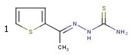
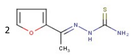
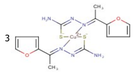
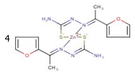
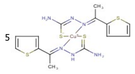
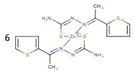
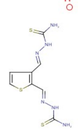
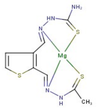
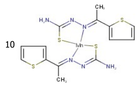
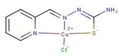
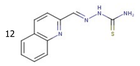
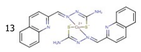
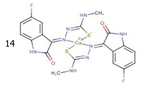
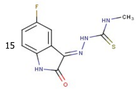
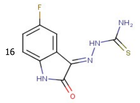
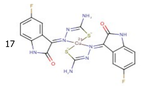
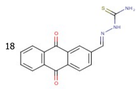
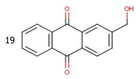
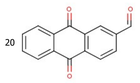
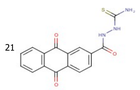
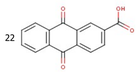
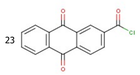
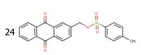
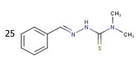
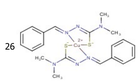
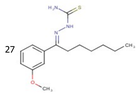
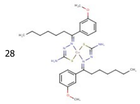
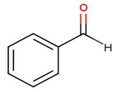
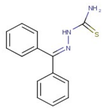
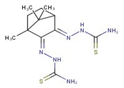
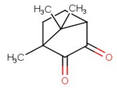
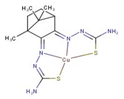
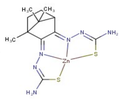
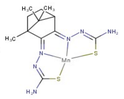
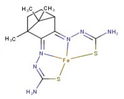
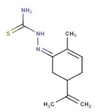
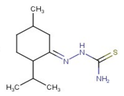
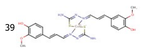
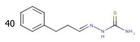
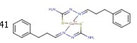
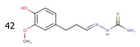
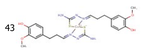
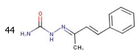
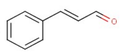
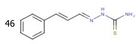
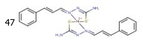
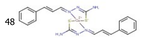
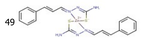
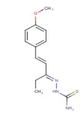
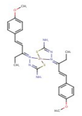
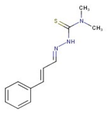
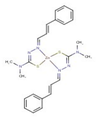
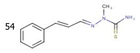
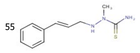
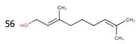
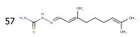
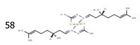
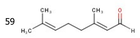
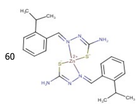
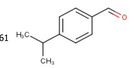
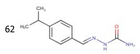
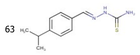
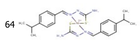
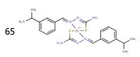
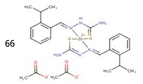
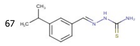
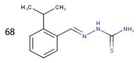
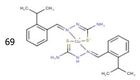
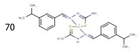
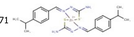
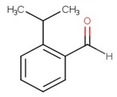
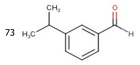
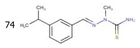
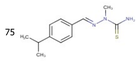
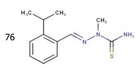
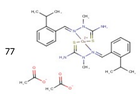
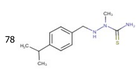
CdId	Structure	Mol Weight	Formula	LogP	LogD	TPSA	H bond acce	H bond donors	Group	growth inhibition (%) - 50uM	growth inhibiti	AF inhibition 5	AF inhibition 100	CRL1790 (GI5	HS27 (GI50)	HFL1 (GI50)	U937 (G	COMET 1h (genotoxicity	COMET 24h (genotoxicity)	Ames (mutagenesis)	EC50 Allium cepa (uM)	Mitotic index reduction .	Genotoxicity Micronucleus Allium	Genotoxicity Chromosomal aberration Allium cepa (u
			C7H9N3S2						2-acetylthiophene									yes	no	Not mutagen				
1		199.29		1.42	1.42	50.41	1	2		22.20	35.70	58.30	88.40	101.00	101.00	101.00	101.00				100.00	101.00		25.00
			C7H9N3OS						2-acetylthiophene															
2		183.23		0.57	0.57	63.55	1	2		13.9	35.9	19.06	28.44											
			C14H16CuN6O2S2						2-acetylthiophene															
3		427.99				141.46	0	0		41.08	63.42	47.49	65.71	10.00	33.50	25.00	101.00							
			C14H16N6O2S2Zn						2-acetylthiophene															
4		429.82				141.46	0	0		13.31	19.00	34.48	48.04		30.50									
			C14H17CuN6S4						2-acetylthiophene															
5		461.12				114.85	0	0		12.40	29.30	56.56	88.59		6.20									
			C14H16N6S4Zn						2-acetylthiophene															
6		461.94				115.18	0	0		0.00	4.10	60.49	85.42		15.40									
			C6H4O2S						2-acetylthiophene															
7		140.16		1.31	1.31	34.14	2	0		8.00	22.00	1.00	4.00											
			C8H10N6S3						2-acetylthiophene															
8		286.39		1.27	1.27	100.82	2	4		48.00	65.00	2.00	8.00											
			C9H11MgN5S3						2-acetylthiophene															
9		309.71				88.50	0	0		15.00	26.00													
			C14H16MnN6S4						2-acetylthiophene															
10		451.50				115.18	0	0		40.00	53.00	61.00	92.00											
			C7H7ClCuN4S						2-formylpyridine															
11		278.22				76.80	0	0		0.00	0.00	0.00	0.00											
			C11H10N4S						2-Quinolinecarboxaldehyde															
12		230.29		2.50	2.50	63.30	2	2		0.00	0.00	0.00	0.00											
			C22H18CuN8S2						2-Quinolinecarboxaldehyde															
13		522.11				140.96	0	0		32.9	60.7	55.7	88											

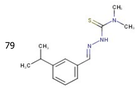
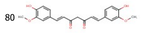
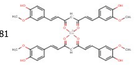
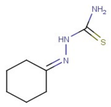
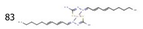
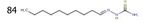
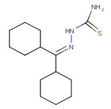
		C20H16CuF2N8O2S2					5-fluoroisatin																
14		566.06			145.40	0	0	0.00	0.00	0.00	0.00												
		C10H9FN4OS					5-fluoroisatin																
15		252.27	1.30	1.30	65.52	2	3	0.00	0.00	0.00	0.00												
		C9H7FN4OS					5-fluoroisatin																
16		238.24	1.07	1.07	79.51	2	3	0.00	0.00	0.00	0.00												
		C18H12CuF2N8O2S2					5-fluoroisatin																
17		538.01			173.38	0	0	0.00	0.00	0.00	0.00												
		C16H11N3O2S					anthraquinone											Weakly mutagen					
18		309.34	2.61	2.61	84.55	3	2	8.00	2.00	4.00	0.00	101.00	101.00	101.00	101.00				101.00	101.00		10.00
		C15H10O3					anthraquinone																
19		238.24	2.15	2.15	54.37	3	1	42.00	62.00			101.00	101.00	58.00	101.00							
		C15H8O3					anthraquinone											Not mutagen					
20		236.23	2.63	2.63	51.21	3	0	43.00	58.00			101.00	96.00	85.00	101.00				101.00	50.00		10.00
		C16H11N3O3S					anthraquinone																
21		325.34	1.74	1.73	101.29	3	3	48.00	58.00	11.00	26.00												
		C15H8O4					anthraquinone									no	no	Not mutagen					
22		252.23	2.58	-0.77	71.44	4	1	2.00	14.00	56.00	80.00	101.00	101.00	101.00	101.00				50.00	101.00		10.00
		C15H7ClO3					anthraquinone																
23		270.67	3.11	3.11	51.21	3	0	6.0	11.0	18.0	47.0												
		C22H16O5S					anthraquinone																
24		392.43	4.72	4.72	77.51	4	0	66.00	87.00														
		C10H13N3S					benzaldehyde									yes		Not mutagen					
25		207.30	2.11	2.11	27.63	1	1	22.00	44.00	76.00	90.00	101.00	101.00	101.00	101.00				100.00	100.00	101.00	25.00
		C20H24CuN6S2					benzaldehyde											Not mutagen					
26		476.12			69.62	0	0	0.00	0.00	35.00	67.00	3.00	3.00	1.00	5.00				100.00			

27		C15H23N3OS	293.43	3.83	3.83	59.64	2	2	benzaldehyde	23.00	36.00	28.67	47.06	34.00	27.00	42.50	101.00							
28		C30H44CuN6O2S2	648.39			133.64	0	0	benzaldehyde	8.20	15.30	82.51	95.24	36.50	1.00	34.00	101.00							
29		C7H6O	106.12	1.69	1.69	17.07	1	0	benzaldehyde	0.00	0.00	0.00	0.00											
30		C14H13N3S	255.34	3.41	3.41	50.41	1	2	Benzophenone	39.00	53.00	25.00	41.00	101.00	101.00	101.00	73.00	yes	yes	Not mutagen	100.00	101.00	10.00	
31		C12H20N6S2	312.45	2.61	2.61	100.82	2	4	camphorquinone	21.00	58.00	30.00	43.00											
32		C10H14O2	166.22	2.65	2.65	34.14	2	0	camphorquinone	2.00	10.00	17.00	18.00											
33		C12H18CuN6S2	373.98			115.18	0	0	camphorquinone	34.00	32.00	30.00	53.00											
34		C12H18N6S2Zn	375.82			115.18	0	0	camphorquinone	26.00	27.00													
35		C12H18MnN6S2	365.38			115.18	0	0	camphorquinone	8.00	10.00	23.00	34.00											
36		C12H18FeN6S2	366.28			115.18	0	0	camphorquinone	39.00	40.00	27.00	34.00											
37		C11H17N3S	223.34	2.53	2.53	50.41	1	2	carvone	0.00	0.00	16.70	34.50											
38		C11H21N3S	227.37	3.03	3.03	50.41	1	2	carvone	0	18.3	12.40	15.00											
39		C22H24CuN6O4S2	564.14			174.10	0	0	cinnamaldehyde															
										58	49													

		C10H13N3S					cinnamaldehyde														
40		207.30	1.88	1.88	50.41	1	2	102.00	107.00	48.00	48.00										
		C20H24CuN6S2					cinnamaldehyde														
41		476.12			115.18	0	0	69.00	68.00	15.00	46.00										
		C11H15N3O2S					cinnamaldehyde														
42		253.32	1.42	1.41	79.87	3	3			20.00	2.00										
		C22H28CuN6O4S2					cinnamaldehyde														
43		568.17			174.10	0	0			26.00	34.00										
		C11H13N3O					cinnamaldehyde														
44		203.25	1.56	1.56	67.48	2	2	0.00	0.00	0.00	0.00	101.00									
		C9H8O					cinnamaldehyde														
45		132.16	1.98	1.98	17.07	1	0	0.00	0.00	0.00	0.00	77.00									
		C10H11N3S					cinnamaldehyde									Not mutagen					
46		205.28	1.96	1.96	50.41	1	2	45.00	56.00	73.10	79.00	101					0.10	10.00	101.00	0.01	
		C20H20N6NiS2					cinnamaldehyde														
47		467.24			115.18	0	0	87.9	100	95	100										
		C20H20CuN6S2					cinnamaldehyde														
48		472.09			115.18	0	0	25.00	32.00	24.00	20.00	7.50									
		C20H20N6S2Zn					cinnamaldehyde									Not mutagen					
49		473.92			115.18	0	0	56.00	76.00	99.00	100.00	23.00					1.00	10.00	101.00	0.01	
		C13H17N3OS					cinnamaldehyde														
50		263.36	2.99	2.99	59.64	2	2	62.00	74.00												
		C26H32N6O2S2Zn					cinnamaldehyde														
51		590.08			133.64	0	0	86.00	89.00												
		C12H15N3S					cinnamaldehyde						yes	tox		Weakly mutagen					
52		233.33	2.40	2.40	27.63	1	1	20.00	42.00	100.00	100.00	101.00	101.00	101.00	101.00		50.00	101.00		10.00	

53		C24H28N6S2Zn	530.03			69.62	0	0	cinnamaldehyde	17.00	40.00	75.00	100.00	101.00	41.00	39.50	101.00								
54		C11H13N3S	219.31	2.18	2.18	41.62	1	1	cinnamaldehyde	-8.00	0.00	41.00	64.00	101.00	101.00	101.00	101.00	no	yes	Not mutagen	100.00	50.00		10.00	
55		C11H15N3S	221.32	2.01	2.01	41.29	1	2	cinnamaldehyde	2.00	15.00	37.00	45.00	101.00	101.00	101.00	101.00	no	no	Not mutagen	100.00	101.00		10.00	
56		C11H20O	168.28	2.95	2.95	20.23	1	1	citral	3.00	26.00	0.00	4.00												
57		C12H21N3S	239.38	3.09	3.09	50.41	1	2	citral	24.00	57.00	0.00	20.00												
58		C22H40N6NiS2	511.42			115.18	0	0	citronellal	41.52	58.90	29.01	82.10							Not mutagen	0.01	10.00	101.00	10.00	
59		C10H16O	152.24	2.66	2.66	17.07	1	0	citronellal	2.00	5.00	24.00	41.00				10								
60		C22H28N6S2Zn	506.01			115.18	0	0	cuminaldehyde	8.40	11.20	55.30	100.00	30.00	36.00	33.00	32.00								
61		C10H12O	148.21	2.93	2.93	17.07	1	0	cuminaldehyde	0.00	0.00	0.00	0.00	77.50	91.00	101.00	101.00								
62		C11H15N3O	205.26	2.02	2.02	67.48	2	2	cuminaldehyde	0.00	0.00	0.00	0.00	101.00	96.00	101.00	101.00								
63		C11H15N3S	221.32	2.91	2.91	50.41	1	2	cuminaldehyde	80.00	90.00	100.00	100.00	101.00	101.00	85.00	53.00			Not mutagen	100.00	101.00	101.00	25.00	
64		C22H28N6NiS2	499.32			115.18	0	0	cuminaldehyde	84.00	90.00	91.50	96.00												
65		C22H28N6S2Zn	506.01			115.18	0	0	cuminaldehyde	25.00	11.20	93.78	100.00	54.00	41.50	42.00	101.00								

66		C26H35N6O4S2Zn	625.10			114.85	0	0	cuminaldehyde			69.30	81.90	30.00	36.00	33.00	32.00					
67		C11H15N3S	221.32	2.91	2.91	50.41	1	2	cuminaldehyde	19.00	21.00	67.00	97.00	101.00	101.00	101.00	73.00	Not mutagen				
68		C11H15N3S	221.32	2.91	2.91	50.41	1	2	cuminaldehyde	0.00	0.00	0.00	0.00	101.00	101.00	101.00	101.00	Not mutagen	100.00	101.00	10.00	10.00
69		C22H29CuN6S2	505.18			114.85	0	0	cuminaldehyde	0.00	0.00	46.00	73.51	16.00	18.00	32.00	24.00					
70		C22H29CuN6S2	505.18			114.85	0	0	cuminaldehyde	3.40	24.00	65.93	80.83	31.50	26.00	32.50	20.00					
71		C22H28N6S2Zn	506.01			115.18	0	0	cuminaldehyde	56.00	60.30	97.10	100.00	33.50	21.00	26.00	36.00	Not mutagen	1.00	0.01	101.00	0.10
72		C10H12O	148.21	2.93	2.93	17.07	1	0	cuminaldehyde	0.0	0.0	0.0	13.9									
73		C10H12O	148.21	2.93	2.93	17.07	1	0	cuminaldehyde	0.0	0.0	0.0	0.0									
74		C12H17N3S	235.35	3.13	3.13	41.62	1	1	cuminaldehyde	47.7	70.6	19.46	62.74	101.00	97.00	101.00	66.00					
75		C12H17N3S	235.35	3.13	3.13	41.62	1	1	cuminaldehyde	29.2	32.5	7.40	41.80									
76		C12H17N3S	235.35	3.13	3.13	41.62	1	1	cuminaldehyde	19.1	22.1	38.44	37.69									
77		C28H40CuN6O4S2	652.33			96.94	0	0	cuminaldehyde	90	95	71.40	86.70	9.50	31.00	17.50	20.00					
78		C12H19N3S	237.37	2.65	2.65	41.29	1	2	cuminaldehyde	0.00	4.00	13.00	10.00									

		C13H19N3S					cuminaldehyde								
79		249.38	3.36	3.36	27.63	1	1								
		C21H20O6					curcumin								
80		368.39	4.12	4.12	93.06	6	2	14.00	41.00	0.00	0.00				
		C42H38CuO12					curcumin								
81		798.30			254.40	0	0	0.00	14.00	0.00	0.00				
		C7H13N3S					cyclohexanone								
82		171.26	1.47	1.47	50.41	1	2	80.00	95.00	0.00	11.00				
		C22H36CuN6S2					decanal								
83		512.24			115.18	0	0	91	80						
		C11H23N3S					decanal								
84		229.39	3.41	3.41	50.41	1	2	96.00	96.00	8.00	62.00	65	33.00	insolubile	30
		C10H20O					decanal								
85		156.27	3.43	3.43	17.07	1	0	0.00	17.00	0.00	0.00				
		C14H25N3S					Dicyclohexyl ketone								
86		267.44	4.31	4.31	50.41	1	2	90.00	99.00	18.00	32.00				
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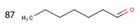
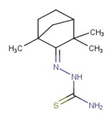
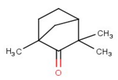
87		114.19	2.10	2.10	17.07	1	0	0.00	0.00	0.00	0.00				
		C11H19N3S					fenchone								
88		225.35	3.04	3.04	50.41	1	2	17.00	41.00	2.00	7.00				
		C10H16O					fenchone								
89		152.24	3.06	3.06	17.07	1	0	10.00	27.00	0.00	0.00				
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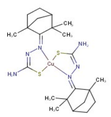
90		512.24			115.18	0	0	45.00	57.00	62.00	84.00				
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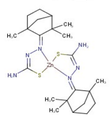
91		514.07			115.18	0	0	20.00	18.00	0.00	0.00				

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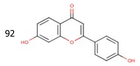
92		254.24	2.36	1.42	66.76	4	2	24.00	25.00	26.00	22.00											
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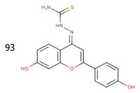
93		327.36	2.34	2.17	100.10	4	4	18.00	29.00	9.00	9.00											
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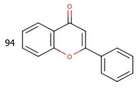
94		222.24	2.97	2.97	26.30	2	0	66.00	83.00													
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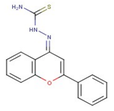
95		295.36	2.95	2.95	59.64	2	2	100.00	100.00													
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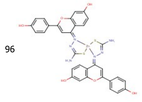
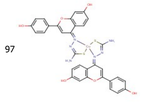
96		718.08			214.56	0	0	4.00	18.00													
		C32H24CuN6O6S2					flavone															
97		716.25			214.56	0	0	100.00	100.00	31.00	41.00								27.00			
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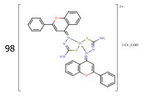
98		654.08			133.64	0	0	15.00	23.00													
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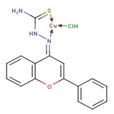
99		395.36			66.49	3	2	60.00	79.00													
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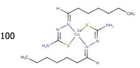
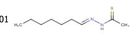
100		436.14			115.18	0	0	16.3	49.5	62.80	85.50	30.50	29.00	10.00	29.00							
		C9H18N2S					heptanal									no	yes	Weakly mutagen				
101		186.32	2.41	2.41	24.39	1	1	42.00	58.00	22.00	51.00	101.00	101.00	101.00	101.00				50.00	101.00	10.00	
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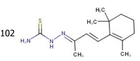
102		265.42	3.26	3.26	50.41	1	2	0.00	0.00	0.00	0.00											
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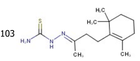
103		267.44	3.26	3.26	50.41	1	2	0.00	0.00	0.00	0.00											
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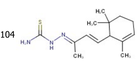
104		265.42	3.30	3.30	50.41	1	2	0.00	0.00	0.00	0.00											

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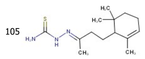
105		267.44	3.30	3.30	50.41	1	2	0.00	0.00	0.00	0.00														
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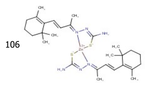
106		594.20			115.18	0	0	0.00	0.00	0.00	0.00														
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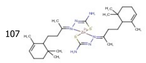
107		598.23			115.18	0	0	0.00	0.00	0.00	0.00														
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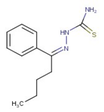
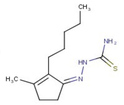
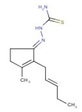
108		235.35	3.10	3.10	50.41	1	2	44.00	54.00	34.00	55.00	101.00	79.50	101.00	58.00										
		C12H21N3S					jasmone									yes	yes	Not mutagen							
109		239.38	3.44	3.44	50.41	1	2	16.90	24.70	51.54	63.18	101.00	101.00	101.00	101.00							101.00	101.00		10.00
		C12H19N3S					jasmone									yes		Not mutagen							
110		237.37	3.08	3.08	50.41	1	2	22	44	88.00	90.00	101.00	101.00	101.00	40.00							101.00	100.00		10.00
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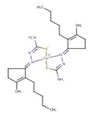
111		540.29			115.18	0	0	0	11	66.00	80.00														
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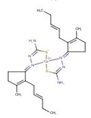
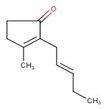
112		536.26			115.18	0	0	37.5	74.3	78.00	97.00	38.00	28.00	5.00	18.00										
		C11H16O					jasmone									no	yes								
113		164.25	3.10	3.10	17.07	1	0	0.0	23.0	20.0	28.0	101.00	101.00	101.00	101.00										
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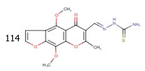
114		361.37	1.12	1.12	108.31	5	2	5.00	5.00	6.00	25.00														
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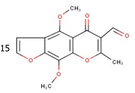
115		288.26	1.14	1.14	74.97	5	0	-7.00	-12.00	3.00	10.00														
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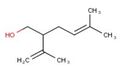
116		154.25	2.32	2.32	20.23	1	1	18.00	29.00	26.00	34.00														
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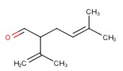
117		152.24	2.46	2.46	17.07	1	0	17.00	34.00	0.00	13.00														

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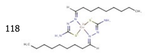
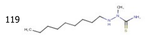
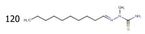
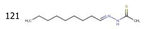
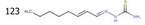
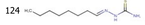
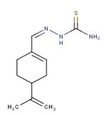
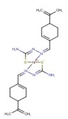
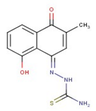
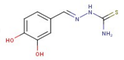
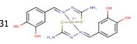
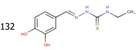
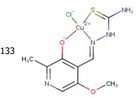
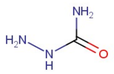
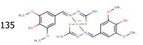
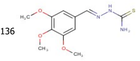
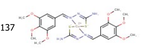
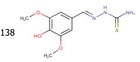
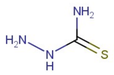
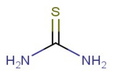
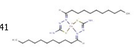
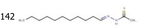
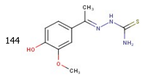
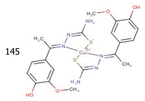
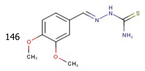
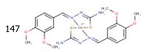
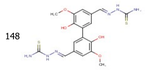
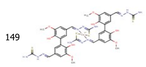
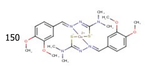
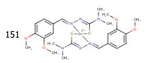
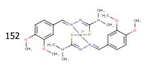
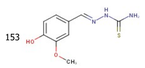
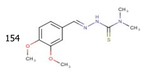
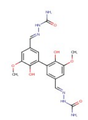
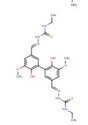
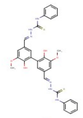
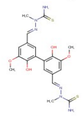
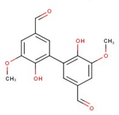
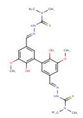
118		492.25			115.18	0	0	34.2	84.1	90.00	100.00	44.00	30.50	35.00	101.00			
		C11H25N3S					nonanal											
119		231.40	3.22	3.22	41.29	1	2	43.00	50.00	-17.00	-6.00							
		C12H25N3S					nonanal											
120		243.41	3.63	3.63	41.62	1	1	35.00	47.00	11.00	26.00							
		C11H22N2S					nonanal											
121		214.37	3.30	3.30	24.39	1	1	95.0	100.0	91.00	101.00	32.00	63.00	80.00	41.00			
		C9H18O					nonanal											
122		142.24	2.99	2.99	17.07	1	0	0.00	0.00	0.00	0.00							
		C9H17N3S					octanal											
123		199.32	2.52	2.52	50.41	1	2	93.00	96.00	76.00	96.00	101	101.00	insolubile	101			
		C9H19N3S					octanal											
124		201.33	2.52	2.52	50.41	1	2	82.00	93.00	0.00	31.00	101	93.00	insolubile	94			
		C8H16O					octanal											
125		128.22	2.54	2.54	17.07	1	0	0.00	0.00	0.00	8.00							
		C8H14O					octanal											
126		126.20	2.54	2.54	17.07	1	0	7.00	32.00	6.00	3.00							
		C11H17N3S					perillaldehyde									no	no	Not mutagen
127		223.34	2.23	2.23	50.41	1	2	46	73.5	78.00	87.30	71.00	34.00		101.00			
		C22H32N6NiS2					perillaldehyde									yes	tox	Not mutagen
128		503.35			115.18	0	0	3.7	14.2	85.20	90.10	49.00	35.00		101.00			
		C12H11N3O2S					plumbagin											
129		261.30	1.57	1.50	87.71	3	3	36.7	61.9	50.00	83.00	100.00	97.00	57.00	101.00			
		C8H9N3O2S					protocatechualdehyde											
130		211.24	1.06	1.05	90.87	3	4	53.00	77.00	5.00	0.00							

		C16H16CuN6O4S2					protocatechualdehyde								
131		484.01			196.10	0	0	0.00	0.00	0.00	6.00				
		C10H13N3O2S					protocatechualdehyde								
132		239.29	1.64	1.63	76.88	3	4	17.00	24.00	0.00	5.00				
		C9H11ClCuN4O2S					pyridoxal								
133		338.27			88.61	0	0	0.00	0.00	0.00	0.00				
		CH5N3O					semicarbazide								
134		75.07	-1.66	-1.66	81.14	2	3	0.00	0.00	0.00	0.00				
		C20H24CuN6O6S2					syringaldehyde								
135		572.11			192.56	0	0	48.00	61.00	29.00	61.00				
		C11H15N3O3S					syringaldehyde								
136		269.32	1.19	1.19	78.10	4	2	0.00	0.00	6.00	0.00				
		C22H28CuN6O6S2					syringaldehyde								
137		600.17			170.56	0	0	55.00	54.00	47.00	76.00				
		C10H13N3O3S					syringaldehyde								
138		255.29	1.05	1.04	89.10	4	3	3.00	0.00	0.00	2.00				
		CH5N3S					thiosemicarbazide								
139		91.13	-0.77	-0.77	64.07	1	3	0.00	0.00	0.00	0.00			101.00	
		CH4N2S					thiourea								
140		76.12	-0.47	-0.47	52.04	0	2	0.00	0.00	0.00	0.00			101.00	
		C24H48CuN6S2					undecanal								
141		548.36			115.18	0	0	60.4	94	84.80	96.00				
		C13H26N2S					undecanal								
142		242.43	4.19	4.19	24.39	1	1	78.00	62.00	72.00	93.00	77.00	28.00	46.50	101.00
		C11H22O					undecanal								
143		170.30	3.88	3.88	17.07	1	0	0.00	14.00	7.00	19.00				

144		C10H13N3O2S	239.29	1.05	1.05	79.87	3	3	vanillin	48.00	50.00	26.00	12.00									
145		C20H24CuN6O4S2	540.12			174.10	0	0	vanillin	61.00	72.00	52.00	72.00	31.00	16.00	30.00	27.00					
146		C10H13N3O2S	239.29	1.35	1.35	68.87	3	2	vanillin	20.00	3.00	26.00	25.00									
147		C20H24CuN6O4S2	540.12			152.10	0	0	vanillin	41.00	51.00	62.00	80.00	37.50	17.00	29.00	27.00					
148		C18H20N6O4S2	448.52	2.08	2.07	159.74	6	6	vanillin	39	57	43.00	61.00	101.00	101.00	101.00	101.00	Not mutagen	100.00	25.00	10.00	101.00
149		C36H38CuN12O8S4	958.56			333.84	0	0	vanillin	44.2	65.5	53.00	77.00	46.00	101.00	43.00	24.00					
150		C24H32CuN6O4S2	596.22			106.54	0	0	vanillin	0.00	5.00	61.40	84.60	0.75	2.50	0.50	3.00					
151		C24H32N6O4S2Zn	598.06			106.54	0	0	vanillin	1.00	16.00	0.00	28.00									
152		C24H32N6NiO4S2	591.37			106.54	0	0	vanillin	0.00	0.00	0.00	0.00									
153		C9H11N3O2S	225.27	1.20	1.20	79.87	3	3	vanillin	3.00	0.00	16.00	18.00									
154		C12H17N3O2S	267.35	1.80	1.80	46.09	3	1	vanillin	0.00	0.00	0.00	7.10									
155		C18H20N6O6	416.39	0.30	0.29	193.88	8	6	vanillin	0.0	11.0											
156		C22H28N6O4S2	504.62	3.24	3.23	131.76	6	6	vanillin	5.0	13.0											

157		C30H28N6O4S2	600.71	6.56	6.55	131.76	6	vanillin 6	4.0	11.0
158		C20H24N6O4S2	476.57	2.53	2.51	142.16	6	vanillin 4	17.0	17.0
159		C16H14O6	302.28	2.12	1.53	93.06	6	vanillin 2	0.0	8.0
160		C22H28N6O4S2	504.62	2.98	2.96	114.18	6	vanillin 4	1.0	8.0

M)