

GC-MS

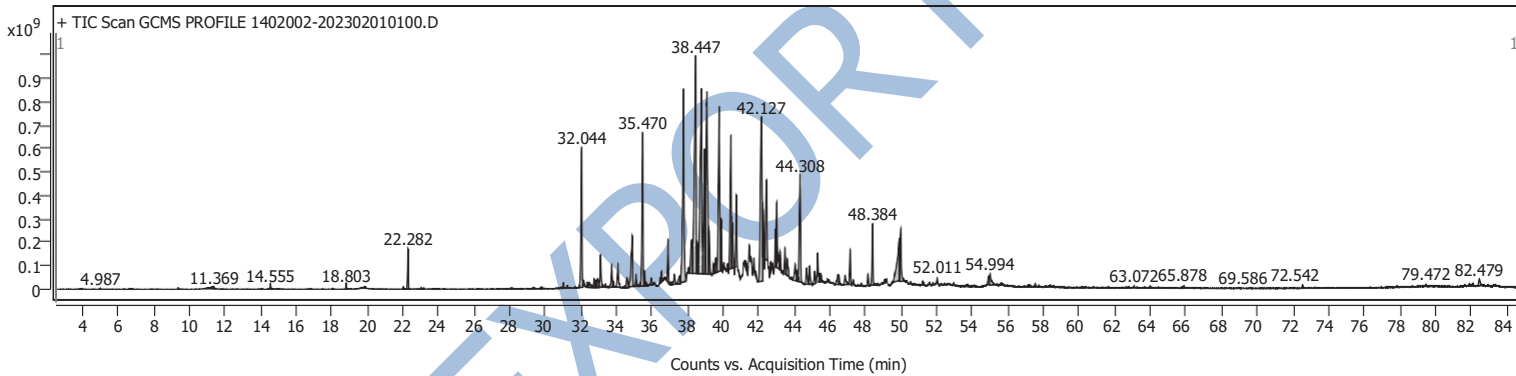
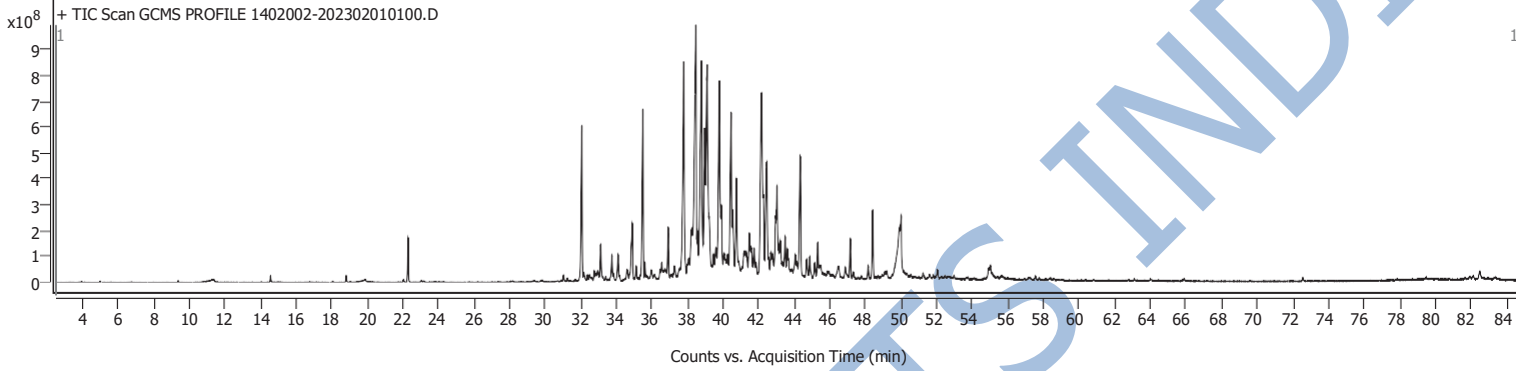
Analysis Report



Sample Information

Name	AGARWOOD OIL 202302010100	Data File Path	J:\GCMS\Data\YEAR 2023\FEBRUARY\GCMS PROFILE\14022023\GCMS PROFILE 1402002-202302010100.D
Sample ID		Acq. Time (Local)	14-02-2023 17:48:29 (UTC+05:30)
Instrument	GCMSMS	Method Path (Acq)	J:\GCMS\Method\GCMS PROFILE.M
MS Type	QQQ	Version (Acq SW)	MassHunter GC/MS Acquisition 10.1.49 02-Nov-2020 Copyright © 1989-2020 Agilent Technologies, Inc.
Inj. Vol. (ul)	1	IRM Status	
Position	1	Method Path (DA)	
Plate Pos.		Target Source Path	J:\Mass Hunter old\Library\NIST17.L
Operator	Sanjay Kumar Sharma	Result Summary	211 found

Sample Chromatograms



Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	3.780	3.949	3.997	2453437	11595084	0.02	
2	4.960	4.987	5.074	4936643	11723736	0.02	
3	6.515	6.738	6.876	1577720	11368946	0.01	
4	9.324	9.361	9.432	6820689	18930332	0.02	
5	10.877	11.369	11.490	9484386	143807737	0.19	
6	13.968	14.040	14.153	2483967	8820408	0.01	
7	14.494	14.555	14.685	25872566	81239954	0.11	
8	14.842	15.017	15.060	1085324	6671747	0.01	
9	17.984	18.047	18.129	4556535	15289178	0.02	
10	18.736	18.803	18.947	26537364	85762229	0.11	
11	19.749	19.904	19.956	6732136	38212574	0.05	
12	21.941	22.021	22.131	11194242	41064589	0.05	
13	22.189	22.282	22.450	172342964	614976975	0.80	
14	22.953	23.021	23.106	7463555	25704458	0.03	
15	23.106	23.169	23.241	4838866	17435288	0.02	
16	23.592	23.740	23.770	1629985	7828240	0.01	
17	23.770	23.826	23.933	2545563	12017863	0.02	
18	23.933	24.039	24.096	1745439	7816885	0.01	
19	26.122	26.186	26.331	1417866	7277672	0.01	
20	26.898	27.026	27.086	1759104	8037878	0.01	
21	27.225	27.404	27.495	833190	6756456	0.01	
22	27.764	27.863	27.936	1865990	8206759	0.01	
23	27.999	28.048	28.091	3109417	10171721	0.01	
24	28.091	28.156	28.209	3065186	11032877	0.01	
25	28.547	28.640	28.694	1677903	6924652	0.01	
26	29.220	29.269	29.317	3230247	10346015	0.01	
27	29.317	29.369	29.472	5068396	21202811	0.03	
28	29.642	29.740	29.765	6003914	25758629	0.03	
29	29.765	29.815	29.907	7054835	33347940	0.04	
30	30.551	30.668	30.718	2564812	10768127	0.01	
31	30.836	30.888	30.941	5188468	17034086	0.02	
32	30.941	31.016	31.151	25300639	98501991	0.13	
33	31.178	31.234	31.294	13299265	42731783	0.06	

Analysis Report

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
34	31.323	31.382	31.432	2396376	7771473	0.01	
35	31.623	31.678	31.729	6480198	21763551	0.03	
36	31.906	32.044	32.104	597824195	2655086457	3.44	
37	32.104	32.156	32.254	22003221	89707187	0.12	
38	32.299	32.359	32.414	21893448	74458420	0.10	
39	32.414	32.475	32.575	21933479	124684079	0.16	
40	32.575	32.615	32.662	10644263	38062755	0.05	
41	32.673	32.738	32.785	39274430	146347445	0.19	
42	32.785	32.828	32.881	26489746	132901900	0.17	
43	32.881	32.933	33.016	38780854	221072817	0.29	
44	33.016	33.101	33.216	138928980	641599503	0.83	
45	33.216	33.239	33.296	8524005	25116762	0.03	
46	33.319	33.387	33.442	14314313	49904389	0.06	
47	33.475	33.532	33.580	6021204	19881881	0.03	
48	33.597	33.730	33.793	95978260	437138172	0.57	
49	33.793	33.828	33.888	24315039	79067243	0.10	
50	33.965	34.076	34.229	99857811	520012200	0.67	
51	34.322	34.389	34.437	5668238	24496545	0.03	
52	34.437	34.487	34.507	9433116	30735970	0.04	
53	34.507	34.580	34.678	43997314	276652338	0.36	
54	34.678	34.873	34.949	217608653	1361144200	1.76	
55	34.956	34.993	35.021	3199775	6918260	0.01	
56	35.021	35.089	35.166	51983026	196396240	0.25	
57	35.166	35.209	35.247	5083669	16711358	0.02	
58	35.337	35.470	35.532	656844331	3004216780	3.89	
59	35.532	35.585	35.640	61740538	211610709	0.27	
60	35.640	35.685	35.775	11681768	62600441	0.08	
61	35.867	35.941	36.036	30199909	145623846	0.19	
62	36.054	36.101	36.165	8944449	31649416	0.04	
63	36.391	36.435	36.472	24688631	79727308	0.10	
64	36.472	36.530	36.590	44854701	179225292	0.23	
65	36.590	36.625	36.643	5777979	17119739	0.02	
66	36.643	36.703	36.744	8351013	28377959	0.04	
67	36.821	36.889	36.965	184702075	677529379	0.88	
68	36.984	37.051	37.111	11885171	50899239	0.07	
69	37.111	37.252	37.371	40667905	245429196	0.32	
70	37.402	37.535	37.578	29991718	202363191	0.26	
71	37.580	37.771	37.903	823833989	4901852783	6.35	
72	37.981	38.051	38.090	23003157	70968869	0.09	
73	38.107	38.219	38.277	142306191	984826864	1.28	
74	38.277	38.447	38.500	929898434	6585409194	8.53	
75	38.500	38.528	38.585	134890916	486218343	0.63	
76	38.585	38.768	38.853	790483148	5630425386	7.30	
77	38.853	38.946	38.991	532834241	2601397294	3.37	
78	38.991	39.079	39.172	778373572	5306255694	6.88	
79	39.172	39.189	39.299	191690174	780027685	1.01	
80	39.305	39.325	39.360	4180877	8436948	0.01	
81	39.392	39.440	39.492	42785352	128998198	0.17	
82	39.498	39.573	39.635	63822597	320951332	0.42	
83	39.635	39.763	39.851	704394125	4178767858	5.42	
84	39.851	39.881	39.944	219471942	737734079	0.96	
85	39.994	40.032	40.104	27718878	91061446	0.12	
86	40.189	40.235	40.275	32948363	93142146	0.12	
87	40.316	40.425	40.470	569708649	2859473751	3.71	
88	40.470	40.505	40.592	192631934	887186888	1.15	
89	40.655	40.726	40.793	306402650	1255156557	1.63	
90	40.839	40.844	40.906	2936790	16583218	0.02	
91	41.129	41.142	41.162	7001408	6603742	0.01	
92	41.182	41.210	41.363	19337345	206499470	0.27	
93	41.417	41.455	41.518	60497996	185067303	0.24	
94	41.522	41.558	41.589	18198590	41828859	0.05	
95	41.681	41.718	41.766	55404010	161027825	0.21	
96	41.791	41.826	41.897	24632230	84831140	0.11	
97	41.947	42.127	42.215	700303767	5382120150	6.97	
98	42.215	42.230	42.283	204810654	603978188	0.78	
99	42.333	42.430	42.491	341251629	1877781147	2.43	
100	42.618	42.661	42.701	37279050	112373741	0.15	
101	42.731	42.754	42.801	20343745	49518426	0.06	
102	42.871	42.939	42.957	163389852	565229459	0.73	
103	42.957	43.007	43.117	281662741	1316773057	1.71	
104	43.117	43.185	43.260	80965778	408985702	0.53	
105	43.280	43.305	43.343	8676332	19301449	0.03	
106	43.383	43.461	43.528	113623245	437917785	0.57	
107	43.528	43.583	43.713	73888090	390758820	0.51	
108	43.786	43.839	43.894	8754700	31449112	0.04	
109	43.906	44.032	44.085	71870554	383666636	0.50	
110	44.085	44.125	44.180	44089679	196468495	0.25	
111	44.180	44.308	44.438	459088420	2635898870	3.42	
112	44.574	44.675	44.774	68659418	370973881	0.48	
113	44.774	44.849	44.985	80327574	370587689	0.48	
114	45.020	45.127	45.203	53311135	237090341	0.31	
115	45.226	45.299	45.361	123857931	507170587	0.66	
116	45.361	45.416	45.443	33917045	154723800	0.20	
117	45.443	45.471	45.621	32951891	134505568	0.17	
118	45.784	45.847	45.884	14184998	46706973	0.06	
119	45.884	45.935	45.988	11252409	45898826	0.06	
120	46.262	46.431	46.449	41635810	202930154	0.26	

Analysis Report

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
121	46.449	46.466	46.638	41145393	173145512	0.22	
122	46.747	46.837	47.016	41409003	241734848	0.31	
123	47.031	47.122	47.184	150284027	588147470	0.76	
124	47.223	47.293	47.401	24704567	108442729	0.14	
125	47.520	47.554	47.634	3324326	11481583	0.01	
126	47.667	47.757	47.827	11108518	45960391	0.06	
127	48.034	48.123	48.222	48913847	208550771	0.27	
128	48.274	48.384	48.468	263213851	1127829857	1.46	
129	48.482	48.537	48.632	3643436	19153951	0.02	
130	48.632	48.685	48.728	6779505	21459496	0.03	
131	48.833	48.903	48.990	6592674	29788001	0.04	
132	48.990	49.068	49.118	15147376	63503442	0.08	
133	49.118	49.166	49.209	15611205	51342779	0.07	
134	49.414	49.477	49.499	3841334	16604202	0.02	
135	49.513	49.878	49.893	169121280	1599607340	2.07	
136	49.893	49.981	50.103	228366197	1429010956	1.85	
137	50.252	50.307	50.358	5989755	20871252	0.03	
138	50.450	50.517	50.578	9825822	41149101	0.05	
139	50.632	50.700	50.745	3123341	10511172	0.01	
140	50.745	50.783	50.843	3002906	10884085	0.01	
141	50.951	50.983	51.038	3759771	11874405	0.02	
142	51.076	51.216	51.346	21008623	122302956	0.16	
143	51.490	51.582	51.684	13356227	65804198	0.09	
144	51.721	51.783	51.848	11851362	41034094	0.05	
145	51.940	52.011	52.114	26773148	109668520	0.14	
146	52.162	52.237	52.362	5699972	39333421	0.05	
147	52.362	52.440	52.511	9488052	38998575	0.05	
148	52.533	52.628	52.665	5650731	27780248	0.04	
149	52.665	52.701	52.783	4623593	19699316	0.03	
150	52.891	52.944	53.028	12825043	46907056	0.06	
151	53.068	53.114	53.177	2400183	7727647	0.01	
152	53.428	53.468	53.550	2811754	10675098	0.01	
153	53.572	53.638	53.676	7805922	27577949	0.04	
154	53.676	53.723	53.783	10409118	38038057	0.05	
155	53.814	53.901	53.943	1760089	8248352	0.01	
156	53.977	54.084	54.155	6831350	31803832	0.04	
157	54.582	54.648	54.691	2289245	8699564	0.01	
158	54.774	54.902	54.934	35556786	173441100	0.22	
159	54.934	54.994	55.304	50040464	396355348	0.51	
160	55.328	55.391	55.465	4446201	21625538	0.03	
161	55.514	55.624	55.849	11964370	101868854	0.13	
162	55.893	55.955	56.030	2771262	11580112	0.02	
163	56.563	56.617	56.696	2618333	10190083	0.01	
164	56.807	56.910	56.966	5272960	20431983	0.03	
165	57.018	57.100	57.138	6830426	27587322	0.04	
166	57.138	57.168	57.211	8304277	29165747	0.04	
167	57.211	57.246	57.333	7322711	31358068	0.04	
168	57.407	57.524	57.605	14941507	67760397	0.09	
169	57.647	57.737	57.797	6918120	27492095	0.04	
170	58.238	58.374	58.447	7249534	41163554	0.05	
171	58.449	58.549	58.639	5640710	30826940	0.04	
172	58.698	58.758	58.868	2264259	12816224	0.02	
173	58.868	58.918	58.976	2688342	90222702	0.01	
174	58.976	59.046	59.146	3778115	16786938	0.02	
175	59.817	59.876	59.923	2234509	8042310	0.01	
176	60.277	60.340	60.405	1979456	8232640	0.01	
177	60.723	60.791	60.865	5078305	19505870	0.03	
178	61.538	61.628	61.714	2883286	14325740	0.02	
179	62.330	62.431	62.502	1861306	7620395	0.01	
180	62.551	62.609	62.658	1881311	6877132	0.01	
181	62.669	62.746	62.819	4760806	19449880	0.03	
182	63.015	63.072	63.154	6348945	25704906	0.03	
183	63.171	63.238	63.304	3678167	13823144	0.02	
184	63.579	63.669	63.719	2391787	12106155	0.02	
185	63.884	63.972	64.213	6998147	48136288	0.06	
186	64.366	64.439	64.521	2789525	13325748	0.02	
187	64.608	64.687	64.734	2292838	8629107	0.01	
188	65.710	65.783	65.813	4104154	15153260	0.02	
189	65.813	65.878	66.013	10746545	51396874	0.07	
190	67.110	67.179	67.239	2589997	9242022	0.01	
191	69.513	69.586	69.651	2179300	8457539	0.01	
192	72.457	72.542	72.643	15389709	62368818	0.08	
193	73.169	73.261	73.357	2297607	13819284	0.02	
194	76.260	76.318	76.405	1648147	7553701	0.01	
195	77.485	77.536	77.611	2157852	8846756	0.01	
196	77.707	77.830	77.954	4492157	29897124	0.04	
197	78.469	78.557	78.612	1861076	8549118	0.01	
198	78.612	78.707	78.837	2944726	18488153	0.02	
199	79.328	79.472	79.580	6686290	42727315	0.06	
200	79.580	79.796	79.891	2593356	25394779	0.03	
201	79.956	80.056	80.157	2796149	19121898	0.02	
202	80.706	80.766	80.865	2820389	13352355	0.02	
203	81.574	81.671	81.743	4857890	23486633	0.03	
204	81.822	81.932	82.007	9937034	49927329	0.06	
205	82.007	82.113	82.204	11759414	73616632	0.10	
206	82.365	82.479	82.619	27854236	185656824	0.24	
207	82.672	82.725	82.768	2349870	8518190	0.01	

Analysis Report

Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
208	82.880	82.955	82.960	3314144	9563412	0.01	
209	82.960	82.975	83.093	3479792	16044397	0.02	
210	83.230	83.362	83.471	5484797	40826892	0.05	
211	83.504	83.522	83.670	1104943	8861732	0.01	

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1	Butanoic acid	C4 H8 O2	3.949		107-92-6	LibSearch	71.99	71.99			Integrate
2	3-Furaldehyde	C5 H4 O2	4.987		498-60-2	LibSearch	69.40	69.40			Integrate
3	Urea	C H4 N2 O	6.738		57-13-6	LibSearch	60.43	60.43			Integrate
4	Benzoyl isothiocyanate	C8 H5 N O S	9.361		532-55-8	LibSearch	88.29	88.29			Integrate
5	Hexanoic acid	C6 H12 O2	11.369		142-62-1	LibSearch	72.89	72.89			Integrate
6	Benzoyl isothiocyanate	C8 H5 N O S	14.040		532-55-8	LibSearch	78.44	78.44			Integrate
7	p-Cresol	C7 H8 O	14.555		106-44-5	LibSearch	74.06	74.06			Integrate
8	Propionic acid, 3-tetrazol-1-yl-	C4 H6 N4 O2	15.017		1000304-09-3	LibSearch	63.93	63.93			Integrate
9	Benzene, 1-ethenyl-4-methoxy-	C9 H10 O	18.047		637-69-4	LibSearch	73.55	73.55			Integrate
10	Phenol, 3,5-dimethyl-	C8 H10 O	18.803		108-68-9	LibSearch	77.50	77.50			Integrate
11	Octanoic acid	C8 H16 O2	19.904		124-07-2	LibSearch	71.07	71.07			Integrate
12	4,5,6,7-Tetrahydroindazole-3-spirocyclohexane	C12 H18 N2	22.021		1000098-34-3	LibSearch	67.87	67.87			Integrate
13	2-Butanone, 4-phenyl-	C10 H12 O	22.282		2550-26-7	LibSearch	76.04	76.04			Integrate
14	Phenol, 3-propyl-	C9 H12 O	23.021		621-27-2	LibSearch	70.75	70.75			Integrate
15	Cyclohexane, 1-ethenyl-3-methylene-5-(1-propenylidene)-	C12 H16	23.169		61142-28-7	LibSearch	75.06	75.06			Integrate
16	n-Dodecylpyridinium chloride	C17 H30 Cl N	23.740		104-74-5	LibSearch	55.76	55.76			Integrate
17	3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	C13 H20 O	23.826		6901-97-9	LibSearch	73.71	73.71			Integrate
18	Oxacyclotetradeca-4,11-diyne	C13 H18 O	24.039		6568-32-7	LibSearch	65.31	65.31			Integrate
19	Cyclohexane, 1-ethenyl-3-methylene-5-(1-propenylidene)-	C12 H16	26.186		61142-28-7	LibSearch	66.79	66.79			Integrate
20	2,3-Diazabicyclo[2.2.1]hept-2-ene, 7,7-dimethyl-5-phenyl-, (1.alpha.,4.alpha.,5.beta.)-	C13 H16 N2	27.026		1000221-85-6	LibSearch	70.33	70.33			Integrate
21	1,8-Cyclopentadecadiyne	C15 H22	27.404		4722-42-3	LibSearch	65.17	65.17			Integrate
22	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	27.863		1000221-85-9	LibSearch	75.50	75.50			Integrate
23	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	28.048		1000221-85-9	LibSearch	73.15	73.15			Integrate
24	Benzene, 1,3,5-trimethyl-2-(1,2-propadienyl)-	C12 H14	28.156		29555-07-5	LibSearch	63.97	63.97			Integrate
25	2,3-Diazabicyclo[2.2.1]hept-2-ene, 7,7-dimethyl-5-phenyl-, (1.alpha.,4.alpha.,5.beta.)-	C13 H16 N2	28.640		1000221-85-6	LibSearch	62.37	62.37			Integrate
26	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	29.269		1000221-85-9	LibSearch	81.22	81.22			Integrate
27	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	29.369		1000185-64-0	LibSearch	68.30	68.30			Integrate
28	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	29.740		1000221-85-9	LibSearch	55.78	55.78			Integrate
29	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	29.815		1000221-85-9	LibSearch	58.60	58.60			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
30	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	30.668		1000221-85-9	LibSearch	75.58	75.58			Integrate
31	5,6-Decadien-3-yne, 5,7-diethyl-	C14 H22	30.888		61227-89-2	LibSearch	69.76	69.76			Integrate
32	4,5,6,7-Tetrahydroindazole-3-spirocyclohexane	C12 H18 N2	31.016		1000098-34-3	LibSearch	63.08	63.08			Integrate
33	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	31.234		1000221-85-9	LibSearch	76.39	76.39			Integrate
34	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	31.382		1000221-85-9	LibSearch	53.83	53.83			Integrate
35	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	31.678		1000221-85-9	LibSearch	72.46	72.46			Integrate
36	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1a-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-	C15 H24 O	32.044		6750-60-3	LibSearch	66.83	66.83			Integrate
37	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	32.156		1000221-85-9	LibSearch	77.37	77.37			Integrate
38	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	32.359		1000221-85-9	LibSearch	75.71	75.71			Integrate
39	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	32.475		1000221-85-9	LibSearch	75.22	75.22			Integrate
40	trans-Valerenyl acetate	C17 H26 O2	32.615		101527-74-6	LibSearch	71.04	71.04			Integrate
41	Aristol-1(10)-en-9-yl isovalerate	C20 H32 O2	32.738		1000414-30-6	LibSearch	82.15	82.15			Integrate
42	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	32.828		14113-61-2	LibSearch	63.68	63.68			Integrate
43	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	32.933		1000221-85-9	LibSearch	71.01	71.01			Integrate
44	Undeca-3,4-diene-2,10-dione, 5,6,6-trimethyl-	C14 H22 O2	33.101		90165-10-9	LibSearch	64.35	64.35			Integrate
45	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	33.239		1000221-85-9	LibSearch	65.93	65.93			Integrate
46	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	33.387		1000221-85-9	LibSearch	75.54	75.54			Integrate
47	Oxacyclotetradeca-4,11-diyne	C13 H18 O	33.532		6568-32-7	LibSearch	68.02	68.02			Integrate
48	4,5,6,7-Tetrahydroindazole-3-spirocyclohexane	C12 H18 N2	33.730		1000098-34-3	LibSearch	65.36	65.36			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
49	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	33.828		1000221-85-9	LibSearch	76.13	76.13			Integrate
50	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	C15 H24	34.076		483-76-1	LibSearch	67.94	67.94			Integrate
51	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	34.389		1000221-85-9	LibSearch	65.90	65.90			Integrate
52	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	34.487		1000221-85-9	LibSearch	75.34	75.34			Integrate
53	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	34.580		1000221-85-9	LibSearch	73.29	73.29			Integrate
54	2,3-Diazabicyclo[2.2.1]hept-2-ene, 7,7-dimethyl-5-phenyl-, (1.alpha.,4.alpha.,5.beta.)-	C13 H16 N2	34.873		1000221-85-6	LibSearch	53.52	53.52			Integrate
55	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	34.993		14113-61-2	LibSearch	70.87	70.87			Integrate
56	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	35.089		1000221-85-9	LibSearch	82.43	82.43			Integrate
57	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	35.209		14113-61-2	LibSearch	69.59	69.59			Integrate
58	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R-cis)-	C15 H22 O	35.470		15764-04-2	LibSearch	60.03	60.03			Integrate
59	Adamantane, 1-isothiocyanato-3-methyl-	C12 H17 N S	35.585		136860-48-5	LibSearch	58.55	58.55			Integrate
60	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	35.685		1000221-85-9	LibSearch	72.53	72.53			Integrate
61	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	35.941		14113-61-2	LibSearch	64.93	64.93			Integrate
62	Oxacyclotetradeca-4,11-diyne	C13 H18 O	36.101		6568-32-7	LibSearch	68.66	68.66			Integrate
63	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	36.435		14113-61-2	LibSearch	68.88	68.88			Integrate
64	1,8-Cyclotetradecadiyne	C14 H20	36.530		1540-80-3	LibSearch	71.12	71.12			Integrate
65	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	36.625		14113-61-2	LibSearch	68.93	68.93			Integrate
66	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	36.703		14113-61-2	LibSearch	72.94	72.94			Integrate
67	2-Cyclopropylvinylidene-3-methoxy-1,1-dimethylcyclopropane	C11 H16 O	36.889		1000301-08-9	LibSearch	60.37	60.37			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
68	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	37.051		1000221-85-9	LibSearch	74.45	74.45			Integrate
69	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	37.252		1000185-64-0	LibSearch	74.71	74.71			Integrate
70	Oxacyclotetradeca-4,11-diyne	C13 H18 O	37.535		6568-32-7	LibSearch	67.82	67.82			Integrate
71	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)-	C15 H24	37.771		515-17-3	LibSearch	72.05	72.05			Integrate
72	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	38.051		1000221-85-9	LibSearch	71.36	71.36			Integrate
73	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)-	C15 H24	38.219		515-17-3	LibSearch	72.38	72.38			Integrate
74	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	38.447		1000221-85-9	LibSearch	76.06	76.06			Integrate
75	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	38.528		1000221-85-9	LibSearch	75.65	75.65			Integrate
76	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	38.768		1000221-85-9	LibSearch	73.69	73.69			Integrate
77	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	38.946		1000185-64-0	LibSearch	73.70	73.70			Integrate
78	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	39.079		1000221-85-9	LibSearch	74.09	74.09			Integrate
79	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	39.189		1000221-85-9	LibSearch	71.67	71.67			Integrate
80	1,8-Cyclotetradecadiyne	C14 H20	39.325		1540-80-3	LibSearch	66.46	66.46			Integrate
81	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	39.440		1000221-85-9	LibSearch	71.37	71.37			Integrate
82	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	39.573		1000221-85-9	LibSearch	70.14	70.14			Integrate
83	Tricyclo[4.4.0.0(2,7)]dec-8-ene-3-methanol, .alpha.,.alpha.,6,8-tetramethyl-, stereoisomer	C15 H24 O	39.763		41370-56-3	LibSearch	65.44	65.44			Integrate
84	1,8-Cyclotetradecadiyne	C14 H20	39.881		1540-80-3	LibSearch	68.07	68.07			Integrate
85	Oxacyclotetradeca-4,11-diyne	C13 H18 O	40.032		6568-32-7	LibSearch	71.29	71.29			Integrate
86	Heneicosapentaenoic Acid methyl ester	C22 H34 O2	40.235		65919-53-1	LibSearch	72.04	72.04			Integrate
87	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	40.425		1000185-64-0	LibSearch	67.51	67.51			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
88	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	40.505		1000221-85-9	LibSearch	70.01	70.01			Integrate
89	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	40.726		14113-61-2	LibSearch	70.16	70.16			Integrate
90	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	40.844		14113-61-2	LibSearch	71.58	71.58			Integrate
91	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	41.142		1000185-64-0	LibSearch	74.21	74.21			Integrate
92	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	41.210		1000185-64-0	LibSearch	68.68	68.68			Integrate
93	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	41.455		14113-61-2	LibSearch	69.04	69.04			Integrate
94	9-Borabicyclo[3.3.1]nonane, 9-(2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)-	C18 H31 B	41.558		73624-47-2	LibSearch	70.38	70.38			Integrate
95	9-Borabicyclo[3.3.1]nonane, 9-(2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)-	C18 H31 B	41.718		73624-47-2	LibSearch	70.21	70.21			Integrate
96	Arachidonoyl-N-methylamide, N-(trifluoroacetyl)-	C23 H34 F3 N O2	41.826		1000452-13-9	LibSearch	73.16	73.16			Integrate
97	1(2H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-4a,5-dimethyl-3-(1-methylethenyl)-, [3S-(3.alpha.,4a.alpha.,5.alpha.ha.)]-	C15 H22 O	42.127		562-23-2	LibSearch	67.73	67.73			Integrate
98	1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-1,4,9-tetramethyl-, (1.alpha.,4.alpha.,4a.alpha.ha.,8a.alpha.)-	C13 H22 N2	42.230		109746-14-7	LibSearch	72.43	72.43			Integrate
99	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.ha.,10a.alpha.)-	C13 H20 N2	42.430		1000221-85-9	LibSearch	70.31	70.31			Integrate
100	2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)prop-2-en-1-ol	C15 H24 O	42.661		515-20-8	LibSearch	70.81	70.81			Integrate
101	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	42.754		1000185-64-0	LibSearch	67.19	67.19			Integrate
102	9-Borabicyclo[3.3.1]nonane, 9-(2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)-	C18 H31 B	42.939		73624-47-2	LibSearch	70.06	70.06			Integrate
103	(E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahydronaphthalen-2(1H)-ylidene)propanal	C15 H22 O	43.007		137695-18-2	LibSearch	67.43	67.43			Integrate
104	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.ha.,10a.alpha.)-	C13 H20 N2	43.185		1000221-85-9	LibSearch	69.48	69.48			Integrate
105	O-Arachidonoylglycidol	C23 H36 O3	43.305		439146-24-4	LibSearch	71.51	71.51			Integrate
106	10,12-Tricosadynoic acid, methyl ester	C24 H40 O2	43.461		1000333-59-4	LibSearch	73.37	73.37			Integrate
107	Butyl 5,8,11,14,17-icosapentaenoate	C24 H38 O2	43.583		1000336-76-3	LibSearch	70.03	70.03			Integrate
108	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	43.839		14113-61-2	LibSearch	73.42	73.42			Integrate
109	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.ha.,10a.alpha.)-	C13 H20 N2	44.032		1000221-85-9	LibSearch	69.97	69.97			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
110	(E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahydronaphthalen-2(1H)-ylidene)propanal	C15 H22 O	44.125		137695-18-2	LibSearch	66.03	66.03			Integrate
111	Boron, (1,3-butanediiminato-N,N')-1,5-cyclooctanediyl-, (t-4)-	C12 H21 B N2	44.308		136704-98-8	LibSearch	63.10	63.10			Integrate
112	Oxacyclotetradeca-4,11-diyne	C13 H18 O	44.675		6568-32-7	LibSearch	69.29	69.29			Integrate
113	2aS,3aR,5aS,9bR)-2a,5a,9-Trimethyl-2a,4,5,5a,6,7,8,9b-octahydro-2H-naphtho[1,2-b]oxireno[2,3-c]furan	C15 H22 O2	44.849		352457-43-3	LibSearch	68.05	68.05			Integrate
114	Cyclopropane, 1-ethoxy-2,2-dimethyl-3-(2-phenylethenylidene)-	C15 H18 O	45.127		1000271-76-2	LibSearch	64.87	64.87			Integrate
115	1(2H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-4a,5-dimethyl-3-(1-methylethenyl)-, [3s-(3.alpha.,4a.alpha.,5.alpha.ha.)]-	C15 H22 O	45.299		562-23-2	LibSearch	65.97	65.97			Integrate
116	Oxacyclotetradeca-4,11-diyne	C13 H18 O	45.416		6568-32-7	LibSearch	66.25	66.25			Integrate
117	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	45.471		1000185-64-0	LibSearch	64.15	64.15			Integrate
118	Oxacyclotetradeca-4,11-diyne	C13 H18 O	45.847		6568-32-7	LibSearch	67.69	67.69			Integrate
119	Oxacyclotetradeca-4,11-diyne	C13 H18 O	45.935		6568-32-7	LibSearch	66.91	66.91			Integrate
120	Diazoprogesterone	C21 H30 N4	46.431		1000255-30-9	LibSearch	60.55	60.55			Integrate
121	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	46.466		14113-61-2	LibSearch	64.49	64.49			Integrate
122	Methyl 10,12-pentacosadiynoate	C26 H44 O2	46.837		1000342-58-7	LibSearch	63.22	63.22			Integrate
123	2,6-Diisopropyl-naphthalene	C16 H20	47.122		24157-81-1	LibSearch	65.39	65.39			Integrate
124	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	47.293		1000185-64-0	LibSearch	69.06	69.06			Integrate
125	Oxacyclotetradeca-4,11-diyne	C13 H18 O	47.554		6568-32-7	LibSearch	66.24	66.24			Integrate
126	Selenofenchone	C10 H16 Se	47.757		61849-83-0	LibSearch	61.91	61.91			Integrate
127	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	48.123		1000185-64-0	LibSearch	67.09	67.09			Integrate
128	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	48.384		14113-61-2	LibSearch	69.44	69.44			Integrate
129	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	48.537		14113-61-2	LibSearch	73.21	73.21			Integrate
130	Oxacyclotetradeca-4,11-diyne	C13 H18 O	48.685		6568-32-7	LibSearch	69.21	69.21			Integrate
131	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	48.903		1000210-42-6	LibSearch	69.31	69.31			Integrate
132	Andrographolide	C20 H30 O5	49.068		5508-58-7	LibSearch	73.41	73.41			Integrate
133	1-[3-(2,6,6-Trimethylcyclohex-2-enyl)-4,5-dihydro-3H-pyrazol-4-yl]-ethanone	C14 H22 N2 O	49.166		1000185-64-0	LibSearch	70.68	70.68			Integrate
134	1,4-Methano-1H-cycloheptal[d]pyridazine, 4,4a,5,6,7,8,9,9a-octahydro-10,10-dimethyl-	C12 H20 N2	49.477		1000221-85-4	LibSearch	57.80	57.80			Integrate
135	n-Hexadecanoic acid	C16 H32 O2	49.878		57-10-3	LibSearch	65.75	65.75			Integrate
136	n-Hexadecanoic acid	C16 H32 O2	49.981		57-10-3	LibSearch	69.21	69.21			Integrate
137	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	50.307		1000210-42-6	LibSearch	64.00	64.00			Integrate
138	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	50.517		1000210-42-6	LibSearch	60.59	60.59			Integrate
139	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	50.700		1000210-42-6	LibSearch	59.21	59.21			Integrate
140	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	50.783		1000210-42-6	LibSearch	60.87	60.87			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
141	3-(3-Methylbutyl)thiophene-1,1-dioxide	C9 H14 O2 S	50.983		142076-46-8	LibSearch	61.47	61.47			Integrate
142	Oxacyclotetradeca-4,11-diyne	C13 H18 O	51.216		6568-32-7	LibSearch	71.84	71.84			Integrate
143	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	51.582		1000221-85-9	LibSearch	58.64	58.64			Integrate
144	Benzene, 1,3-bis(1-allyl-5-tetrazolylthiomethyl)-	C16 H18 N8 S2	51.783		329081-94-9	LibSearch	55.29	55.29			Integrate
145	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	52.011		1000221-85-9	LibSearch	65.13	65.13			Integrate
146	Diazoprogesterone	C21 H30 N4	52.237		1000255-30-9	LibSearch	63.36	63.36			Integrate
147	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	52.440		1000210-42-6	LibSearch	68.24	68.24			Integrate
148	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	52.628		1000210-42-6	LibSearch	64.20	64.20			Integrate
149	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	52.701		1000221-85-9	LibSearch	61.33	61.33			Integrate
150	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	52.944		14113-61-2	LibSearch	64.03	64.03			Integrate
151	Oxacyclotetradeca-4,11-diyne	C13 H18 O	53.114		6568-32-7	LibSearch	63.51	63.51			Integrate
152	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	53.468		1000210-42-6	LibSearch	63.47	63.47			Integrate
153	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	53.638		1000221-85-9	LibSearch	65.73	65.73			Integrate
154	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	53.723		1000210-42-6	LibSearch	70.06	70.06			Integrate
155	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	53.901		1000210-42-6	LibSearch	66.34	66.34			Integrate
156	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	54.084		1000210-42-6	LibSearch	67.42	67.42			Integrate
157	Diazoprogesterone	C21 H30 N4	54.648		1000255-30-9	LibSearch	63.30	63.30			Integrate
158	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	54.902		1000210-42-6	LibSearch	75.72	75.72			Integrate
159	Nona-2,3-dienoic acid, ethyl ester	C11 H18 O2	54.994		1000187-19-2	LibSearch	74.07	74.07			Integrate
160	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	55.391		1000210-42-6	LibSearch	65.96	65.96			Integrate
161	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	55.624		1000210-42-6	LibSearch	63.32	63.32			Integrate
162	Diazoprogesterone	C21 H30 N4	55.955		1000255-30-9	LibSearch	62.11	62.11			Integrate
163	Diazoprogesterone	C21 H30 N4	56.617		1000255-30-9	LibSearch	63.38	63.38			Integrate
164	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	56.910		1000221-85-9	LibSearch	70.03	70.03			Integrate

Analysis Report

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
165	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	57.100		14113-61-2	LibSearch	68.27	68.27			Integrate
166	1,8-Cyclotetradecadiyne	C14 H20	57.168		1540-80-3	LibSearch	68.52	68.52			Integrate
167	1,8-Cyclopentadecadiyne	C15 H22	57.246		4722-42-3	LibSearch	59.40	59.40			Integrate
168	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	57.524		1000221-85-9	LibSearch	70.38	70.38			Integrate
169	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	57.737		1000221-85-9	LibSearch	67.06	67.06			Integrate
170	.beta.-D-Mannofuranoside, 2,3:5,6-diethylboranediyl-cis-nerolidyl	C25 H42 B2 O6	58.374		1000155-68-3	LibSearch	63.76	63.76			Integrate
171	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	58.549		1000221-85-9	LibSearch	69.26	69.26			Integrate
172	Diazoprogesterone	C21 H30 N4	58.758		1000255-30-9	LibSearch	61.27	61.27			Integrate
173	Diazoprogesterone	C21 H30 N4	58.918		1000255-30-9	LibSearch	59.98	59.98			Integrate
174	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	59.046		1000210-42-6	LibSearch	67.26	67.26			Integrate
175	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	59.876		14113-61-2	LibSearch	63.57	63.57			Integrate
176	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	60.340		1000221-85-9	LibSearch	66.33	66.33			Integrate
177	Phosphonofluoridic acid, methyl-, nonyl ester	C10 H22 F O2 P	60.791		211192-74-4	LibSearch	63.24	63.24			Integrate
178	1-(10,10-Dimethyl-3,3-dioxo-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-yl)-3-methylpent-4-en-1-one	C16 H25 N O3 S	61.628		1000210-42-6	LibSearch	61.50	61.50			Integrate
179	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	62.431		1000221-85-9	LibSearch	67.53	67.53			Integrate
180	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	62.609		14113-61-2	LibSearch	62.67	62.67			Integrate
181	1,8-Cyclotetradecadiyne	C14 H20	62.746		1540-80-3	LibSearch	66.93	66.93			Integrate
182	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	63.072		1000221-85-9	LibSearch	70.92	70.92			Integrate
183	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	63.238		1000221-85-9	LibSearch	65.58	65.58			Integrate
184	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	63.669		1000221-85-9	LibSearch	63.84	63.84			Integrate

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
185	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	63.972		1000221-85-9	LibSearch	64.11	64.11			Integrate
186	Diazoprogesterone	C21 H30 N4	64.439		1000255-30-9	LibSearch	59.81	59.81			Integrate
187	n-Dodecylpyridinium chloride	C17 H30 Cl N	64.687		104-74-5	LibSearch	58.48	58.48			Integrate
188	Diazoprogesterone	C21 H30 N4	65.783		1000255-30-9	LibSearch	63.15	63.15			Integrate
189	Cyclopentyl-methyl-phosphinic acid, 2-isopropyl-5-methyl-cyclohexyl ester	C16 H31 O2 P	65.878		1000194-56-2	LibSearch	65.91	65.91			Integrate
190	2-Azido-2,4,4,6,6,8,8-heptamethylnonane	C16 H33 N3	67.179		1000293-29-1	LibSearch	56.70	56.70			Integrate
191	n-Dodecylpyridinium chloride	C17 H30 Cl N	69.586		104-74-5	LibSearch	54.51	54.51			Integrate
192	2-Azidomethyl-1,3,3-trimethyl-cyclohexene	C10 H17 N3	72.542		90073-44-2	LibSearch	63.72	63.72			Integrate
193	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	73.261		1000221-85-9	LibSearch	59.76	59.76			Integrate
194	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	76.318		1000221-85-9	LibSearch	54.45	54.45			Integrate
195	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	77.536		1000221-85-9	LibSearch	55.64	55.64			Integrate
196	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	77.830		1000221-85-9	LibSearch	58.71	58.71			Integrate
197	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	78.557		1000221-85-9	LibSearch	59.38	59.38			Integrate
198	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	78.707		1000221-85-9	LibSearch	57.83	57.83			Integrate
199	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	79.472		1000221-85-9	LibSearch	63.48	63.48			Integrate
200	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	79.796		1000221-85-9	LibSearch	59.36	59.36			Integrate
201	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	80.056		1000221-85-9	LibSearch	58.95	58.95			Integrate
202	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	80.766		1000221-85-9	LibSearch	57.61	57.61			Integrate

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
203	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	81.671		1000221-85-9	LibSearch	59.25	59.25			Integrate
204	Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	C22 H32	81.932		14113-61-2	LibSearch	65.25	65.25			Integrate
205	1,8-Cyclotetradecadiyne	C14 H20	82.113		1540-80-3	LibSearch	57.32	57.32			Integrate
206	Boron, (1,3-butanediiminato-N,N')-1,5-cyclooctanediyl-, (t-4)-	C12 H21 B N2	82.479		136704-98-8	LibSearch	64.99	64.99			Integrate
207	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	82.725		1000221-85-9	LibSearch	57.67	57.67			Integrate
208	Boron, (1,3-butanediiminato-N,N')-1,5-cyclooctanediyl-, (t-4)-	C12 H21 B N2	82.955		136704-98-8	LibSearch	62.23	62.23			Integrate
209	Boron, (1,3-butanediiminato-N,N')-1,5-cyclooctanediyl-, (t-4)-	C12 H21 B N2	82.975		136704-98-8	LibSearch	58.96	58.96			Integrate
210	.gamma.-HIMACHALENE	C15 H24	83.362		1000140-08-0	LibSearch	58.67	58.67			Integrate
211	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13 H20 N2	83.522		1000221-85-9	LibSearch	54.48	54.48			Integrate

MassHunter Qual 10.0
(End of Report)