	2.9839954178	2.1238580284

		C 6.0 1.4952280848 1.4688562901 1.9959410523 C 6.0 -0.6522051352 3.3204851501 2.6085391649 H 1.0 0.9632023183 4.6677084979 3.2080750595 N 7.0 3.1637398377 3.3958573074 2.4074736389 H 1.0 -0.2480575773 0.1572589419 1.7942655199 H 1.0 -2.7281550971 3.5933754397 3.1201799224 C 6.0 0.7729886248 3.5921648843 3.1238393845 O 8.0 -0.8417137742 1.8922355687 2.6032602677 H 1.0 -1.7044467110 5.0105563510 3.4455266106 H 1.0 4.1517967704 0.7892810747 3.0215964578 C 6.0 -1.7477840139 3.9168871366 3.4793850189 C 6.0 4.7571002383 1.6725274044 3.2822490854 H 1.0 1.7370569884 0.9615745819 2.9365611692 C 6.0 3.8580840319 2.8765918819 3.5882023242 H 1.0 4.5019551505 3.6776650928 3.9841327314 H 1.0 5.3729469623 1.4193798332 4.1524922701 H 1.0 -1.6318272567 3.6019431932 4.5194977011 O 8.0 0.8973989703 3.0538104843 4.4461499284 H 1.0 3.1236791807 2.6346829598 4.3577617427 H 1.0 0.3957008064 2.2228566686 4.4242015147
NSC 286628	NSC 286628 / 67903-59-7	H 1.0 -0.7766465836 -1.7356223512 -6.4479628919 H 1.0 -3.0862655898 -2.1378662528 -7.0561646145 H 1.0 -5.4585098384 -2.3810726051 -6.3833704276 H 1.0 -0.9056820657 -0.0388004741 -5.9997551008 C 6.0 -3.4035502154 -1.8155431800 -6.0662384671 C 6.0 -4.7402512450 -1.9541201433 -5.6880338810 H 1.0 -0.0817499090 -3.5093521994 -5.7483068995 C 6.0 -1.0283470123 -1.0596189380 -5.6185961521 C 6.0 -2.4660421827 -1.2721209564 -5.1821567563 C 6.0 -5.1470880179 -1.5581341547 -4.4133707411 H 1.0 -6.1850118974 -1.6723107994 -4.1119035308 C 6.0 -2.8772656771 -0.8744148800 -3.9029795594 C 6.0 -4.2116834170 -1.0228873332 -3.5243194184 H 1.0 -2.1391352885 -0.4648908136 -3.2165921220 H 1.0 0.6246206049 -5.6379259571 -4.7079059759 H 1.0 -4.5217356962 -0.7202480614 -2.5278159349 C 6.0 0.1998879768 -3.5205920530 -4.7017567388 O 8.0 -0.0981403740 -1.1341989883 -4.5524641021 C 6.0 0.6154843985 -4.7290960494 -4.1112227154 C 6.0 0.1825502642 -2.3446035447 -3.9640863592 C 6.0 1.0257019858 -4.7511853533 -2.7964941508 C 6.0 0.5372144730 -2.3370861082 -2.5768891227 H 1.0 1.3735370683 -5.6583144752 -2.3158446826

O	8.0	-0.0727642086	-0.0463523413	-2.1488998664
C	6.0	0.9980459164	-3.5748559711	-2.0170561490
C	6.0	0.4234821091	-1.1539033488	-1.7285591802
H	1.0	0.0921305824	0.8211734256	-0.9645195476
C	6.0	1.4478781117	-3.6686496987	-0.6359760411
O	8.0	1.8948252751	-4.7748267347	-0.1664399356
C	6.0	0.8702333856	-1.2588543692	-0.3485573906
H	1.0	0.3728482374	5.4833025457	-0.2495801537
O	8.0	0.3424254739	1.0551081896	0.0067647485
C	6.0	1.3786282101	-2.4805670120	0.1798927127
H	1.0	-2.0063126298	4.2651301206	0.0344639574
C	6.0	0.8026102181	-0.1139431023	0.4989796366
N	7.0	0.4401508189	5.4307886362	0.7657213532
H	1.0	0.2020754330	3.3557973526	0.6078693176
H	1.0	-0.1376333958	6.1947342463	1.1183621052
C	6.0	-0.1824531859	4.1794438379	1.2178492277
H	1.0	-4.1524057871	2.7502689671	0.5899561137
H	1.0	2.2605047018	-4.3389391294	1.2654399244
C	6.0	-1.7245573983	4.1842330861	1.0921281400
C	6.0	1.8265329523	-2.5315709087	1.5268590330
H	1.0	-1.8521426784	2.0367043475	1.2060582579
C	6.0	1.2298728095	-0.1853923311	1.8368947657
O	8.0	2.3322177493	-3.6780113868	2.0364787330
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C	6.0	-2.3089517703	2.9013650035	1.6974459460
H	1.0	1.7172258525	1.8557172235	2.1646731273
C	6.0	1.7597371773	-1.3950532678	2.3417137047
H	1.0	4.6877214296	-1.3340165044	2.2135713550
C	6.0	-3.8252426140	2.8127469689	1.6328681696
H	1.0	1.2900990146	3.8041456489	2.7645026314
C	6.0	0.2063778891	3.9215592818	2.6829700145
C	6.0	1.1588442757	1.0705961664	2.6881304534
H	1.0	6.0194841403	-0.2145096387	2.6318634559
O	8.0	-0.2253957232	1.4618421191	2.7733396816
H	1.0	-4.2892799543	3.6942374238	2.0842509884
H	1.0	-4.1710942632	1.9199657075	2.1604573129
H	1.0	-2.3235505483	5.0931770538	2.6787591345
C	6.0	5.1199059115	-0.7088081246	3.0016835799
H	1.0	-0.0485562082	4.8050602137	3.2838419501
O	8.0	4.3450775289	1.5302297550	3.3250837659
C	6.0	-0.5498997937	2.7328541399	3.2989465357
O	8.0	-1.9464211798	2.8895527684	3.1022067168
C	6.0	4.1216452859	0.3364630538	3.4477834495
H	1.0	3.0742833105	-2.2598761702	3.7957511473

		C	6.0	2.3083840263	-1.4830643619	3.7474138781
		H	1.0	5.3682427803	-1.3693724037	3.8386970692
		C	6.0	1.7307248444	0.8994278848	4.1118748222
		C	6.0	2.8506682255	-0.1339210056	4.2032181997
		H	1.0	1.5329143862	-1.7810951015	4.4668597651
		H	1.0	-0.4223961639	2.7369081654	4.3927476508
		H	1.0	2.0887429134	1.8655808886	4.4845316007
		H	1.0	0.9231825820	0.5541235346	4.7662086946
		O	8.0	3.2941600753	-0.2945265384	5.5687342097
		H	1.0	3.5316643768	0.5897466230	5.8840446128
		C	6.0	5.2914247370	2.8526786991	2.1053505330
		C	6.0	4.6516431829	1.4751982195	1.8845678920
		C	6.0	5.3220138670	0.3112779711	2.6514400601
		C	6.0	4.8716114517	0.2297641082	4.1364942277
		C	6.0	3.3258709925	0.3140604478	4.2261950367
		C	6.0	2.8085315111	1.5523780351	3.4765774888
		O	8.0	3.2454341943	1.4760567760	2.1036665661
		O	8.0	1.4223484639	1.5207585848	3.4575727011
		C	6.0	0.7746206337	2.7207029310	2.9472510675
		C	6.0	0.1675687875	2.3358112789	1.5946958587
		C	6.0	-0.9224261577	3.2947432196	1.1238551734
		C	6.0	-2.0812920045	3.2301150131	2.1652281770
		C	6.0	-1.5995385117	3.4676884655	3.6032976467
		C	6.0	-0.2436301863	3.2338659113	3.9446407226
		C	6.0	0.1846886927	3.5493921293	5.2427400045
		C	6.0	-0.7265293963	4.0282052150	6.2332688297
		C	6.0	-2.0904091114	4.1993756392	5.8755287784
		C	6.0	-2.4991846390	3.9115726110	4.5639408273
		C	6.0	-3.0874444330	4.6624032019	6.8483161328
		O	8.0	-4.3166911248	4.6107830680	6.5739523365
		C	6.0	-2.5657400794	5.1139183129	8.1422147729
		C	6.0	-3.4041312452	5.7361553855	9.0941765144
		C	6.0	-3.0570747991	5.8178813727	10.4433916439
		C	6.0	-1.7645883418	5.4267269108	10.8343768888
		C	6.0	-0.8314689653	4.9982373424	9.8946061749
		C	6.0	-1.2209728578	4.8091075553	8.5320594588
		C	6.0	-0.2740119494	4.2932038587	7.5761286397
		O	8.0	0.9627540726	4.0669065346	7.9175258071
		O	8.0	0.4248566935	4.7236632220	10.3048835422
		C	6.0	-4.1461637201	6.1879063431	11.4430129407
		C	6.0	-4.9048755988	4.9266893714	11.9481224802
		C	6.0	-5.4385632306	4.1144357156	10.7508857185
		C	6.0	-6.2785186185	5.0049184822	9.8035945609
Nogalamycin	1404-15-5	C	6.0	5.2914247370	2.8526786991	2.1053505330
		C	6.0	4.6516431829	1.4751982195	1.8845678920
		C	6.0	5.3220138670	0.3112779711	2.6514400601
		C	6.0	4.8716114517	0.2297641082	4.1364942277
		C	6.0	3.3258709925	0.3140604478	4.2261950367
		C	6.0	2.8085315111	1.5523780351	3.4765774888
		O	8.0	3.2454341943	1.4760567760	2.1036665661
		O	8.0	1.4223484639	1.5207585848	3.4575727011
		C	6.0	0.7746206337	2.7207029310	2.9472510675
		C	6.0	0.1675687875	2.3358112789	1.5946958587
		C	6.0	-0.9224261577	3.2947432196	1.1238551734
		C	6.0	-2.0812920045	3.2301150131	2.1652281770
		C	6.0	-1.5995385117	3.4676884655	3.6032976467
		C	6.0	-0.2436301863	3.2338659113	3.9446407226
		C	6.0	0.1846886927	3.5493921293	5.2427400045
		C	6.0	-0.7265293963	4.0282052150	6.2332688297
		C	6.0	-2.0904091114	4.1993756392	5.8755287784
		C	6.0	-2.4991846390	3.9115726110	4.5639408273
		C	6.0	-3.0874444330	4.6624032019	6.8483161328
		O	8.0	-4.3166911248	4.6107830680	6.5739523365
		C	6.0	-2.5657400794	5.1139183129	8.1422147729
		C	6.0	-3.4041312452	5.7361553855	9.0941765144
		C	6.0	-3.0570747991	5.8178813727	10.4433916439
		C	6.0	-1.7645883418	5.4267269108	10.8343768888
		C	6.0	-0.8314689653	4.9982373424	9.8946061749
		C	6.0	-1.2209728578	4.8091075553	8.5320594588
		C	6.0	-0.2740119494	4.2932038587	7.5761286397
		O	8.0	0.9627540726	4.0669065346	7.9175258071
		O	8.0	0.4248566935	4.7236632220	10.3048835422
		C	6.0	-4.1461637201	6.1879063431	11.4430129407
		C	6.0	-4.9048755988	4.9266893714	11.9481224802
		C	6.0	-5.4385632306	4.1144357156	10.7508857185
		C	6.0	-6.2785186185	5.0049184822	9.8035945609

C	6.0	-5.6170828301	6.3902418695	9.5947366887
O	8.0	-4.5880725211	6.2768736074	8.6378469227
O	8.0	-5.1670967595	6.9850510306	10.7874559289
O	8.0	-6.5431937472	4.3988805916	8.5552682115
N	7.0	-6.0726023136	2.8753103992	11.2503184883
C	6.0	-7.4040749936	3.0357900022	11.8258846181
C	6.0	-6.0475348651	1.7743715735	10.2842524150
O	8.0	-4.0831861569	4.1149071886	12.7623164154
C	6.0	-3.6552621862	7.0358684368	12.6102695689
O	8.0	1.4867837682	3.3994482001	5.5478937486
C	6.0	-3.1711493352	4.2270449733	1.8070771621
O	8.0	-2.9849140785	5.3530158160	1.3713386337
O	8.0	-4.4058862405	3.7296825451	2.0095471631
C	6.0	-5.4907750736	4.6491831860	1.7930085463
C	6.0	-1.4231484047	2.9004006123	-0.2768257101
O	8.0	-0.3346487202	4.5928027594	1.0743249887
O	8.0	2.9954560504	0.3025072706	5.5993947308
C	6.0	1.6913572304	-0.1626820479	5.9160605960
C	6.0	5.3613615582	-1.0576701172	4.8069666600
O	8.0	5.3495836006	1.4129830329	4.8037132058
C	6.0	6.6814859932	1.4329305908	5.2711783320
O	8.0	5.0023729628	-0.9419297653	2.0408399221
C	6.0	5.8039961552	-1.2777173133	0.9317052192
H	1.0	4.7460822099	1.2403609311	0.8168796926
H	1.0	6.4160852430	0.4489478492	2.6329099356
H	1.0	2.9101443446	-0.5644026280	3.7083423237
H	1.0	3.1723097211	2.4704865973	3.9506689366
H	1.0	1.5443318967	3.4857208282	2.8008293283
H	1.0	-2.5307674037	2.2311540337	2.0987273027
H	1.0	-5.7521447096	5.3232941093	12.5358864859
H	1.0	-4.5614950597	3.7754987166	10.1928778881
H	1.0	-7.2525072395	5.1948283676	10.2741256381
H	1.0	6.3427513138	2.8396125978	1.7934954705
H	1.0	4.7647123087	3.5935908141	1.4969185009
H	1.0	5.2507562843	3.1588451515	3.1505878282
H	1.0	0.9698218333	2.2805152808	0.8536139626
H	1.0	-0.2549968400	1.3290333056	1.6899997655
H	1.0	-3.5493640357	4.0537667556	4.3394887260
H	1.0	-1.4595185869	5.4624883919	11.8731575215
H	1.0	0.9062884230	4.4179893627	9.4812911098
H	1.0	-6.3421000332	7.0807863091	9.1560479350
H	1.0	-5.7636093896	4.5245809331	7.9640063484
H	1.0	-8.1902568968	3.2313902419	11.0765917248
H	1.0	-7.6760209604	2.1174867154	12.3589962020

		H	1.0	-7.4117516016	3.8546526885	12.5508595574
		H	1.0	-5.0267581976	1.6317597947	9.9189998232
		H	1.0	-6.3617936991	0.8507604589	10.7858541904
		H	1.0	-6.6976227604	1.9500941407	9.4157470592
		H	1.0	-4.4580464712	3.2226830819	12.6447546791
		H	1.0	-3.1330899455	7.9221666395	12.2413429963
		H	1.0	-4.5117215409	7.3549044793	13.2124105331
		H	1.0	-2.9822180218	6.4577671615	13.2456650820
		H	1.0	1.5615011841	3.6218698034	6.5276559692
		H	1.0	-6.3979000357	4.0849691628	2.0073157586
		H	1.0	-5.4048634195	5.5028617149	2.4687652595
		H	1.0	-5.4911351700	5.0073773782	0.7605315653
		H	1.0	-1.8448479481	1.8889600606	-0.2899716883
		H	1.0	-2.1881693353	3.5994690834	-0.6302253172
		H	1.0	-0.5863997812	2.9365537946	-0.9804023539
		H	1.0	-1.0736859402	5.2260234534	1.0692554678
		H	1.0	1.6365614230	-0.1972287740	7.0073018196
		H	1.0	0.9161402077	0.5016501606	5.5304654315
		H	1.0	1.5234653626	-1.1774234829	5.5189963906
		H	1.0	6.4452763186	-1.1778403626	4.7119645226
		H	1.0	5.0869344540	-1.0409967573	5.8630274859
		H	1.0	4.8916779621	-1.9187239088	4.3299459672
		H	1.0	6.8566974986	2.4472180552	5.6390262237
		H	1.0	6.8467831698	0.7318186337	6.0993616280
		H	1.0	7.4221793379	1.2200881529	4.4845726525
		H	1.0	5.4809579887	-2.2644006173	0.5891958781
		H	1.0	5.6956232862	-0.5709953567	0.0953948436
		H	1.0	6.8721395912	-1.3273224002	1.2002367999
		H	1.0	2.6523760733	1.3257437971	-1.6935225064
		H	1.0	2.0203545802	1.8774922567	1.8130695907
		O	8.0	3.8655472282	2.0946294734	0.2287448911
		O	8.0	1.0859747065	3.6636004707	-3.8099942583
		H	1.0	0.4552366562	4.0255129432	-4.5249776574
		C	6.0	2.2676824209	2.3416014855	-1.5604014763
		H	1.0	-2.9039161457	4.6924583057	-6.4019417820
		H	1.0	3.2119875119	-1.7617615738	-0.5178666545
		H	1.0	2.8064187677	2.9875609077	-2.2571674713
		H	1.0	-5.3570289473	4.6683762942	-6.9150154730
		H	1.0	4.3772803742	2.7897112963	0.6794522887
		C	6.0	0.2616898764	2.9999130962	-2.9634125715
		C	6.0	1.5115510438	2.2223309067	0.9083626118
		O	8.0	-0.9090211362	4.2388041962	-5.1967530463
		C	6.0	-3.6177639777	4.1971646373	-5.7540823497
Pirarubicin	72496-41-4	H	1.0	2.6523760733	1.3257437971	-1.6935225064
		H	1.0	2.0203545802	1.8774922567	1.8130695907
		O	8.0	3.8655472282	2.0946294734	0.2287448911
		O	8.0	1.0859747065	3.6636004707	-3.8099942583
		H	1.0	0.4552366562	4.0255129432	-4.5249776574
		C	6.0	2.2676824209	2.3416014855	-1.5604014763
		H	1.0	-2.9039161457	4.6924583057	-6.4019417820
		H	1.0	3.2119875119	-1.7617615738	-0.5178666545
		H	1.0	2.8064187677	2.9875609077	-2.2571674713
		H	1.0	-5.3570289473	4.6683762942	-6.9150154730
		H	1.0	4.3772803742	2.7897112963	0.6794522887
		C	6.0	0.2616898764	2.9999130962	-2.9634125715
		C	6.0	1.5115510438	2.2223309067	0.9083626118
		O	8.0	-0.9090211362	4.2388041962	-5.1967530463
		C	6.0	-3.6177639777	4.1971646373	-5.7540823497

C	6.0	0.7875174329	2.3661612838	-1.8384624621
H	1.0	3.0816722553	-4.5942984249	0.5913107239
C	6.0	2.6169070392	2.7044047489	-0.0892034706
C	6.0	-4.9661146937	4.1776707496	-6.0267019584
H	1.0	0.8621433039	3.0500544100	1.2135543546
C	6.0	-1.6746323140	3.6194777825	-4.3731262549
C	6.0	-1.1427754143	2.9635601292	-3.2036121960
C	6.0	-3.1118545262	3.5596968402	-4.5987911585
O	8.0	1.2590505531	-0.0745454291	-0.0417539248
C	6.0	-0.0654804781	1.7115326308	-0.9229020050
C	6.0	2.5818367482	-1.9877368118	0.3496923243
H	1.0	1.7292322376	-2.5852797737	0.0088829909
C	6.0	-5.8584555202	3.5212760806	-5.1557002599
C	6.0	0.5685417370	1.1536636825	0.3238572730
H	1.0	-6.9157573657	3.5158021778	-5.3895936228
C	6.0	-2.0063213928	2.2904347912	-2.2907070352
C	6.0	-3.9896767943	2.8840015792	-3.6908004986
H	1.0	-7.8287229225	1.7250331841	-4.3895308246
N	7.0	3.8785256508	-4.0764269655	0.9595716537
C	6.0	-1.4478827310	1.6683995786	-1.1312697360
C	6.0	-5.3880263205	2.8864143672	-4.0102847902
H	1.0	2.8567049706	-0.0386404577	1.2643202796
C	6.0	2.0285240681	-0.6917573848	0.9337823211
C	6.0	-3.4469735228	2.2362358207	-2.4966991552
H	1.0	4.2615615212	-2.1707285100	1.6892050899
C	6.0	3.3813536770	-2.7664445700	1.4078678290
C	6.0	2.7908657181	4.2167950627	0.0650642430
H	1.0	4.5007311464	-3.9352382657	0.1654056158
O	8.0	-6.2284384769	2.2411552481	-3.1483280281
H	1.0	0.7632189096	4.9327986122	-0.1109294411
H	1.0	-0.1991455808	0.9053950002	1.0593493927
C	6.0	-7.6080643794	2.2248260390	-3.4349988301
O	8.0	-4.1855831082	1.6372000625	-1.6444741674
O	8.0	-2.2405981736	1.0581826141	-0.2307734145
O	8.0	3.7953332882	4.6570598440	0.6207030353
H	1.0	0.7772702883	-6.2404840317	1.4610431918
H	1.0	-3.1776487994	1.1714360148	-0.6267276998
H	1.0	-8.0742477651	1.6633732374	-2.6224591965
C	6.0	1.7654845733	5.2044120386	-0.4661911478
H	1.0	2.9754259216	6.4500156340	0.3166548813
H	1.0	-8.0383835833	3.2364738473	-3.4655201221
O	8.0	1.2135253208	-0.9905414955	2.0708982556
H	1.0	2.6737675365	-5.5263413141	2.9287258988
O	8.0	2.0877876436	6.5190752457	-0.0754029407

		C	6.0	2.5526736542	-2.9425653488	2.6931889459
		O	8.0	1.5018722507	-3.8998584484	2.4564411690
		H	1.0	1.5818299074	-7.9533054949	3.0554337350
		H	1.0	1.7350759422	5.0980226569	-1.5630730494
		C	6.0	0.6060224894	-6.0919218029	2.5326240668
		H	1.0	2.8008437457	-0.9475819394	3.3987842527
		C	6.0	1.6534586335	-5.1308150465	3.0867728053
		C	6.0	1.9434450197	-1.5953531522	3.1310075503
		H	1.0	3.2000707598	-3.3127334457	3.4962786768
		H	1.0	-0.1699822810	-8.0797128102	2.9594744703
		C	6.0	0.6454885190	-7.4278091435	3.2919347399
		H	1.0	-0.3709238887	-5.6088835165	2.6465423769
		H	1.0	2.6344181549	-6.5682164528	5.0724132418
		O	8.0	1.4658823771	-4.9461892792	4.4949803358
		C	6.0	1.0040106953	-1.7045217962	4.3222989417
		H	1.0	0.1566425667	-2.3432535331	4.0685443265
		C	6.0	0.5722068753	-7.1905807632	4.8077134362
		H	1.0	0.6345619066	-0.7112901947	4.5908451215
		C	6.0	1.6205140965	-6.1567452698	5.2252351281
		H	1.0	0.7278663135	-8.1257655338	5.3601219828
		H	1.0	1.5173340402	-2.1443292162	5.1819158915
		H	1.0	-0.4206958034	-6.8103141580	5.0775544370
		H	1.0	1.5246818739	-5.8894344105	6.2819768157
		H	1.0	4.2146338889	-0.5489346461	-7.4039228016
		O	8.0	2.8543365450	1.4861623607	-6.5798517482
		C	6.0	3.6544015558	-0.7446755703	-6.4947278062
		H	1.0	2.2381768659	2.0475895715	-6.0052066677
		H	1.0	4.3043745081	-2.8008226672	-6.2913549797
		C	6.0	2.8820860134	0.2896091090	-5.9594473631
		C	6.0	3.7042918726	-1.9970065183	-5.8755392675
		O	8.0	1.2918447073	2.2915748648	-4.7827213439
		C	6.0	2.1363107316	0.0657318467	-4.7674007469
		C	6.0	2.9860354069	-2.2513230518	-4.7069669988
		C	6.0	1.3395952930	1.1460854932	-4.2196913002
		C	6.0	2.1879579300	-1.2198851141	-4.1328928017
		O	8.0	3.0662171356	-3.4811348903	-4.1445335503
		H	1.0	-5.4810035648	2.8526141561	-2.5910801896
		H	1.0	2.4838831950	-3.4350791245	-3.3365863660
		H	1.0	-0.2326519594	2.8591609681	-2.9325931476
		C	6.0	0.5883257390	0.8848179482	-2.9981101981
		C	6.0	1.4396269099	-1.4650320660	-2.9290360027
		H	1.0	-4.3599182339	2.3007136717	-3.8535510831
		C	6.0	-0.2030469356	1.8990202880	-2.4275703068
Pyrrromycin	668-17-7	H	1.0	4.2146338889	-0.5489346461	-7.4039228016
		O	8.0	2.8543365450	1.4861623607	-6.5798517482
		C	6.0	3.6544015558	-0.7446755703	-6.4947278062
		H	1.0	2.2381768659	2.0475895715	-6.0052066677
		H	1.0	4.3043745081	-2.8008226672	-6.2913549797
		C	6.0	2.8820860134	0.2896091090	-5.9594473631
		C	6.0	3.7042918726	-1.9970065183	-5.8755392675
		O	8.0	1.2918447073	2.2915748648	-4.7827213439
		C	6.0	2.1363107316	0.0657318467	-4.7674007469
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		C	6.0	1.3395952930	1.1460854932	-4.2196913002
		C	6.0	2.1879579300	-1.2198851141	-4.1328928017
		O	8.0	3.0662171356	-3.4811348903	-4.1445335503
		H	1.0	-5.4810035648	2.8526141561	-2.5910801896
		H	1.0	2.4838831950	-3.4350791245	-3.3365863660
		H	1.0	-0.2326519594	2.8591609681	-2.9325931476
		C	6.0	0.5883257390	0.8848179482	-2.9981101981
		C	6.0	1.4396269099	-1.4650320660	-2.9290360027
		H	1.0	-4.3599182339	2.3007136717	-3.8535510831
		C	6.0	-0.2030469356	1.8990202880	-2.4275703068

C	6.0	-4.7804776245	2.0616746329	-2.8735679923
C	6.0	0.6429422330	-0.3977307986	-2.3797880066
O	8.0	1.4753108140	-2.6310110187	-2.3389161116
H	1.0	-5.2854848628	1.0956199516	-2.9022987545
O	8.0	-3.1831240182	4.0740788511	-2.3048528020
C	6.0	-2.9663282125	3.0318254893	-1.7226148976
O	8.0	-3.7389913769	1.9268953367	-1.8987294283
C	6.0	-0.9258598564	1.6807851359	-1.2627855908
C	6.0	-0.1012701895	-0.6052384713	-1.1810185995
H	1.0	-1.2662692999	3.7375062245	-0.7438394099
H	1.0	0.5338128091	-2.3776606454	-1.1628250712
C	6.0	-1.8255475870	2.7986299027	-0.7377008281
C	6.0	-0.8725738968	0.4200081572	-0.6212547466
O	8.0	-0.0702441510	-1.8083266601	-0.5720628525
H	1.0	-4.3148407317	3.3453834890	0.4507253246
H	1.0	-3.5428320224	0.8901905483	0.3267992115
C	6.0	-2.2974244672	2.6067550556	0.7447299559
H	1.0	-3.1127782600	4.5899340035	0.7620354847
C	6.0	-1.5541145393	0.1660536002	0.6922282863
H	1.0	-1.9187472317	-0.8663536992	0.7173866972
C	6.0	-3.4432183445	3.5903497595	1.0693354948
C	6.0	-2.7011029190	1.1400571019	0.9798608424
H	1.0	2.2482673564	-3.4286319348	0.6059061256
O	8.0	-1.2091165670	2.9715191602	1.5948909976
H	1.0	4.0272554912	-2.8404474938	2.4992525594
H	1.0	-0.7195506605	2.1589891613	1.8131948089
O	8.0	-0.5265880924	0.2973824506	1.7369322786
H	1.0	1.7624800626	-1.3561202562	1.8359347755
H	1.0	-3.0342815591	1.0116852557	2.0154563339
C	6.0	1.7120472918	-3.9230664238	1.4359729926
H	1.0	2.0536408153	-4.9618993925	1.4927898328
H	1.0	1.5387845847	0.8035297821	2.9228421505
C	6.0	-3.8464698705	3.6298768417	2.5462450291
H	1.0	0.6521861605	-3.9373553860	1.1762514737
H	1.0	-0.5008155209	-2.3165618111	1.8120263665
C	6.0	3.3207763258	-3.4131078421	3.1326261438
H	1.0	-4.5718096943	4.4310209624	2.7251157162
H	1.0	-4.3096407640	2.6928348895	2.8738584956
H	1.0	3.6044162993	-4.4681901278	3.0604411619
C	6.0	1.4222104358	-1.8935174026	2.7407442318
N	7.0	1.9243904706	-3.2808257832	2.7336869037
C	6.0	-0.7143863292	-0.4900163752	2.9082402220
H	1.0	-2.9681187142	3.8085180512	3.1705820746
C	6.0	-0.1203252623	-1.8926983440	2.7421238331

		H	1.0	3.4499748158	-3.1077039206	4.1729324827
		H	1.0	3.0142641026	-0.9509592399	3.8895827611
		H	1.0	-1.7845782532	-0.5543959363	3.1485387011
		C	6.0	1.2972986466	0.3394574685	3.8866106789
		C	6.0	1.9266600627	-1.0622565080	3.9429322210
		O	8.0	-0.1380993342	0.2032450399	3.9943770538
		H	1.0	2.8084523543	1.4553287759	4.9473431118
		H	1.0	1.1939124633	2.1976400167	4.9730685194
		H	1.0	-0.4682530952	-2.5268863675	3.5670718610
		C	6.0	1.7358190512	1.2497552508	5.0222624695
		O	8.0	1.6613694416	-1.6777702023	5.2022350572
		H	1.0	1.5437252064	0.7764312623	5.9881996794
		H	1.0	0.7081537423	-1.5857010641	5.3449851198
Rhodomycinone	21288-60-8	H	1.0	-3.5798127508	-2.7389638094	3.3939182702
		H	1.0	-1.8748050815	-3.2338977143	3.4249145850
		C	6.0	-2.7969420880	-3.2645947574	2.8388618183
		H	1.0	-3.0926092578	-4.2973137155	2.6493432323
		O	8.0	-2.0565545199	-0.7581546991	2.6055707731
		H	1.0	-2.8886217522	1.3186386867	1.5255925900
		O	8.0	-2.5961312717	-2.6748384199	1.5506353375
		C	6.0	-2.1907857012	-1.3800130962	1.5696042178
		H	1.0	-4.6118036661	-0.5961928562	1.1234576172
		H	1.0	-1.3421857851	2.9461967049	0.7445570495
		H	1.0	-3.7201580174	2.1863656412	0.2176003004
		C	6.0	-2.9058682955	1.4916376391	0.4455560203
		H	1.0	-5.7931202017	1.3048065724	-0.0120663651
		H	1.0	-6.6275271825	-0.2115174773	-0.3598200462
		C	6.0	-1.5941815059	2.1530297855	0.0283243952
		C	6.0	-4.5050641448	-0.4684677883	0.0393977126
		C	6.0	-5.6889627326	0.3340897881	-0.5084313772
		O	8.0	0.9248703582	3.0736652417	-0.5012136265
		H	1.0	1.9083730765	3.2373090173	-0.6573187969
		C	6.0	-0.4327199935	1.1871723144	-0.0572345067
		C	6.0	-1.9791663339	-0.8386457912	0.1607855788
		C	6.0	-3.1229246388	0.1479727525	-0.2672647430
		C	6.0	0.8321011465	1.7253077944	-0.3097468666
		C	6.0	-0.6033183356	-0.2075904192	0.0330542401
		O	8.0	3.4086615507	2.7596617653	-0.7993845797
		H	1.0	1.2778218991	-2.7636458729	0.0020700969
		H	1.0	-4.5210790208	-1.4741709579	-0.3979094593
		C	6.0	1.9776645936	0.8972025442	-0.3977722390
		C	6.0	0.5164354997	-1.0494569720	-0.0369026843
		C	6.0	3.2740442913	1.4705717377	-0.6462626322

		C 6.0 1.8169359700 -0.5146291412 -0.2448716941 O 8.0 0.3394671070 -2.3802353454 0.0916706406 O 8.0 -1.8220886798 2.7793521454 -1.2637455842 H 1.0 -5.5549835645 0.5152447109 -1.5773354404 H 1.0 -2.0307921348 -1.6930117961 -0.5184596347 H 1.0 4.9930614899 2.8555758240 -1.0276004434 O 8.0 2.8110161141 -2.6733310689 -0.1957398167 H 1.0 -0.9564657930 3.1481547771 -1.5075673681 C 6.0 2.9524744582 -1.4084832637 -0.3241357866 C 6.0 4.4138677111 0.5915877744 -0.7195762462 H 1.0 -2.5527586574 1.1185580527 -1.8720859705 O 8.0 -3.0575422574 0.3061436609 -1.6852833532 O 8.0 5.9067653467 2.4516788163 -1.1139241416 C 6.0 4.2662576641 -0.8208845356 -0.5608818021 C 6.0 5.7206491679 1.1255141233 -0.9562150315 C 6.0 5.3978438080 -1.6564679479 -0.6378473946 H 1.0 5.2488931344 -2.7230233829 -0.5139030601 C 6.0 6.8202751015 0.2734634075 -1.0258000768 C 6.0 6.6511382248 -1.1119541527 -0.8658550514 H 1.0 7.7982759531 0.7090922468 -1.2055980803 H 1.0 7.5216965220 -1.7615983239 -0.9236447805
Steffimycin	11033-34-4	H 1.0 0.6997008141 -1.3898606121 -6.0189235730 H 1.0 -0.9293033649 -1.2761028831 -5.3033309123 H 1.0 -0.3931428112 2.1828641801 -5.7867557754 C 6.0 0.1486272521 -1.2075816567 -5.0914552115 H 1.0 -0.6885925492 3.7360359739 -4.9538511806 H 1.0 -1.8871013519 2.4425251428 -4.8548467421 C 6.0 -0.8140753061 2.6540898557 -4.8951632311 H 1.0 0.4058234929 -1.9778683416 -4.3573470887 O 8.0 0.5010749693 0.0971635371 -4.6619358325 H 1.0 1.8793030373 -3.3904390115 0.5963138048 H 1.0 1.6868141195 1.8608987722 -4.3157641815 C 6.0 -0.0995510298 2.1354296265 -3.6467281116 O 8.0 1.2922114988 2.4866360719 -3.6888981082 H 1.0 -1.2709452635 0.3185382871 -3.5936652089 C 6.0 -0.2112638939 0.6028742781 -3.5264293996 H 1.0 1.2243538244 -4.4953510816 1.8302849087 H 1.0 1.0523830049 -2.2613905948 -1.3119720919 C 6.0 1.0206667389 -3.5929214410 1.2475539820 H 1.0 0.8980387956 -2.7390771730 1.9254319586 O 8.0 -1.4075572698 3.7844310135 -2.4685820769 C 6.0 -0.6634196272 2.8138773097 -2.3737293064 C 6.0 -0.0242605716 -2.3355895288 -1.4627283489

H	1.0	1.3325039938	-0.4111365229	-2.4120236596
C	6.0	0.3392230712	0.0053769966	-2.2088542360
O	8.0	-0.1623813477	-3.8519432553	0.5010184568
H	1.0	-0.6953857546	-1.8453905922	0.5243569812
O	8.0	-0.1911063778	-3.3365304404	-2.4585836375
O	8.0	-0.5620415093	-1.0983767234	-1.8752835751
C	6.0	-0.7373243105	-2.7125920004	-0.1442231388
C	6.0	-0.1853088623	2.2666366063	-1.0961474727
H	1.0	-2.1655910713	-4.1136828676	1.1956661637
C	6.0	0.4163034148	0.9762773935	-1.0491418454
H	1.0	-1.0220120783	-4.2944702521	-4.7853123257
C	6.0	-1.5533572386	-3.6601829352	-2.7853781649
H	1.0	-0.9674680209	-5.5848089348	-3.5688784055
O	8.0	-2.8441313030	-3.5800602049	0.7494312567
H	1.0	-0.7105970801	4.0444450377	-0.0072072468
H	1.0	-2.0724751706	-2.7569984467	-3.1347514003
C	6.0	-2.1894782117	-3.1014237577	-0.4249857228
C	6.0	-1.5177334806	-4.6967412187	-3.8969078595
C	6.0	-0.2415015002	3.0689673259	0.0438956075
H	1.0	-2.7387137297	-2.2148673129	-0.7576392739
H	1.0	-1.7205403237	-5.0614923690	-1.1715218091
C	6.0	-2.2568472236	-4.1651251433	-1.5233827532
C	6.0	1.0428550408	0.5803798987	0.1307095682
O	8.0	1.6942000092	-0.6064253325	0.1686724284
H	1.0	-2.5365735124	-4.9922881117	-4.1592200319
C	6.0	0.3273074717	2.6534248692	1.2497417285
H	1.0	2.0617656539	-0.6690195136	1.1127695720
C	6.0	1.0023985951	1.3928025332	1.3085315253
O	8.0	-3.6128255897	-4.4737608748	-1.8230108452
H	1.0	-4.0490008115	-4.5092783809	-0.9574945812
O	8.0	-0.3297713489	4.6337036068	2.3952548391
C	6.0	0.2443947548	3.5300555563	2.4293686484
C	6.0	1.6100159321	0.9324071879	2.5226165678
O	8.0	2.2188396797	-0.2278864652	2.5729232377
C	6.0	0.8798014354	3.0311220382	3.6705135462
C	6.0	1.5375515466	1.7679077420	3.6975737200
H	1.0	0.3153309867	4.7832049589	4.7705844401
C	6.0	0.8217594169	3.8269699405	4.8182733376
H	1.0	2.6987577230	-0.2427711194	4.0983586419
C	6.0	2.1314317886	1.3429220408	4.9233401366
O	8.0	2.7689263088	0.1598546080	5.0147136916
C	6.0	1.4096606031	3.3874304154	6.0019980934
C	6.0	2.0657226497	2.1480138333	6.0617414108
O	8.0	1.3013261795	4.2363868871	7.0779897016

		H	1.0	2.5331351479	1.7770522856	6.9650282438
		C	6.0	1.8831812721	3.8382919957	8.3024356481
		H	1.0	2.9696928664	3.6999529641	8.2164268569
		H	1.0	1.4418132965	2.9079023947	8.6852784291
		H	1.0	1.6822849072	4.6451657391	9.0109252883
		H	1.0	1.9161156940	-4.4411386499	-1.1961864099
		H	1.0	0.6760941659	-3.3345729949	-1.8359798265
		H	1.0	-5.8797948113	-1.3282064418	-0.7122461332
		C	6.0	1.3370818686	-3.5379932578	-0.9849150890
		H	1.0	2.0175682418	-2.6850501516	-0.8699255876
		O	8.0	0.6043999297	-3.7953788014	0.2069662448
		C	6.0	-4.9674454927	-1.1478239487	-0.1359996486
		H	1.0	-1.1665431835	-2.1694037879	-0.9960389273
		H	1.0	-4.2192986236	-1.9048890412	-0.3928179396
		H	1.0	-5.2030120685	-1.2409939485	0.9351453496
		O	8.0	-4.5438745513	0.1684646552	-0.4511322122
		H	1.0	-3.3964438170	-5.5312950717	0.9617845264
		H	1.0	-4.2146770565	1.9536128035	-1.5802090354
		O	8.0	-2.3123300943	-3.2718434094	0.2221634143
		H	1.0	-1.0656391189	-5.0276251418	1.8964393739
		C	6.0	-1.3267192786	-2.2596871712	0.0777996552
		H	1.0	-2.2940880526	-0.3437670345	-1.2635717488
		C	6.0	-0.0223340829	-2.6499419700	0.7949712775
		H	1.0	-5.6758658388	2.2342485376	0.5149562015
		H	1.0	1.3485240258	-4.0299256270	2.1407908126
		H	1.0	0.6607616600	-1.7934664910	0.7579080410
		H	1.0	-4.6325869476	-4.2612445798	0.9980162982
		C	6.0	-3.7500054012	-4.6528781928	1.5121104232
		O	8.0	-3.5927576774	2.5770201364	-1.1741838408
		C	6.0	-3.4146322730	0.6581994321	0.2830329904
		C	6.0	-2.6556185622	-3.5980860192	1.5753668560
		C	6.0	-1.4130000766	-4.0831352150	2.3449281519
		C	6.0	-2.0922144671	0.0728638972	-0.2701322776
		O	8.0	-1.7492819034	-1.0316541451	0.6270616798
		C	6.0	-0.2812354396	-3.0448334021	2.2561348315
		H	1.0	-4.0303390633	-4.9561799425	2.5230135110
		O	8.0	0.9265664447	-3.5137108860	2.8472202338
		C	6.0	-4.7813186181	2.6911800482	0.9455824063
		H	1.0	-3.4912470716	0.3474254767	1.3344135239
		C	6.0	-3.5377809288	2.1929932047	0.2082270020
		O	8.0	0.2775554264	-0.5132222405	-1.6514129362
		H	1.0	-4.8394772333	3.7765486789	0.8543210229
		H	1.0	-4.7356746712	2.4457512070	2.0112119055
Steffimycin B	NCI 204856					

		H	1.0	-3.0343065454	-2.7000617149	2.0827738234
		H	1.0	1.2179995188	-0.5652790221	-2.0305190861
		O	8.0	-1.8359082295	-4.2988536840	3.6889394840
		C	6.0	-1.0625554432	-5.2315124117	4.4247899431
		H	1.0	-0.5912746411	-2.1557240812	2.8138788083
		C	6.0	-0.9393223620	1.0511876383	-0.3491363423
		C	6.0	0.2361614445	0.6694450589	-0.9929663260
		C	6.0	-2.2614527986	2.8628776879	0.7753976251
		O	8.0	2.6678025061	-0.1055648728	-2.2123263710
		C	6.0	-0.9870733948	2.3333211945	0.2694807638
		C	6.0	1.4070327102	1.4922622306	-0.9623213981
		H	1.0	4.1840356005	-0.0996193454	-2.7203596151
		O	8.0	-2.3522452763	3.8145246019	1.5439313369
		C	6.0	2.6155684550	1.0492641743	-1.5936512460
		C	6.0	0.1471549510	3.1440422976	0.3188959351
		O	8.0	5.0940335468	0.3144958344	-2.8052424844
		C	6.0	1.3472743944	2.7457639429	-0.2742297237
		H	1.0	0.0952561949	4.1141070193	0.7989861046
		C	6.0	3.7824150310	1.8969856921	-1.5353340182
		C	6.0	5.0015237499	1.4908764740	-2.1555577339
		C	6.0	2.5197116121	3.6328471044	-0.2019287261
		C	6.0	3.7539024838	3.1538755638	-0.8655537489
		C	6.0	6.1318106290	2.3082746171	-2.1043753349
		H	1.0	7.0301194474	1.9519081525	-2.5922646826
		O	8.0	2.4850777784	4.7297473761	0.3851815297
		C	6.0	4.8936713940	3.9621380393	-0.8220477537
		C	6.0	6.0706611964	3.5413067372	-1.4364273121
		H	1.0	4.8448283256	4.9131245793	-0.3059431369
		H	1.0	8.2518617887	3.8912085175	-3.0351759330
		O	8.0	7.1389768748	4.4017304221	-1.3416230639
		C	6.0	8.3566481294	4.0219533542	-1.9493653464
		H	1.0	8.7578456938	3.0924372696	-1.5227165393
		H	1.0	9.0597754878	4.8351341526	-1.7551381732
		H	1.0	-1.5588591136	-5.3555986778	5.3921206772
		H	1.0	-0.0364846640	-4.8834644814	4.5766930774
		H	1.0	-1.0294234382	-6.2111176529	3.9203370715
Theprubicin	95343-20-7	O	8.0	-7.7132797762	-1.7978747173	-2.9688600426
		H	1.0	-7.9219983840	-2.2683309831	-2.1412787834
		H	1.0	-6.2984912518	-0.2882247458	-2.9949257734
		H	1.0	-5.7120268138	-1.8670145023	-3.5158154449
		C	6.0	-6.3877887690	-1.3666090396	-2.8017788226
		C	6.0	-5.8822664818	-1.6808564387	-1.3992615688
		H	1.0	-5.4957892610	0.7835056257	-1.0763905190

H	1.0	-3.7520586893	-0.7439622301	-2.8588190351
O	8.0	-6.6082655120	-2.3404983641	-0.6635329093
C	6.0	-4.7275530484	0.2994542052	-0.4555032997
H	1.0	-3.3154973714	-2.3421358565	-2.2510180219
C	6.0	-3.4346370648	-1.2923283141	-1.9638115391
C	6.0	-4.5256901706	-1.1817479719	-0.8870914676
H	1.0	-5.1498924237	0.2898500066	0.5552362233
O	8.0	-4.8107395428	2.8742829939	0.4688406778
H	1.0	-1.4209036631	-0.6819358278	-2.4017705484
H	1.0	6.8345006670	-3.2870171238	0.1715076064
C	6.0	-3.4862312135	1.1630571998	-0.4967361185
H	1.0	-4.9944848261	-2.2869737230	0.6104138564
H	1.0	5.8996076091	-2.2011597516	-1.8340432818
H	1.0	-4.6465562346	3.8410674501	0.7421914393
H	1.0	-1.7090094225	-3.3354476611	-1.2813504610
C	6.0	-2.0890197341	-0.6854052212	-1.5337573637
O	8.0	-4.1563946848	-1.9996630834	0.2121769653
C	6.0	-3.6162906578	2.4746524932	-0.0246519698
O	8.0	4.5522204316	-3.6113796166	-1.3437190956
C	6.0	-2.2584313202	0.7271342621	-1.0333941500
H	1.0	5.1385876982	-5.0885475210	0.9753064673
H	1.0	-0.1694813848	-4.3794165834	0.2649149657
C	6.0	5.2413636093	-2.4088936299	-0.9847452619
O	8.0	0.0856212309	-2.6451825549	-1.8070140831
C	6.0	6.0368039313	-2.5452493962	0.3101571982
H	1.0	3.6667210084	-5.2824160671	-0.7454470558
H	1.0	2.5348318916	-2.8362114032	-2.8845001176
O	8.0	-1.4476103425	-1.4396890258	-0.4819672792
C	6.0	-0.9360274139	-2.7035793722	-0.8245252365
O	8.0	-3.7958113842	5.1220256647	0.9038199959
H	1.0	6.5160253255	-1.5875686692	0.5457477551
C	6.0	-2.5175393955	3.3726137765	-0.0736111813
H	1.0	1.5699835236	-1.4544438851	-3.4700061681
C	6.0	-0.4243846601	-3.3327534212	0.4688668911
C	6.0	3.7240935544	-4.2512060821	-0.3817246628
C	6.0	-1.1633462032	1.6041783461	-1.0977637883
C	6.0	4.3888042964	-4.2871679776	1.0146732100
C	6.0	-2.6781531260	4.7196349936	0.4183262858
H	1.0	-1.2109201924	-3.3041342070	1.2262016243
C	6.0	2.1494023894	-1.8470352636	-2.6304402710
H	1.0	4.5418161735	-1.5670305129	-0.9040461010
O	8.0	2.3639278388	-3.8686834980	-0.4114822229
H	1.0	5.6607000949	-3.1675928678	2.3651321861
C	6.0	5.1024472599	-2.9965094187	1.4370677396

		H	1.0	1.5854713463	-4.1533798434	2.0426388211
		C	6.0	-1.2756632788	2.9397914358	-0.6198288181
		C	6.0	1.2537784893	-1.9048479231	-1.4035201290
		O	8.0	-0.0023774298	1.1738234257	-1.6360006638
		H	1.0	3.6408523099	-4.5918003493	1.7502724089
		H	1.0	-2.6695000751	7.1889056544	1.2398340387
		C	6.0	1.8894078303	-2.5324661809	-0.1434383111
		H	1.0	2.9940504458	-1.1720515741	-2.4626776768
		C	6.0	-1.5313811320	5.6127474119	0.3468606861
		C	6.0	0.8204795871	-2.5992960532	0.9803749414
		H	1.0	0.9488204591	-0.8854610904	-1.1367550285
		H	1.0	4.3761110677	-2.2034064082	1.6523405672
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		N	7.0	1.2547510623	-3.2109126810	2.2389085857
		C	6.0	-1.6971760030	6.9274145715	0.8385822928
		C	6.0	-0.1243765202	3.8272099482	-0.7069833861
		C	6.0	-0.2755528616	5.1882764352	-0.2009660968
		H	1.0	2.7113335476	-1.8867128079	0.1880103404
		O	8.0	0.9671043461	3.3951434245	-1.2168174939
		H	1.0	2.0440786723	-2.6982918541	2.6278109696
		H	1.0	0.5326066900	-1.5648322898	1.1993094254
		C	6.0	-0.6542345673	7.8232774721	0.8008381512
		H	1.0	-0.7807195904	8.8347576955	1.1797389815
		C	6.0	0.7866504097	6.1530705187	-0.2222436913
		C	6.0	0.5943369168	7.4397900198	0.2695633669
		O	8.0	1.9848335707	5.7518949922	-0.7423523403
		H	1.0	1.4021327359	8.1607246491	0.2499566639
		H	1.0	2.8086171514	7.5583216945	-1.3944009590
		C	6.0	3.0471538352	6.6767183825	-0.7817412145
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		C	6.0	7.4180465837	1.3530313625	-2.6112703682
		C	6.0	6.1427998142	3.0970477668	-1.5303511432
		H	1.0	8.5086349670	-1.1850737774	-2.8407700996
		H	1.0	7.8680669809	-0.6947109976	-4.4324586748
		C	6.0	7.6447337683	-1.2612862396	-3.5168057481
		C	6.0	6.3646204449	0.4559523346	-2.4629800509
		C	6.0	5.0573453585	2.2073606991	-1.3641770423
		O	8.0	3.8068437836	3.9363634129	-0.3042227320
Valrubicin	56124-62-0	H	1.0	8.1369788006	3.3604537528	-2.2701151557
		C	6.0	7.3008110188	2.6769080710	-2.1426975378
		H	1.0	8.3392784316	1.0417975387	-3.0879474359
		H	1.0	6.0200983938	4.1073949778	-1.1578058899
		C	6.0	7.4180465837	1.3530313625	-2.6112703682
		C	6.0	6.1427998142	3.0970477668	-1.5303511432
		H	1.0	8.5086349670	-1.1850737774	-2.8407700996
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		C	6.0	7.6447337683	-1.2612862396	-3.5168057481
		C	6.0	6.3646204449	0.4559523346	-2.4629800509
		C	6.0	5.0573453585	2.2073606991	-1.3641770423
		O	8.0	3.8068437836	3.9363634129	-0.3042227320

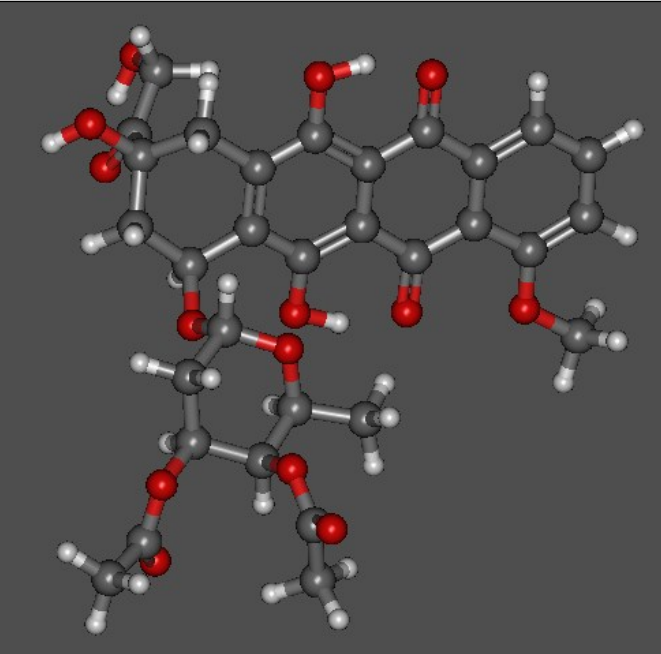
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C	6.0	3.8644545159	2.7177830569	-0.7055320904
H	1.0	2.3915695802	3.9649567519	0.2866523798
C	6.0	4.0030549151	-0.0481627291	-1.6587575232
C	6.0	2.7551035845	1.8150436474	-0.5184141991
O	8.0	1.4880013446	3.5670559706	0.5440978942
O	8.0	4.0138497926	-1.2545978997	-2.0776803046
C	6.0	2.8216253173	0.4696326870	-0.9813314326
C	6.0	1.5753573055	2.2826469940	0.1216443420
C	6.0	1.6984253356	-0.3883333504	-0.7887687046
C	6.0	0.4899293506	1.4229311530	0.3156154657
H	1.0	2.6488711517	-1.7278900852	-1.6784920563
H	1.0	-0.7982065823	3.0458168440	0.8364725581
H	1.0	-3.2486467158	7.1447641133	-0.0442946794
H	1.0	-0.7745173733	1.7777815285	2.0485716041
H	1.0	-2.7709455626	5.8952483954	1.1207182374
C	6.0	0.5479909760	0.0832414031	-0.1308794498
O	8.0	1.7220124843	-1.6512251855	-1.2480302171
C	6.0	-0.7622385852	1.9609052181	0.9642090237
C	6.0	-3.3758721122	6.0940444296	0.2285615034
H	1.0	-5.2864226411	7.6965416735	1.4454932184
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H	1.0	-4.8112793783	6.4459731164	2.5818125390
C	6.0	-2.8333433041	5.2695973673	-0.9197568201
H	1.0	-1.1361841736	3.3373843317	-1.7877620347
C	6.0	-5.4114902744	6.6310501168	1.6809401482
O	8.0	-0.2012203963	-1.9416322166	0.9118048431
H	1.0	0.7699909882	-4.0592101573	1.7248252216
O	8.0	-2.6889060118	3.9665404831	-0.5555072040
C	6.0	-0.6250283897	-0.8572993963	0.0230315520
C	6.0	-2.0116884051	1.2844489128	0.3898487264
C	6.0	-4.8572205099	5.7896795365	0.5253024425
C	6.0	-2.1779718524	3.0719520326	-1.5723909402
H	1.0	-0.5428085744	-3.7312082397	2.8565743086
H	1.0	-1.8986437029	-0.3712158659	1.6928118313
H	1.0	-3.2111689432	2.6848987436	1.0037550244
H	1.0	-0.8353003749	-1.3049010483	-0.9507111846
C	6.0	-2.2271640326	1.6138333171	-1.1042152440
C	6.0	-1.9048783343	-0.2206769750	0.6082594474
H	1.0	-5.4501956526	5.9739821841	-0.3802254463
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		C	6.0	-0.9021174049	-3.1219700193	0.8103006813
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		O	8.0	0.4366634896	-7.8786973715	4.1838069261
		O	8.0	-0.7504703649	-3.6653883206	-0.5155233271
		H	1.0	-7.5145630200	6.5496868288	1.1058748176
		N	7.0	-0.0488183013	-6.4788736796	2.4491008326
		H	1.0	-2.7969020454	-0.7063705152	0.2038324516
		H	1.0	-7.0346995451	5.2888955736	2.2482773375
		O	8.0	0.6256660667	-6.0674569097	-0.2100594727
		C	6.0	-0.3049999440	-7.0814555692	3.6308205379
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		C	6.0	-0.8322748662	-5.5242668290	1.6617200079
		F	9.0	-1.8060869166	-5.3953090759	4.4785831913
		H	1.0	-0.4433333624	-5.3876747145	-2.5326857820
		C	6.0	-0.7387917579	-5.9437584411	0.1783005483
		C	6.0	-1.4530815095	-4.8925110406	-0.6871188715
		H	1.0	-1.8793323327	-5.5916327370	1.9646057807
		C	6.0	-1.6592406317	-6.7298295426	4.3019119230
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		C	6.0	-1.4613366111	-5.2234542091	-2.1723304669
		H	1.0	-1.9009271088	-4.3957844684	-2.7337786275
		H	1.0	-2.4922654528	-4.7859358572	-0.3269392497
		H	1.0	-1.1944184205	-6.9327322120	0.0516824743
		F	9.0	-2.7029425440	-7.1512503506	3.5429191823
		H	1.0	-2.0465883771	-6.1298337594	-2.3589932263
Zorubicin / Rubidazone	36508-71-1	H	1.0	8.3869901817	5.4407643304	1.1864420291
		H	1.0	9.1634838822	5.7605182617	3.5253581246
		C	6.0	7.9028484052	4.9072977864	1.9994655224
		H	1.0	6.5388198749	3.8838965979	0.6945655136
		C	6.0	8.3427293931	5.0814688720	3.3120900678
		H	1.0	2.6710974887	4.3047987316	-0.2822719575
		C	6.0	6.8468819750	4.0372561798	1.7248257422
		H	1.0	3.8932958490	3.3428786780	-1.1389323984
		H	1.0	2.2131934776	3.3170072339	-1.6858682205
		C	6.0	2.8485736276	3.3539681338	-0.8026797565
		H	1.0	-3.3864585246	3.6958354992	0.0645745494
		H	1.0	4.4478276178	3.5096747772	0.9636387049

C	6.0	7.7321811282	4.3708319912	4.3488940454
H	1.0	-0.0330275320	2.9992666613	-0.6177502856
O	8.0	-2.4038988397	3.4315297444	0.0561425331
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H	1.0	8.0766228905	4.4973931326	5.3713409202
N	7.0	4.3230930389	2.6204532520	1.4327327644
O	8.0	-4.9069051848	3.4259828793	0.1127332180
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C	6.0	-2.4370516382	2.0787732581	0.1019317420
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O	8.0	1.4185405483	1.1186939376	-1.6680275082
C	6.0	-4.9092830570	2.1432939525	0.1753421786
H	1.0	6.2055326220	2.9214350500	4.8596438946
C	6.0	-1.2308071941	1.3702524846	0.0926033448
C	6.0	-7.3605764349	2.1543526568	0.2491507057
O	8.0	4.8790980270	1.4405368417	3.3282091633
C	6.0	-3.6785448761	1.3898415758	0.1705498776
H	1.0	-9.5020134735	2.0962225732	0.3162085742
C	6.0	-6.1614079287	1.4056304517	0.2520858992
C	6.0	-8.5792391841	1.5205292702	0.3187501240
H	1.0	1.2140389428	0.1947707667	1.5827504707
C	6.0	1.2627512997	0.0028998901	0.5068278800
C	6.0	-1.2431559345	-0.0397952547	0.1538069255
H	1.0	2.1895473772	-0.5533260228	0.3377622334
C	6.0	-3.6964087872	-0.0328049532	0.2478542733
C	6.0	0.0382881248	-0.8250645942	0.0981165508
C	6.0	-6.1925140162	-0.0256609491	0.3293874049
O	8.0	0.1910462889	-1.2858601799	-1.3029910374
C	6.0	-2.4598781633	-0.7395282127	0.2380863811
H	1.0	1.8453614510	-1.5704075789	-3.3477506825
C	6.0	-8.6468705055	0.1143018764	0.3939568331
C	6.0	-4.9419390669	-0.7832123592	0.3349721755
C	6.0	-7.4830851197	-0.6481402389	0.3996076031
H	1.0	-0.0518688799	-1.7248777485	0.7108516081
H	1.0	-9.6165037891	-0.3649357784	0.4475196359
H	1.0	2.0052738372	-2.2219413644	-0.9625928780
C	6.0	1.3249149055	-2.4740950026	-3.0070599092

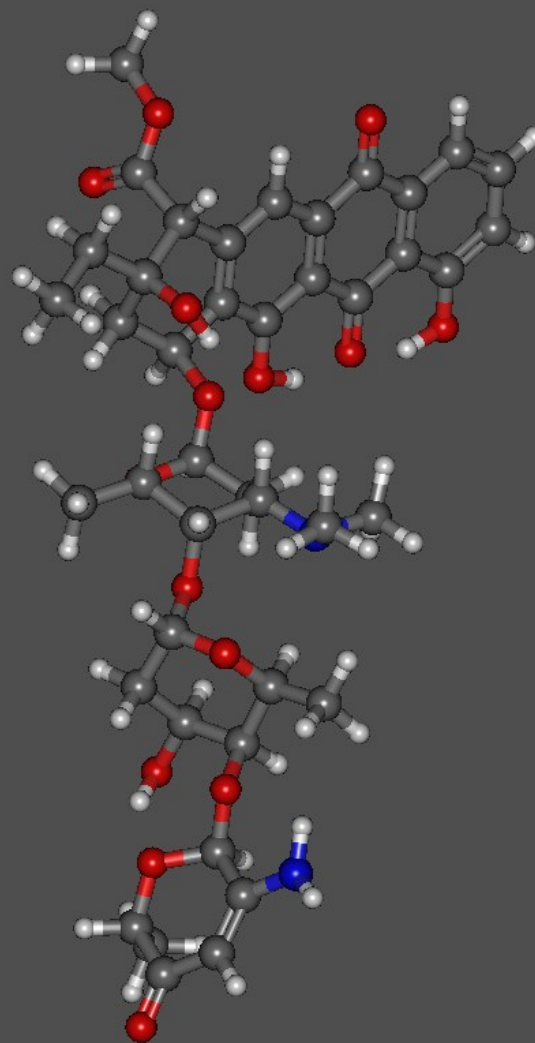
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O	8.0	-4.9082298772	-2.0574148910	0.4128647300
O	8.0	-7.5167231462	-2.0122954271	0.4706509374
H	1.0	-3.4264568068	-2.3321135178	0.3752194693
H	1.0	3.1361327251	-3.6106607062	-2.7825241072
N	7.0	2.3161282699	-3.9441799962	-4.7374324891
C	6.0	2.1608805715	-3.7239785251	-3.2922025077
O	8.0	0.4299669816	-3.5431612662	-1.0193189119
H	1.0	-9.3859885207	-2.4514076523	-0.3540101348
H	1.0	-9.3411186975	-2.3654321691	1.4272689125
C	6.0	-8.7689038855	-2.6546057390	0.5335232096
H	1.0	3.0422228804	-4.6448560640	-4.8733052992
H	1.0	2.2047948253	-4.5739004878	-0.6706399119
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C	6.0	1.4881038857	-4.9493118594	-2.6649654977
H	1.0	0.5187744241	-5.1036526147	-3.1590322394
H	1.0	-8.5530118334	-3.7243242575	0.5799080817
H	1.0	2.0357020214	-6.5515281888	-3.6294046976
O	8.0	2.3204338327	-6.1098117834	-2.8211145667
H	1.0	0.3371236658	-5.6482811715	0.5591483359
C	6.0	0.4800507303	-5.8590501302	-0.5036957247
H	1.0	-0.5078425086	-5.9771182274	-0.9598800241
H	1.0	1.0412649431	-6.7896781281	-0.6172570635

8. Optimized 3D chemical structures of anthracycline's semiquinone free radicals. (Note that $>C=O$ rather than $>C-O$ in quinone moieties appears because the software only reads the Cartesian coordinates to give the pictures.)

Name	NSC No. / CAS No.	3D chemical structures
3'-Acetoxy-4'-O-acetyldoxorubicin	73113-92-5	 A 3D ball-and-stick model of the molecule 3'-Acetoxy-4'-O-acetyldoxorubicin. The structure features a central anthracycline core with two acetoxy groups attached to the 3' and 4' positions of the aglycone moiety. The atoms are represented by spheres: carbon (grey), oxygen (red), and hydrogen (white). The model is set against a dark grey background.

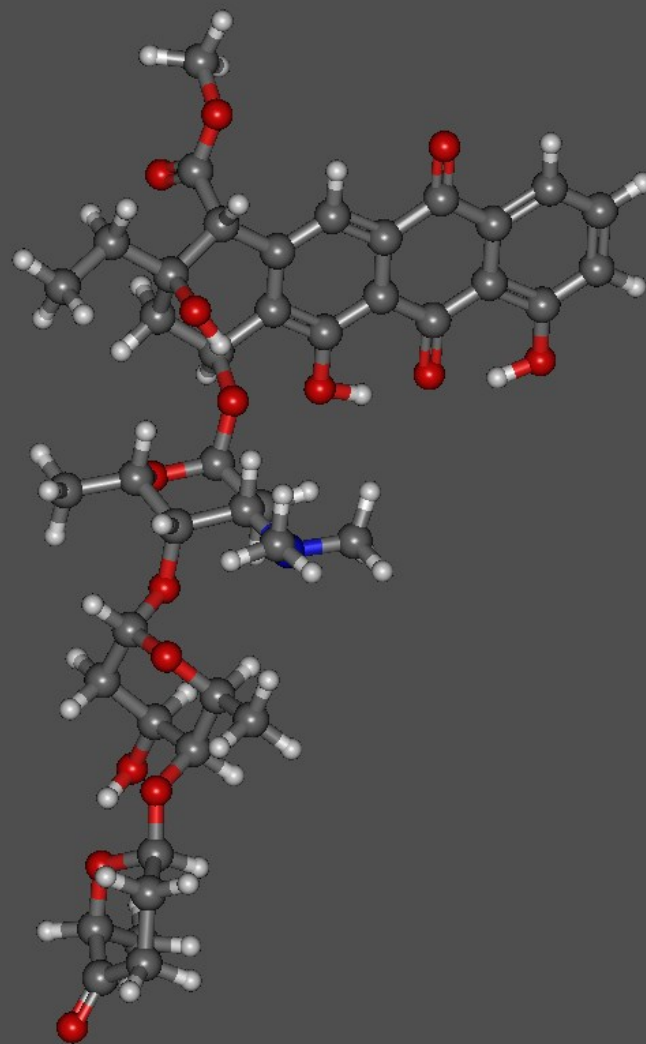
Aclacinomycin X

NSC 670120



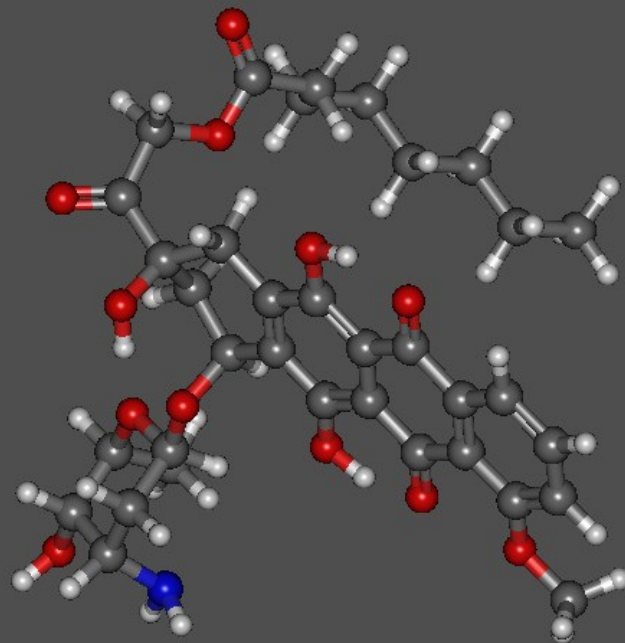
Aclarubicin

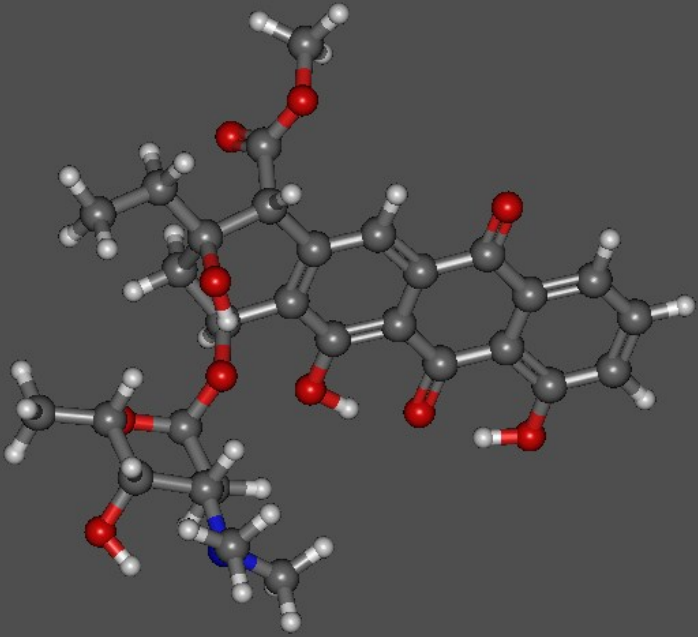
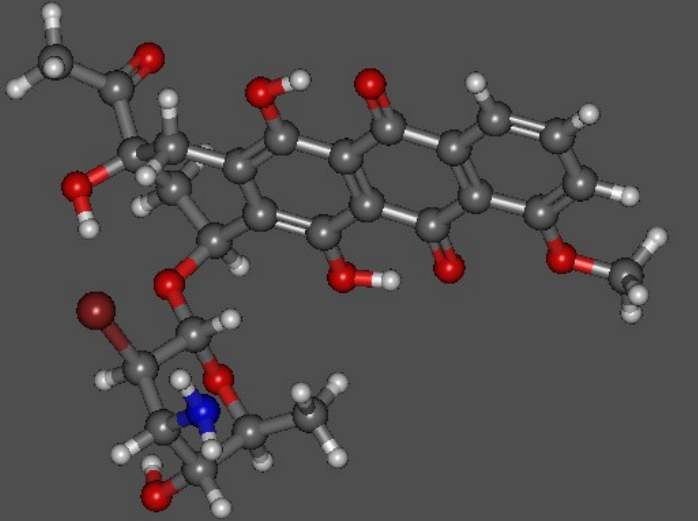
57576-44-0



Adriamycin 14-octanoate

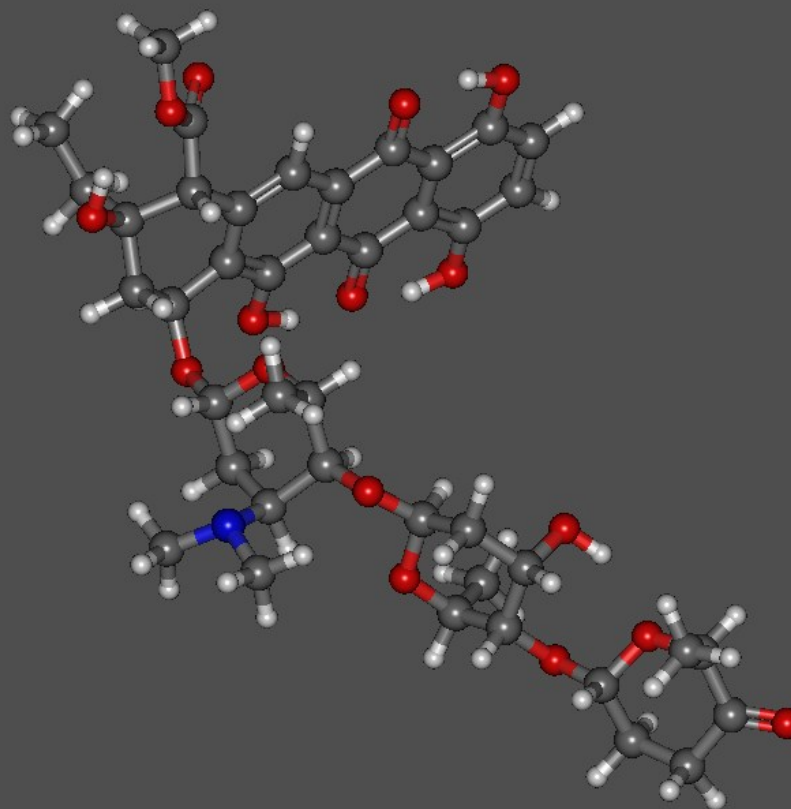
51898-39-6

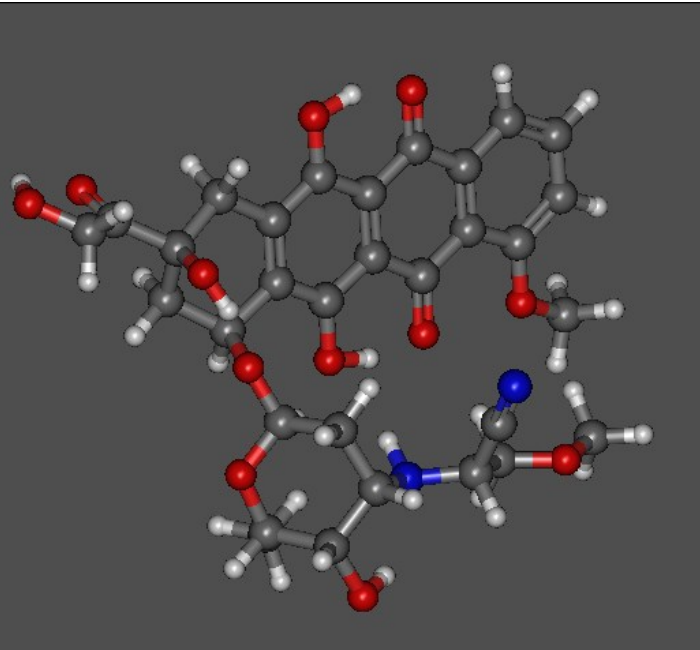
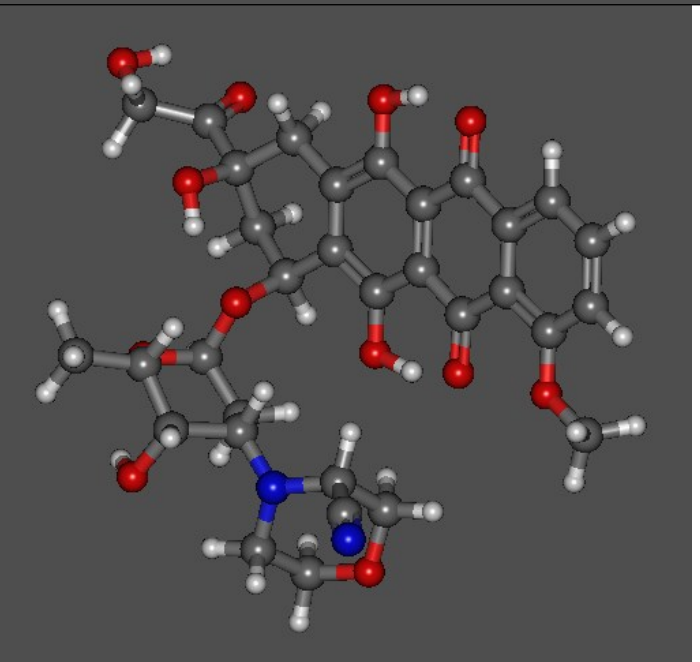


<p>Aklavin</p>	<p>60504-57-6</p>		 A 3D ball-and-stick model of the molecule Aklavin. The structure features a complex polycyclic core with several hydroxyl groups (red and white) and a nitrogen atom (blue) in a ring system. The model is rendered against a dark gray background.	
<p>2'-Bromo-4'-epi-daunorubicin</p>	<p>NSC 650931</p>		 A 3D ball-and-stick model of the molecule 2'-Bromo-4'-epi-daunorubicin. The structure is similar to Aklavin but includes a bromine atom (dark red) at the 2' position. The model is rendered against a dark gray background.	

Cinerubin A

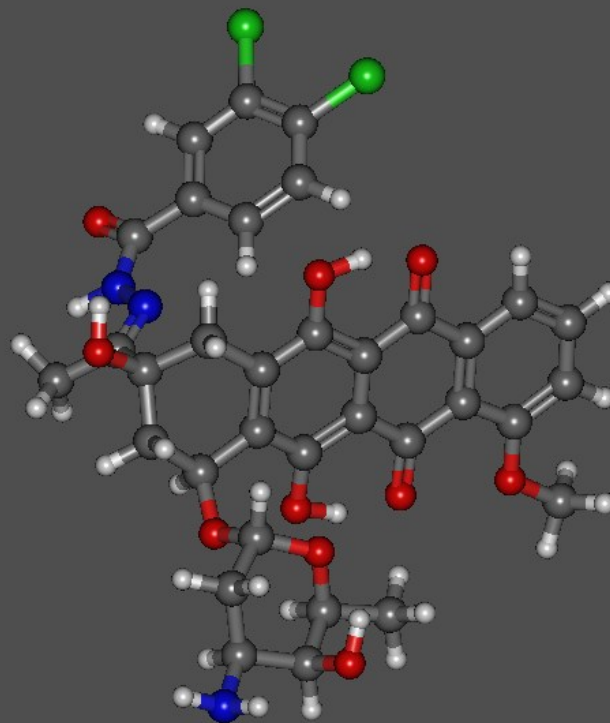
NSC 243022 /
34044-10-5

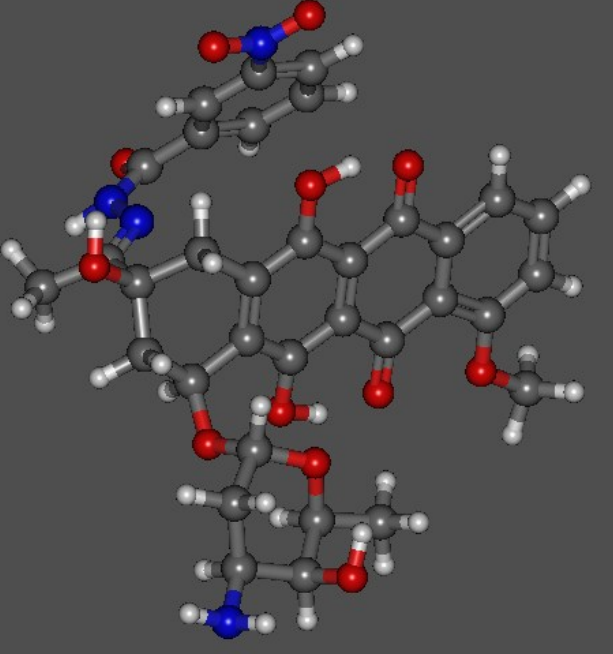
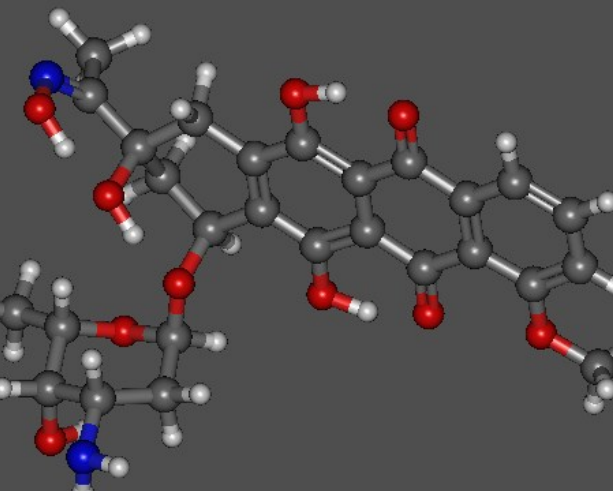


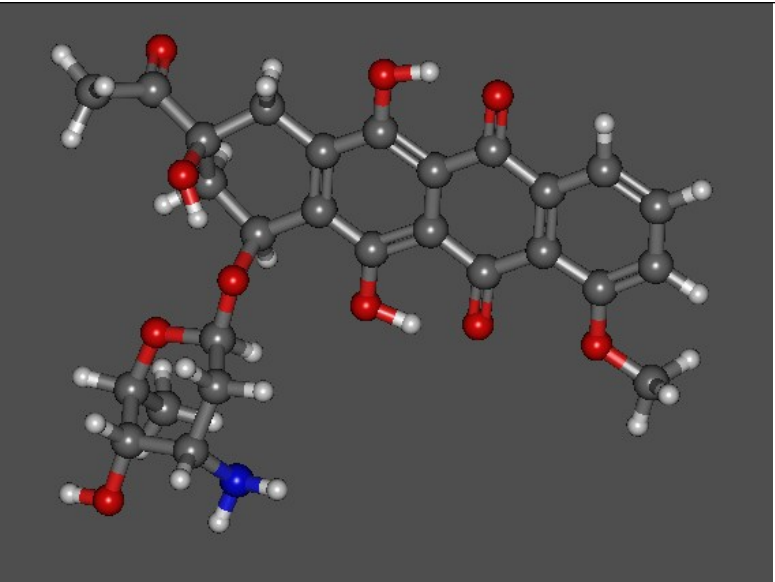
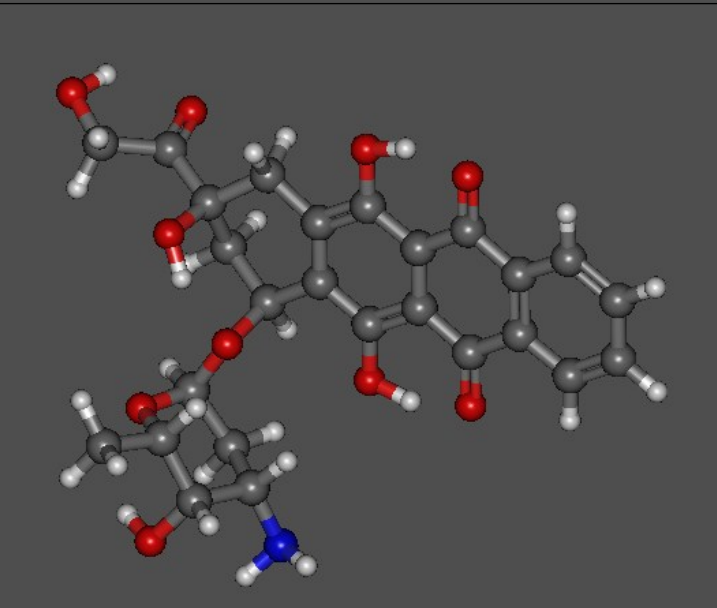
<p>N-(1-Cyano-2-methoxyethyl) doxorubicin</p>	<p>NSC 639659</p>		 A 3D ball-and-stick model of N-(1-Cyano-2-methoxyethyl)doxorubicin. The molecule features a central anthracycline core with a cyanoethyl side chain and a methoxy group. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	
<p>Cyanomorpholino doxorubicin</p>	<p>88254-07-3</p>		 A 3D ball-and-stick model of Cyanomorpholino doxorubicin. The molecule features a central anthracycline core with a cyanomorpholino side chain. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

Daunomycin 3,4-
dichlorobenzoyl hydrazone

66996-54-1

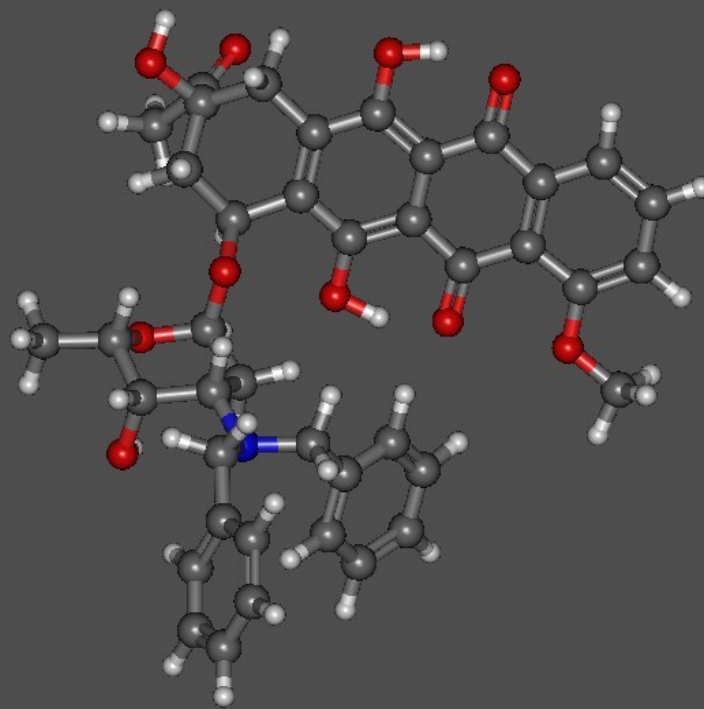


<p>Daunomycin 4-nitrobenzoylhydrazone</p>	<p>66996-56-3</p>		 A 3D ball-and-stick model of Daunomycin 4-nitrobenzoylhydrazone. The molecule features a complex polycyclic core with multiple hydroxyl groups (red and white spheres) and a 4-nitrobenzoylhydrazone group (blue and red spheres) attached to the structure. The model is set against a dark gray background.	
<p>Daunomycin 3-oxime</p>	<p>34610-60-1</p>		 A 3D ball-and-stick model of Daunomycin 3-oxime. The molecule features a complex polycyclic core with multiple hydroxyl groups (red and white spheres) and an oxime group (blue and red spheres) attached to the structure. The model is set against a dark gray background.	

<p>Daunorubicin / Daunomycin</p>	<p>20830-81-3 / 23541-50-6</p>	 A 3D ball-and-stick model of Daunorubicin / Daunomycin. The molecule features a tetracyclic core with a quinone ring system. It has a glycosidic linkage to a D-glucopyranose sugar at the C-10 position and a dimethylamino group at the C-14 position. The model uses grey for carbon, red for oxygen, white for hydrogen, and blue for nitrogen.
<p>4-Demethoxyadriamycin / Medorubicin</p>	<p>64363-63-9</p>	 A 3D ball-and-stick model of 4-Demethoxyadriamycin / Medorubicin. The structure is very similar to Daunorubicin, but it lacks the methoxy group at the C-4 position of the quinone ring. It also features a glycosidic linkage to a D-glucopyranose sugar at the C-10 position and a dimethylamino group at the C-14 position. The model uses grey for carbon, red for oxygen, white for hydrogen, and blue for nitrogen.

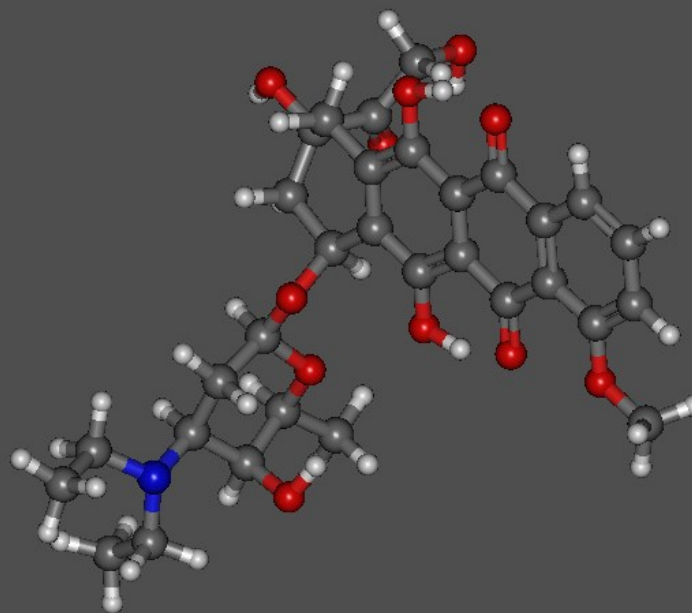
N,N-dibenzyl-daunorubicin

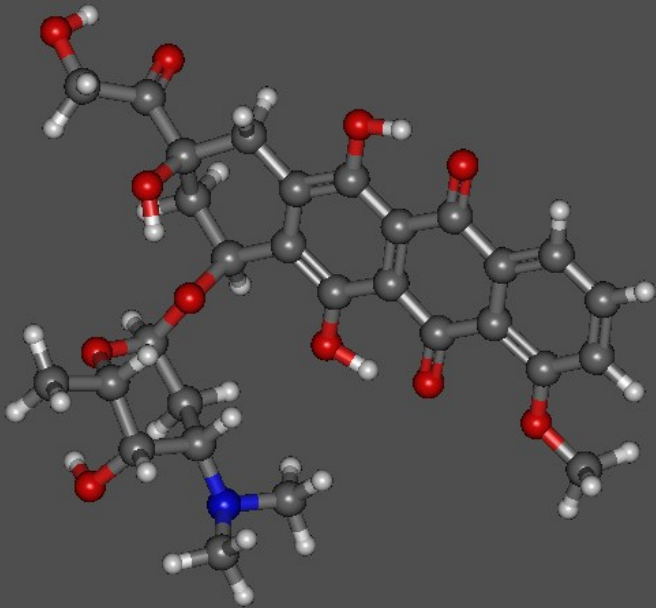
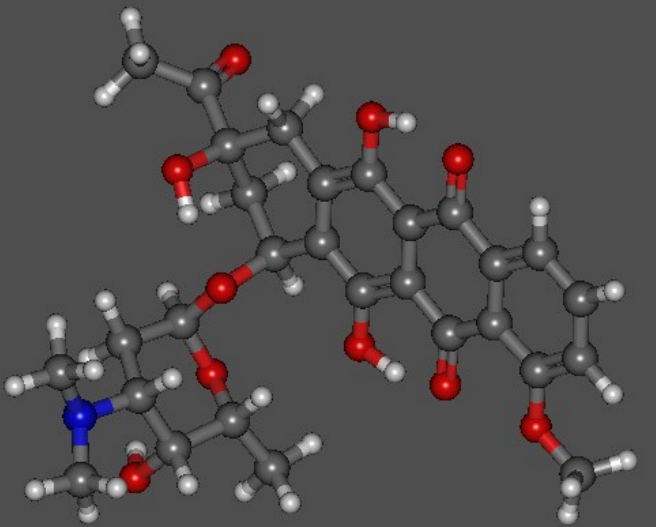
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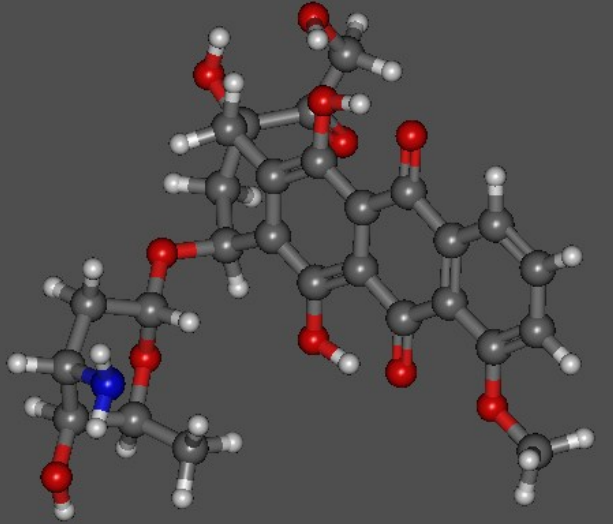
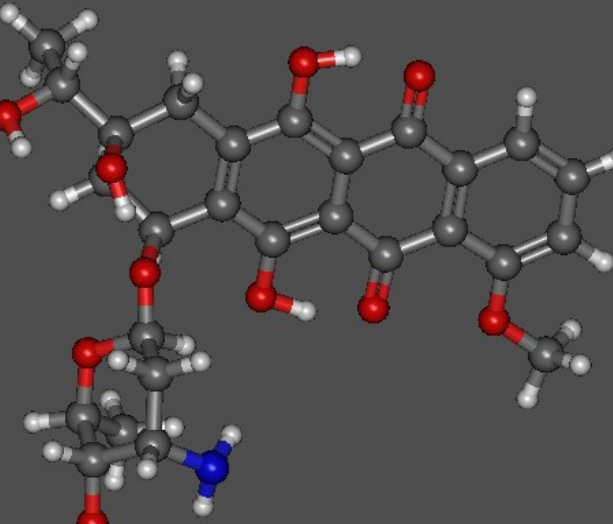


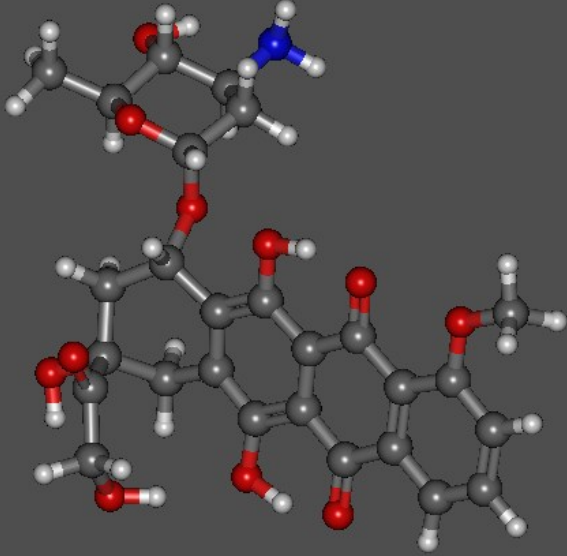
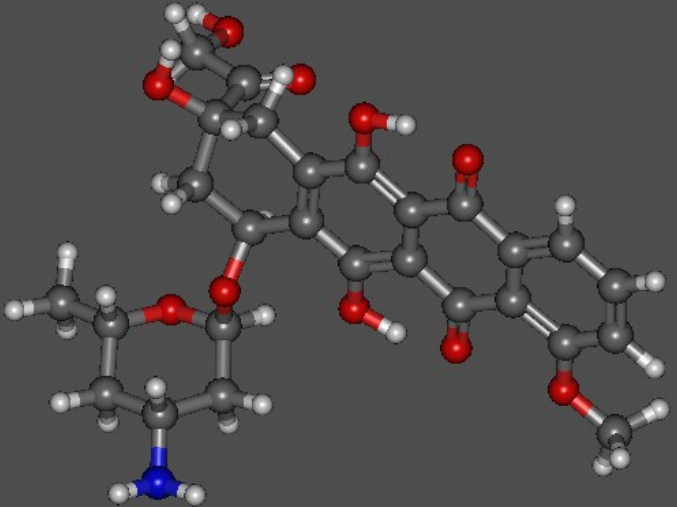
N,N-diethyladriamycin

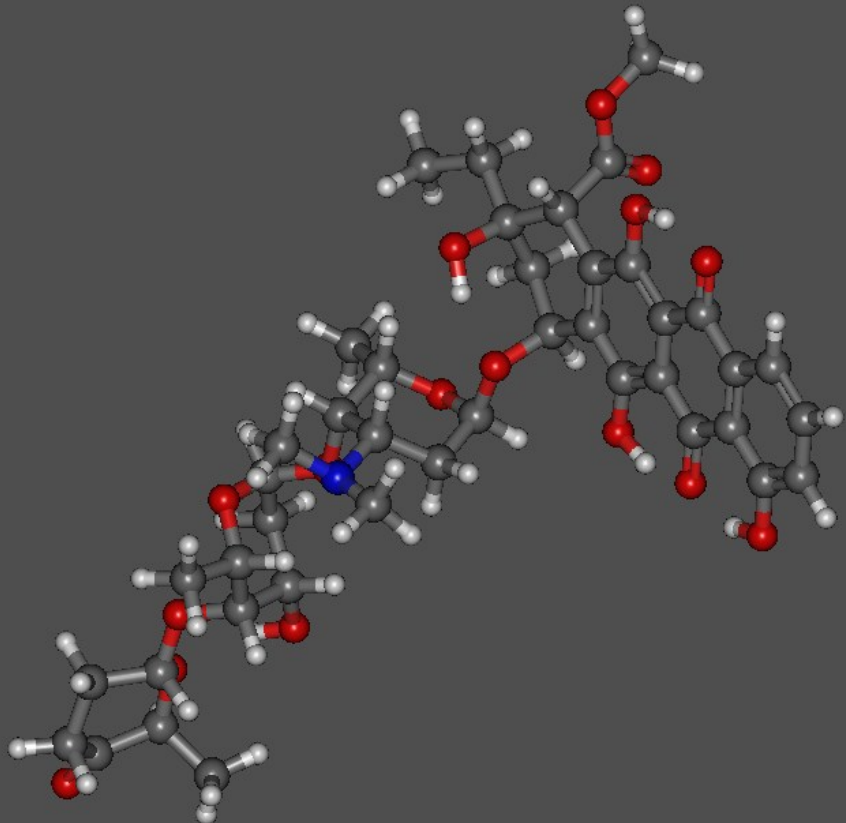
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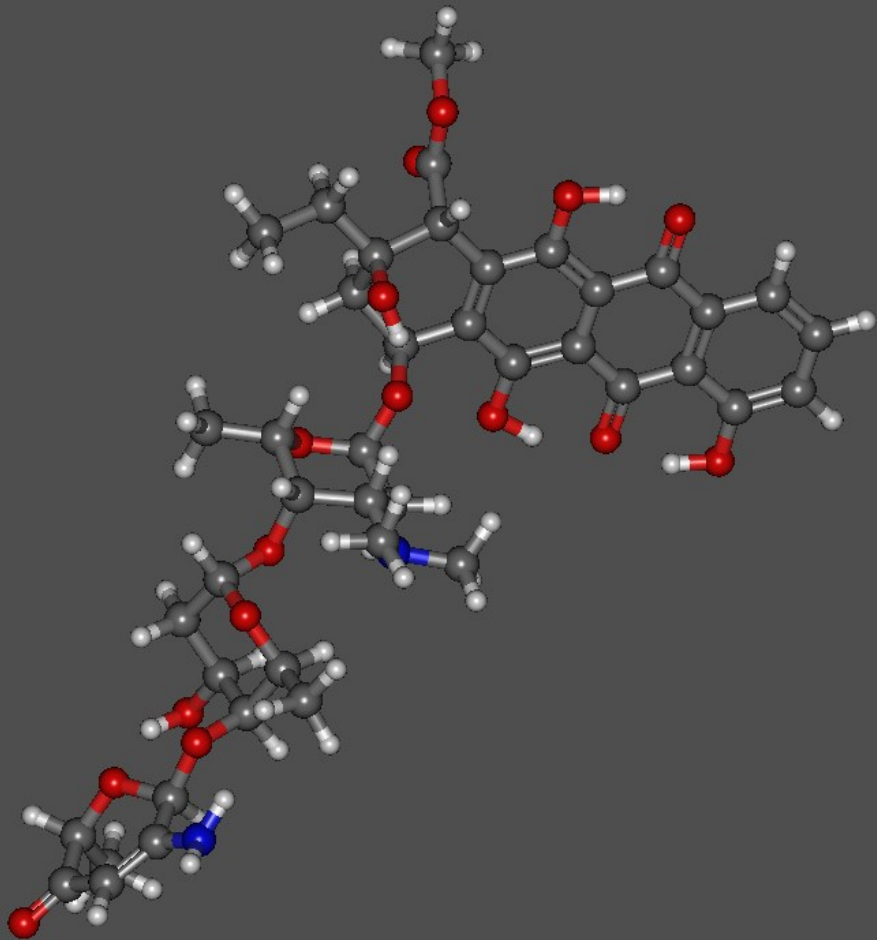


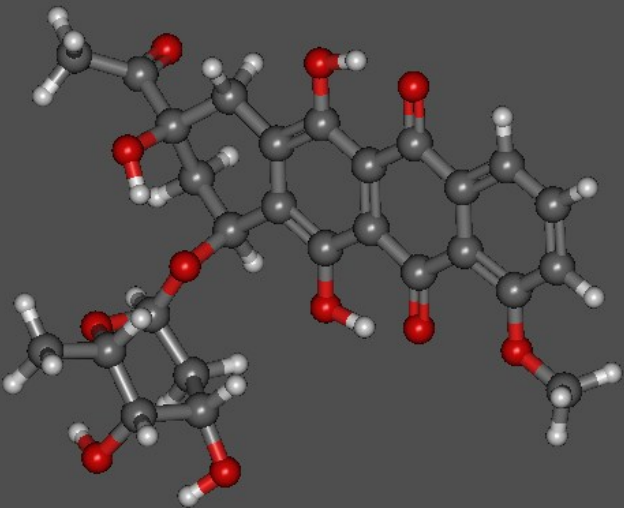
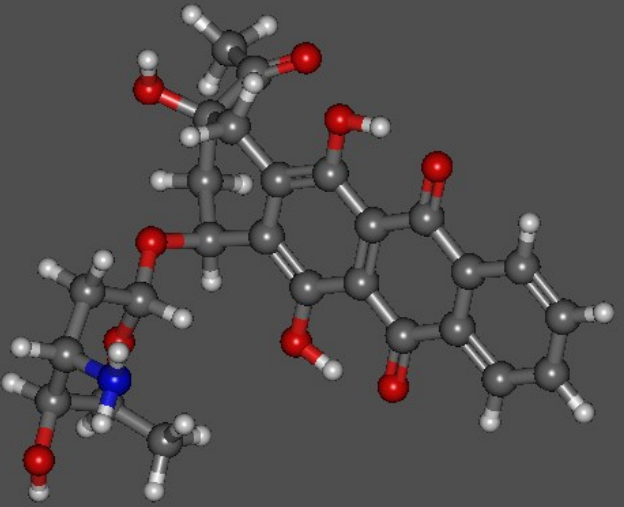
<p>N,N-dimethyladriamycin</p>	<p>67106-76-7</p>		 <p>A 3D ball-and-stick model of N,N-dimethyladriamycin. The molecule features a complex polycyclic core with a central nitrogen atom (blue) bonded to two methyl groups (grey and white). It has multiple hydroxyl groups (red and white) and a dimethylamino group (blue nitrogen with two grey methyl groups) attached to the structure.</p>	
<p>N,N-dimethyldaunomycin</p>	<p>70095-84-0</p>		 <p>A 3D ball-and-stick model of N,N-dimethyldaunomycin. The structure is very similar to N,N-dimethyladriamycin, showing a complex polycyclic core with a central nitrogen atom (blue) bonded to two methyl groups (grey and white). It features multiple hydroxyl groups (red and white) and a dimethylamino group (blue nitrogen with two grey methyl groups).</p>	

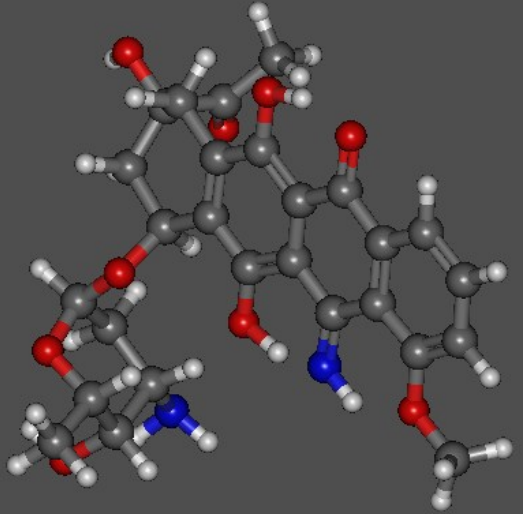
Doxorubicin / Adriamycin	25316-40-9 / 23214-92-8		 A 3D ball-and-stick model of Doxorubicin / Adriamycin. The molecule features a tetracyclic core with a quinone ring system, a decalin ring system, and a glycosaminoglycan side chain. Atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	
Duborimycin	NSC 180510		 A 3D ball-and-stick model of Duborimycin. The molecule features a tetracyclic core with a quinone ring system, a decalin ring system, and a glycosaminoglycan side chain. Atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

Epirubicin	56390-09-1		 A ball-and-stick model of the Epirubicin molecule. The structure features a central anthracycline ring system with a hydroxyl group at the 12-position and an epirubicin side chain at the 14-position. The side chain includes a methoxy group, a hydroxyl group, and a 4-epi-10-hydroxy-10,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine moiety. Atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	
Esorubicin	63950-06-1		 A ball-and-stick model of the Esorubicin molecule. The structure is similar to Epirubicin but with the hydroxyl group at the 12-position in the anthracycline ring system in the opposite orientation. The side chain at the 14-position is identical to Epirubicin. Atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

<p>11-Hydroxy aclacinomycin A</p>	<p>NSC 670121</p>		 A 3D ball-and-stick model of the molecule 11-Hydroxy aclacinomycin A. The structure is a complex polycyclic molecule with a central nitrogen atom (blue) and several oxygen atoms (red). It features a large, multi-ring system with various substituents, including hydroxyl groups and a methyl group. The model is rendered in a semi-transparent style, showing the spatial arrangement of atoms and bonds.	
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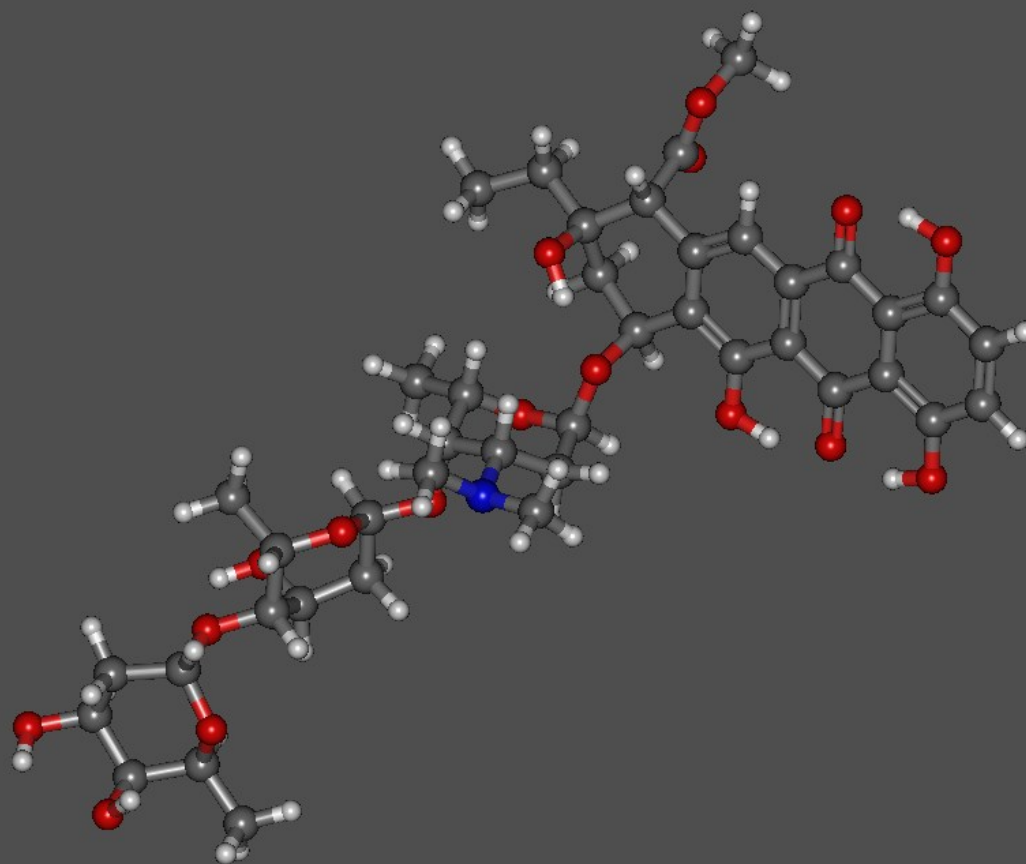
<p>11-Hydroxy aclacinomycin X</p>	<p>NSC 670122</p>	 <p>A 3D ball-and-stick model of the molecule 11-Hydroxy aclacinomycin X. The structure is a complex polycyclic molecule with a central core of fused rings, including a pyridine ring. It features several hydroxyl groups (red oxygen atoms with white hydrogen atoms) and a methylamino group (blue nitrogen atom with two white hydrogen atoms). The molecule is shown in a perspective view against a dark gray background.</p>
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<p>3'-Hydroxy daunorubicin</p>	<p>64842-75-7</p>		 A ball-and-stick model of 3'-Hydroxy daunorubicin. The molecule consists of a tetracyclic anthracycline core with a hydroxyl group at the 3' position of the aglycone moiety. The atoms are color-coded: carbon (grey), oxygen (red), and hydrogen (white).	
<p>Idarubicin</p>	<p>57852-57-0</p>		 A ball-and-stick model of Idarubicin. The molecule features a tetracyclic anthracycline core with a hydroxyl group at the 3' position and an imino group at the 4' position. The atoms are color-coded: carbon (grey), oxygen (red), hydrogen (white), and nitrogen (blue).	

<p>5-Imino daunorubicin</p>	<p>67324-99-6</p>		 A 3D ball-and-stick model of the molecule 5-Imino daunorubicin. The structure is complex, featuring a central anthracycline-like core with a quinone ring system. It has several hydroxyl groups (red and white spheres) and a characteristic imino group (blue and white spheres) at the 5-position. The model is rendered against a dark gray background.	
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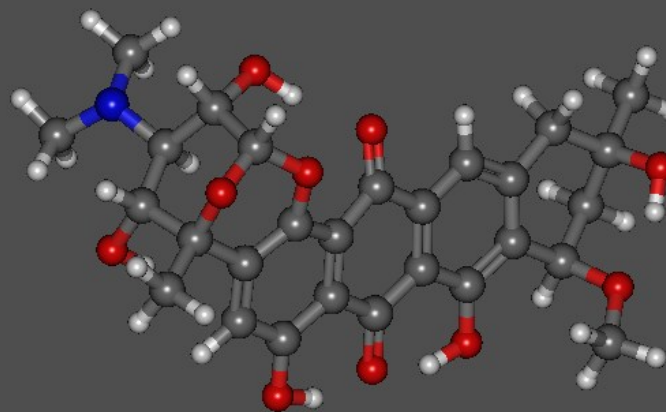
Marcellomycin

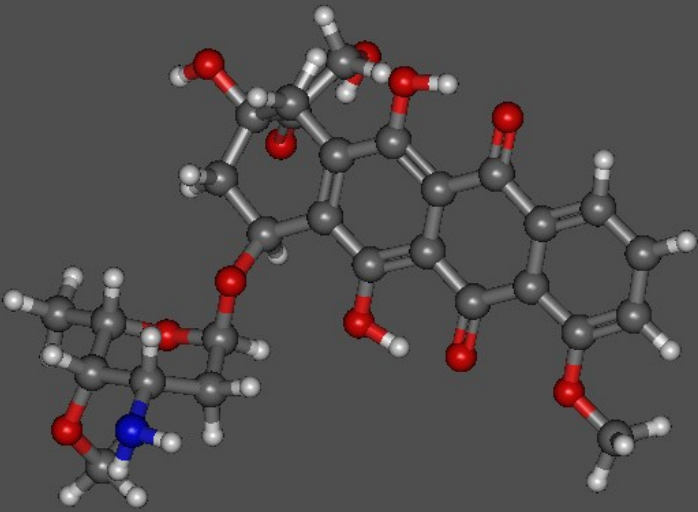
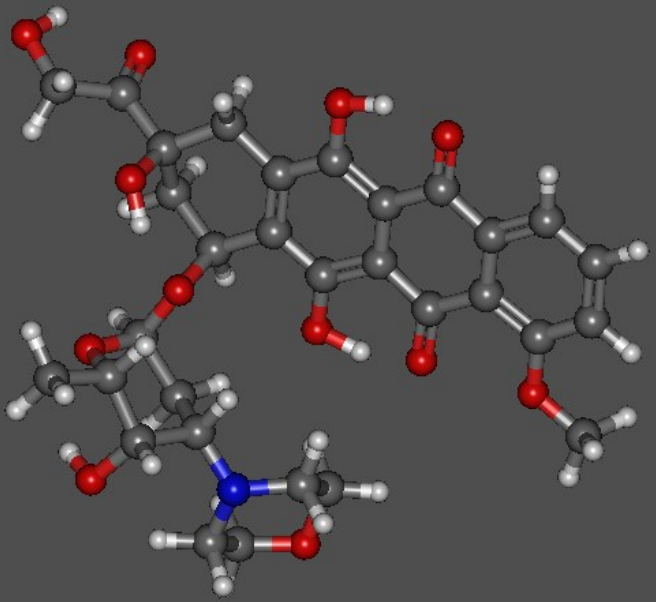
63710-10-1

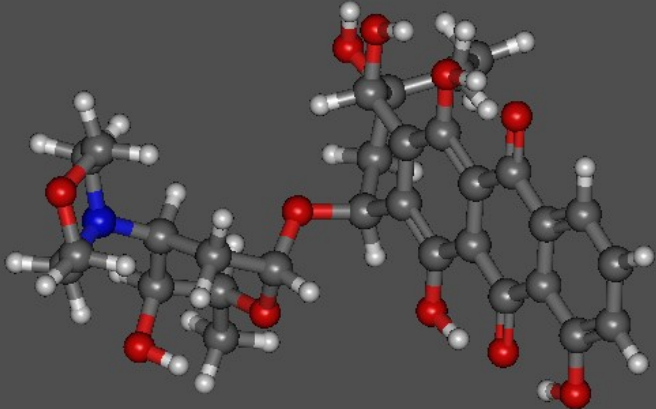
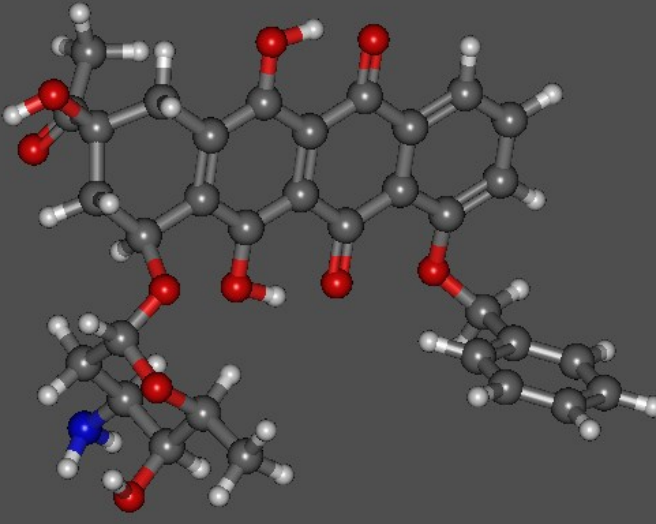


Menogaril

71628-96-1

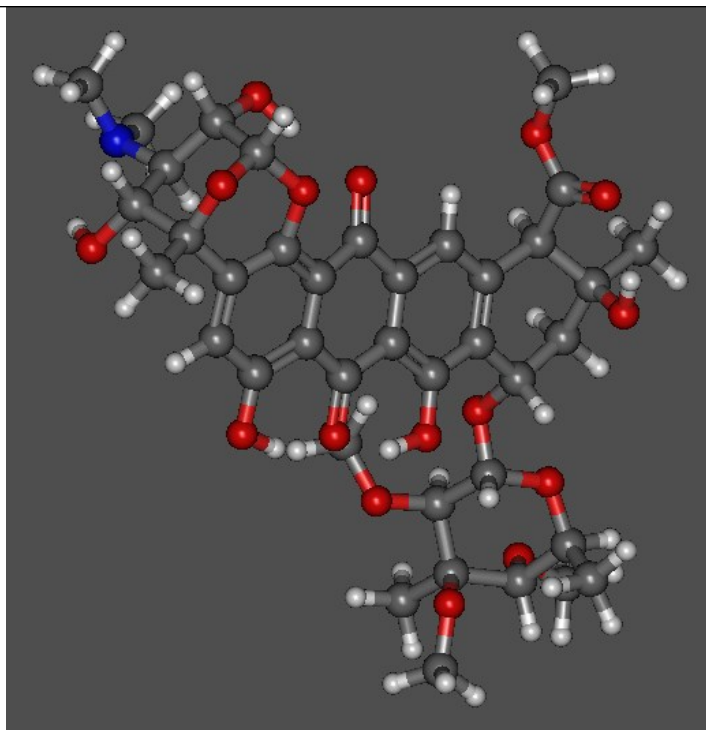


<p>4'-O-methyldoxorubicin</p>	<p>77121-90-5</p>		 A 3D ball-and-stick model of 4'-O-methyldoxorubicin. The molecule features a tetracyclic core with a morpholine ring at the 4' position. The model uses a color scheme where carbon atoms are grey, oxygen atoms are red, hydrogen atoms are white, and the nitrogen atom in the morpholine ring is blue. The structure is shown against a dark grey background.	
<p>Morpholino adriamycin</p>	<p>89196-04-3</p>		 A 3D ball-and-stick model of Morpholino adriamycin. The molecule features a tetracyclic core with a morpholine ring at the 4' position. The model uses a color scheme where carbon atoms are grey, oxygen atoms are red, hydrogen atoms are white, and the nitrogen atom in the morpholine ring is blue. The structure is shown against a dark grey background.	

MX2	NCI 619003		 A ball-and-stick molecular model of NCI 619003. The structure features a central benzene ring with a nitrogen atom (blue) and a carbonyl group (C=O) attached to one side, and a complex side chain containing multiple oxygen atoms (red) and carbon atoms (grey) extending from the other side.	
NSC 286628	NSC 286628 / 67903-59-7		 A ball-and-stick molecular model of NSC 286628. The structure consists of a central benzene ring with a nitrogen atom (blue) and a carbonyl group (C=O) attached to one side, and a complex side chain containing multiple oxygen atoms (red) and carbon atoms (grey) extending from the other side.	

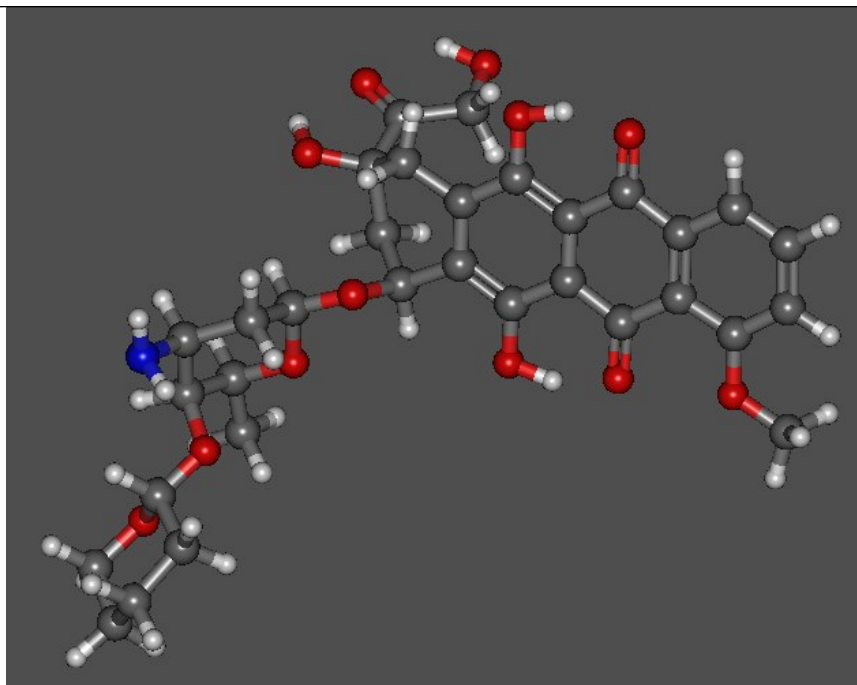
Nogalamycin

1404-15-5



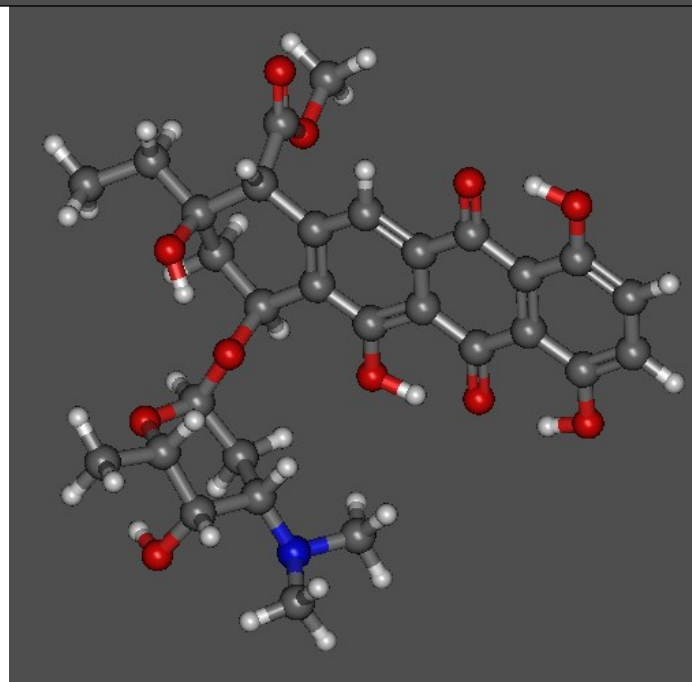
Pirarubicin

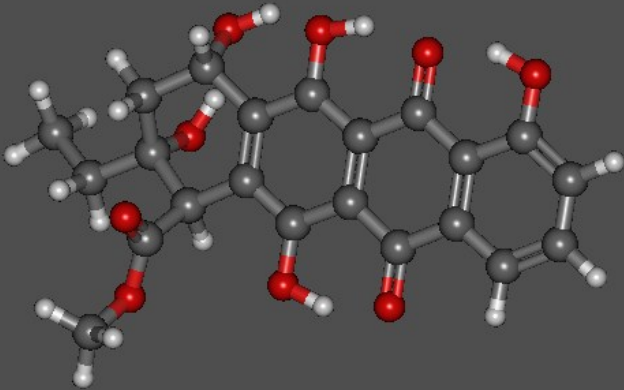
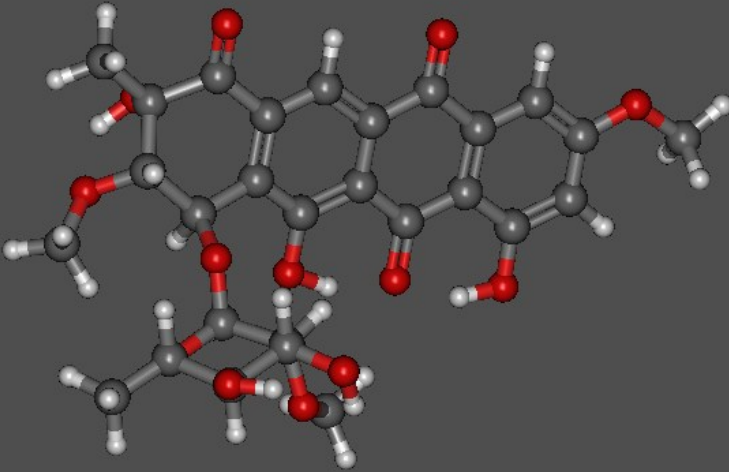
72496-41-4

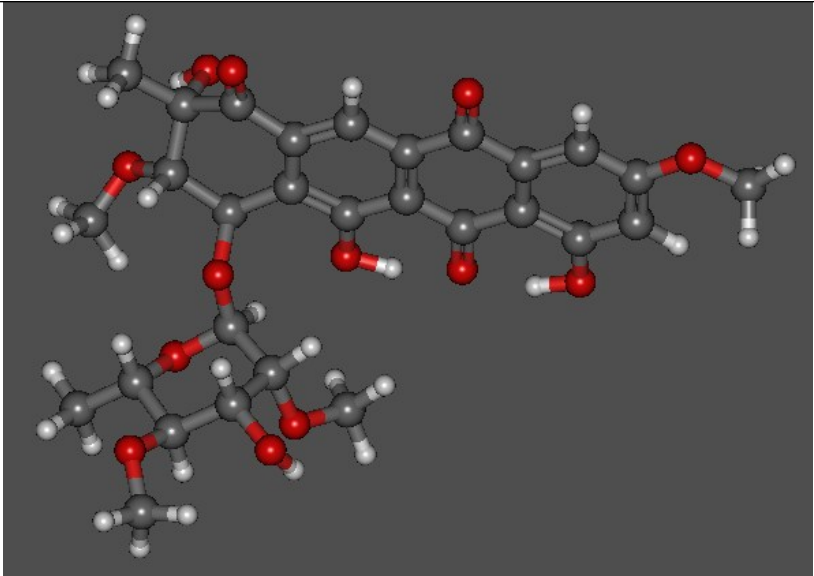
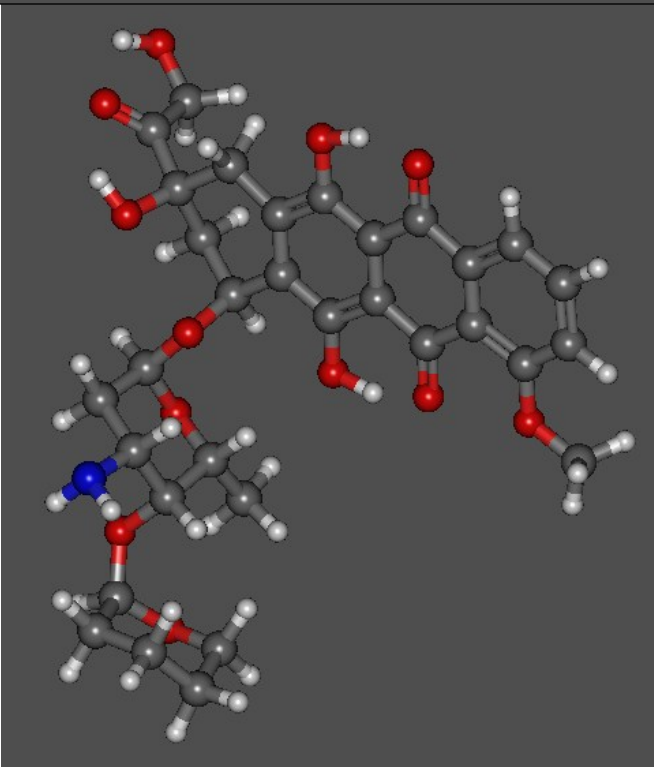


Pyrrromycin

668-17-7

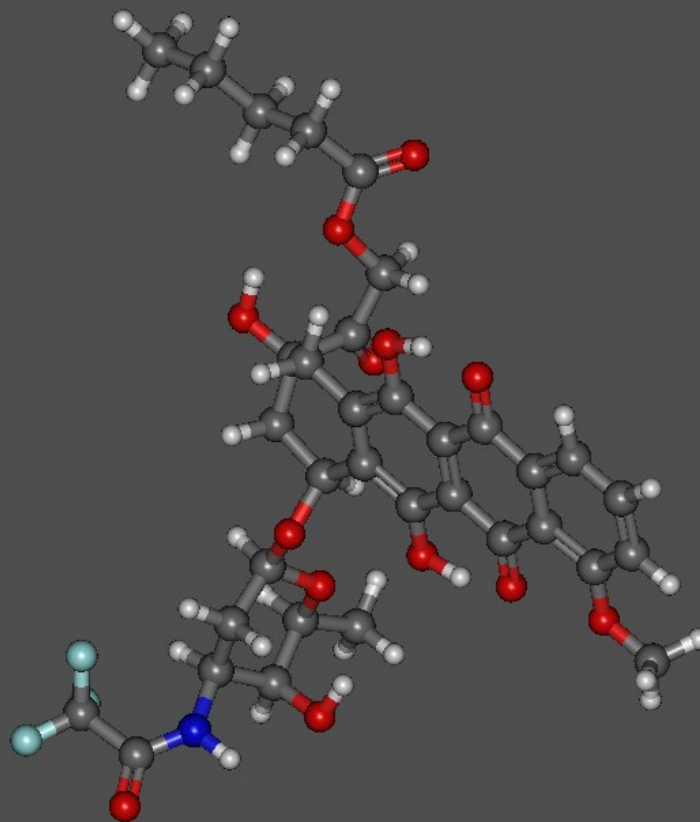


Rhodomycinone	21288-60-8		 A 3D ball-and-stick model of Rhodomycinone, a polyketide. The structure features a long, zig-zagging chain of carbon atoms (grey) with several oxygen atoms (red) and hydrogen atoms (white) attached. The chain is relatively flat and extends horizontally across the frame.	
Steffimycin	11033-34-4		 A 3D ball-and-stick model of Steffimycin, a polyketide. The structure is more complex and folded than Rhodomycinone, with a zig-zagging carbon chain (grey) and numerous oxygen (red) and hydrogen (white) atoms. The molecule is oriented diagonally, with one end pointing towards the top-left and the other towards the bottom-right.	

Steffimycin B	NCI 204856	 A 3D ball-and-stick model of Steffimycin B, a complex polyketide. The molecule features a long, zig-zagging carbon backbone with several hydroxyl groups (red oxygen, white hydrogen) and a methyl group (grey carbon, three white hydrogens) attached. The structure is shown against a dark grey background.
Theprubicin	95343-20-7	 A 3D ball-and-stick model of Theprubicin, a complex polyketide. The molecule features a long, zig-zagging carbon backbone with several hydroxyl groups (red oxygen, white hydrogen) and a methyl group (grey carbon, three white hydrogens) attached. A blue nitrogen atom is also present in the structure. The structure is shown against a dark grey background.

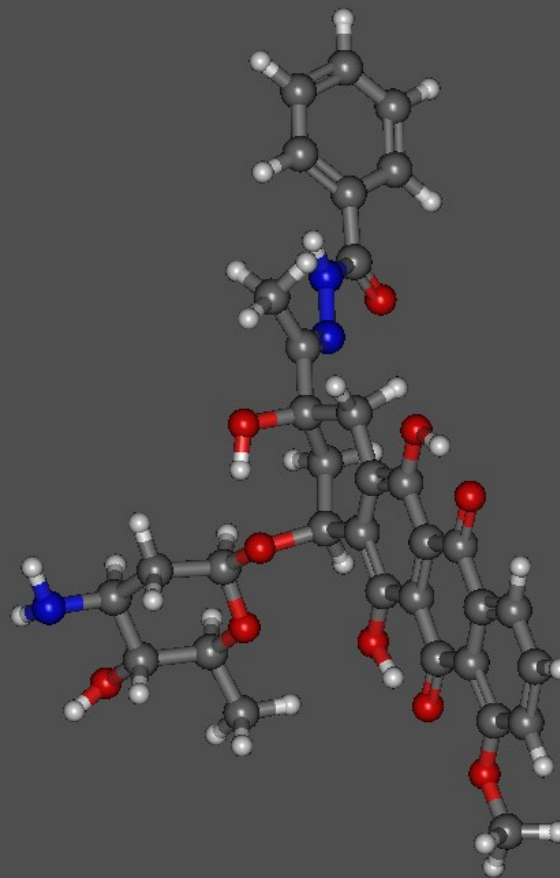
Valrubicin

56124-62-0

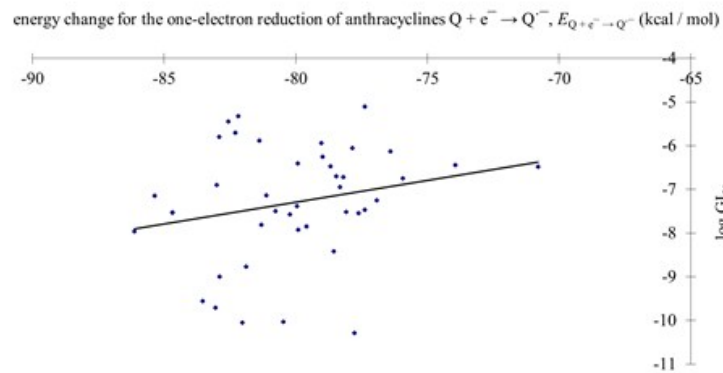
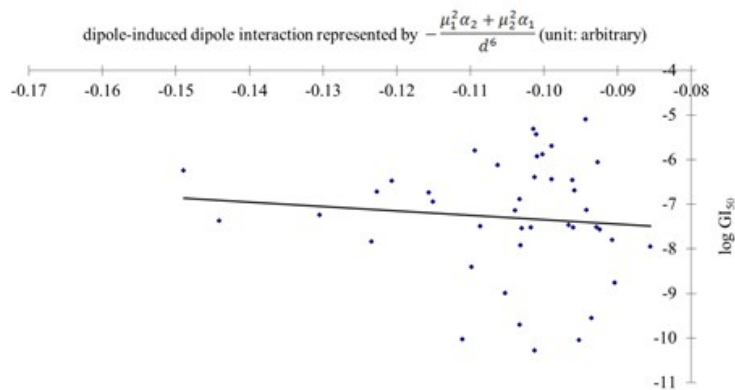
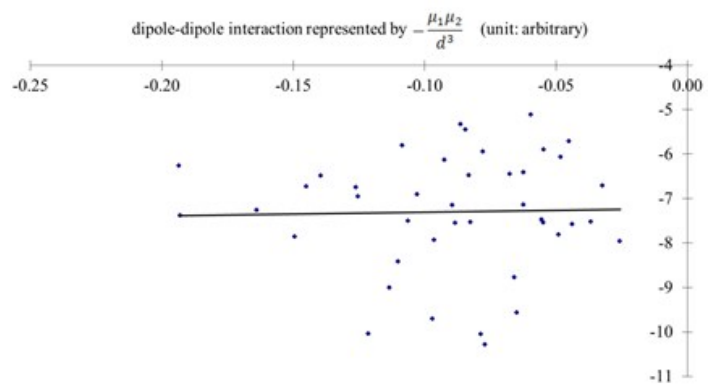
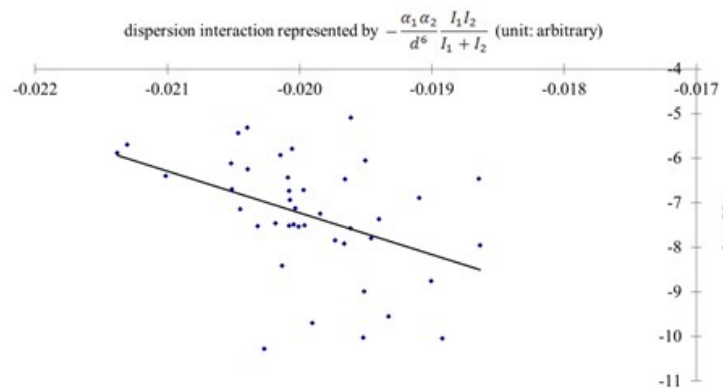
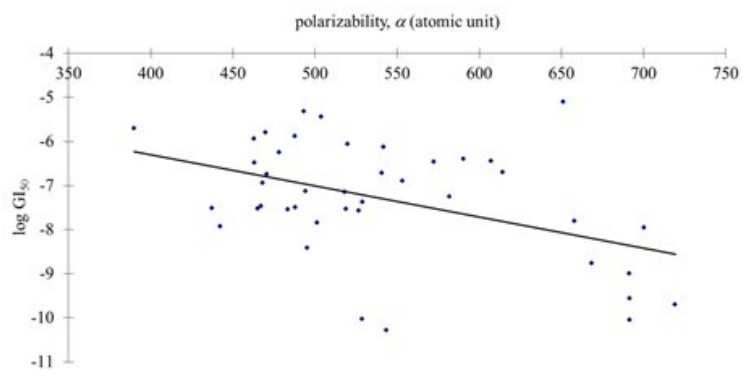


Zorubicin / Rubidazone

36508-71-1



9. Plots of polarizability (α), dispersion interaction ($-\frac{\alpha_1\alpha_2}{d^6} \frac{I_1 I_2}{I_1 + I_2}$), dipole-dipole interaction ($-\frac{\mu_1\mu_2}{d^3}$), dipole-induced dipole interaction ($-\frac{\mu_1^2\alpha_2 + \mu_2^2\alpha_1}{d^6}$), and energy change for the one-electron reduction ($E_{Q+\epsilon^- \rightarrow Q^{\cdot-}}$) of anthracyclines against log GI₅₀ for K562 leukemia.



Representative Firefly inputs used in the study

1. Geometry optimization of one of anthracyenes


```
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$CONTRL SCFTYP=RHF $END
$CONTRL DFTTYP=B3LYP1 $END
$CONTRL ICHARG=0 MULT=1 $END
$CONTRL NZVAR=267 $END
$ZMAT DLC=.T. AUTO=.T. $END
$BASIS GBASIS=N31 NGAUSS=6 $END
$BASIS NDFUNC=1 NPFUNC=1 $END
$SCF DIRSCF=.TRUE. NCONV=9 $END
$$SYSTEM TIMLIM=30000 MWORDS=100 $END
$STATPT NSTEP=200 $END
```

\$DATA

Molecule specification

C1

```
H      1.0  5.8918845272  1.1063231062 -1.7508609126
O      8.0  6.4309807628 -1.3853261070 -1.5039537114
H      1.0  4.2130010362  0.8719841807 -1.2214052890
C      6.0  5.2597672369  0.6736829267 -0.9707811073
```

...

...

...

\$END

2. Calculation of HOMO of one of anthracyclines with taking the solvation into account

```
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$SCF DIRSCF=.TRUE. NCONV=9 $END
$$SYSTEM TIMLIM=30000 MWORDS=100 $END
$BASIS EXTFIL=.T. GBASIS=cc-pvdz $END
$PCM SOLVNT=WATER $END
$DATA
```

Molecule specification

C1

```
H      1.0  5.8918845272  1.1063231062 -1.7508609126
O      8.0  6.4309807628 -1.3853261070 -1.5039537114
H      1.0  4.2130010362  0.8719841807 -1.2214052890
C      6.0  5.2597672369  0.6736829267 -0.9707811073
```

...

...

...

\$END

3. Calculation of dipole moment and polarizability of one of anthracyclines with taking the solvation into account

```
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$BASIS GBASIS=N31 NGAUSS=6 $END
$BASIS NDFUNC=1 NPFUNC=1 $END
$PCM SOLVNT=WATER $END
```

```
$DATA
```

```
Molecule specification
```

```
C1
```

H	1.0	5.8918845272	1.1063231062	-1.7508609126
O	8.0	6.4309807628	-1.3853261070	-1.5039537114
H	1.0	4.2130010362	0.8719841807	-1.2214052890
C	6.0	5.2597672369	0.6736829267	-0.9707811073

```
...
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...
```

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```

```
$END
```