

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031519\
 Data File : VU030022.D
 Acq On : 13 Mar 2019 11:41
 Operator : JC/SP
 Sample : K1763-04RE 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0959RE

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.183	24	29	39	rBV3	12357	13640	0.79%	0.093%
2	1.270	50	56	69	rBV	27684	45041	2.62%	0.307%
3	1.328	69	74	85	rVB	22923	26698	1.56%	0.182%
4	1.386	89	92	104	rVB2	7114	7398	0.43%	0.050%
5	1.473	116	119	123	rBV	7766	6579	0.38%	0.045%
6	1.682	176	184	197	rVB	175619	223592	13.02%	1.524%
7	2.113	312	318	326	rVB	9163	13034	0.76%	0.089%
8	2.273	360	368	376	rBV	40261	58918	3.43%	0.401%
9	2.322	376	383	404	rVB2	28592	58697	3.42%	0.400%
10	2.479	424	432	446	rVB2	5888	9513	0.55%	0.065%
11	2.556	446	456	469	rBV3	3832	8322	0.48%	0.057%
12	2.701	488	501	524	rBV	305461	540068	31.46%	3.680%
13	2.942	567	576	589	rBV	7611	15214	0.89%	0.104%
14	3.174	645	648	650	rBV	1133	808	0.05%	0.006%
15	3.383	707	713	716	rBV2	608	692	0.04%	0.005%
16	3.444	723	732	733	rBV3	1791	1960	0.11%	0.013%
17	3.511	748	753	756	rBV3	656	701	0.04%	0.005%
18	3.553	762	766	775	rVV2	572	699	0.04%	0.005%
19	3.604	775	782	785	rBV	495	542	0.03%	0.004%
20	3.817	835	848	849	rBV2	1167	1419	0.08%	0.010%
21	4.000	897	905	907	rBV5	2470	3682	0.21%	0.025%
22	4.170	945	958	983	rBV	148704	384399	22.39%	2.619%
23	4.665	1087	1112	1142	rBV3	531801	1716673	100.00%	11.698%
24	5.337	1297	1321	1365	rVV2	547662	1645066	95.83%	11.210%
25	5.736	1433	1445	1455	rBV7	3024	6976	0.41%	0.048%
26	5.884	1476	1491	1513	rBV	529376	1060702	61.79%	7.228%
27	6.183	1570	1584	1600	rBV6	25166	57620	3.36%	0.393%
28	6.328	1614	1629	1659	rBV	359632	729295	42.48%	4.970%
29	6.543	1692	1696	1697	rBV2	1233	885	0.05%	0.006%
30	6.630	1719	1723	1728	rVB4	989	869	0.05%	0.006%
31	6.669	1732	1735	1743	rVB4	739	713	0.04%	0.005%
32	6.710	1743	1748	1749	rBV3	1116	758	0.04%	0.005%
33	6.755	1750	1762	1780	rVV3	51078	97436	5.68%	0.664%
34	7.048	1849	1853	1855	rBV3	709	537	0.03%	0.004%

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35	7.161	1877	1888	1894	rBV	1469	2612	0.15%	0.018%
36	7.228	1897	1909	1928	rVV2	22322	44230	2.58%	0.301%
37	7.350	1941	1947	1953	rVV7	1246	1877	0.11%	0.013%
38	7.411	1964	1966	1971	rVB3	659	545	0.03%	0.004%
39	7.466	1971	1983	1995	rBV3	10199	20392	1.19%	0.139%
40	7.540	1997	2006	2011	rBV2	6469	12145	0.71%	0.083%
41	7.652	2035	2041	2049	rBV2	3442	4576	0.27%	0.031%
42	7.739	2066	2068	2073	rVB2	970	587	0.03%	0.004%
43	7.855	2094	2104	2121	rBV3	35471	66322	3.86%	0.452%
44	7.939	2126	2130	2136	rBV5	601	706	0.04%	0.005%
45	8.013	2149	2153	2155	rBV4	1371	1064	0.06%	0.007%
46	8.067	2164	2170	2175	rBV6	2049	2654	0.15%	0.018%
47	8.177	2190	2204	2216	rBV2	130350	260013	15.15%	1.772%
48	8.308	2235	2245	2280	rVB	501955	874099	50.92%	5.956%
49	8.472	2289	2296	2313	rVB3	14509	26247	1.53%	0.179%
50	8.630	2340	2345	2349	rBV4	1467	1293	0.08%	0.009%
51	8.884	2422	2424	2431	rVB5	848	812	0.05%	0.006%
52	8.996	2455	2459	2464	rVB4	834	862	0.05%	0.006%
53	9.042	2464	2473	2476	rBV3	10260	14733	0.86%	0.100%
54	9.087	2476	2487	2503	rVV	802238	1325681	77.22%	9.034%
55	9.164	2504	2511	2525	rVB	33348	61459	3.58%	0.419%
56	9.254	2535	2539	2551	rVB7	1932	3205	0.19%	0.022%
57	9.315	2555	2558	2560	rBV3	916	577	0.03%	0.004%
58	9.328	2560	2562	2565	rBV3	794	514	0.03%	0.004%
59	9.511	2610	2619	2624	rBV6	1349	2185	0.13%	0.015%
60	9.578	2635	2640	2643	rBV3	632	646	0.04%	0.004%
61	9.604	2643	2648	2653	rVV2	695	803	0.05%	0.005%
62	9.707	2676	2680	2684	rBV2	737	547	0.03%	0.004%
63	9.746	2688	2692	2696	rBV2	648	615	0.04%	0.004%
64	9.823	2710	2716	2723	rBV4	1362	1886	0.11%	0.013%
65	9.951	2746	2756	2757	rBV6	1844	2218	0.13%	0.015%
66	10.032	2776	2781	2793	rBV6	2539	3889	0.23%	0.027%
67	10.164	2809	2822	2828	rBV10	2446	5179	0.30%	0.035%
68	10.357	2878	2882	2887	rVB	566	510	0.03%	0.003%
69	10.427	2891	2904	2919	rBV	559788	893616	52.06%	6.089%
70	10.604	2946	2959	2976	rBV	664125	1085389	63.23%	7.396%
71	10.717	2984	2994	3019	rVB	263005	423007	24.64%	2.883%

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72	10.804	3019	3021	3025	rBV3	738	588	0.03%	0.004%
73	10.874	3035	3043	3052	rVB4	3495	5405	0.31%	0.037%
74	10.990	3076	3079	3081	rBV2	828	546	0.03%	0.004%
75	11.035	3082	3093	3104	rVV2	7670	14771	0.86%	0.101%
76	11.099	3106	3113	3120	rVB8	6397	9756	0.57%	0.066%
77	11.151	3120	3129	3140	rBV6	5927	10637	0.62%	0.072%
78	11.221	3144	3151	3156	rVB7	2749	3447	0.20%	0.023%
79	11.376	3190	3199	3202	rBV6	1982	2491	0.15%	0.017%
80	11.418	3206	3212	3220	rVV6	2827	4985	0.29%	0.034%
81	11.479	3220	3231	3257	rVV	823969	1315232	76.62%	8.963%
82	11.643	3279	3282	3284	rBV4	1139	778	0.05%	0.005%
83	11.749	3311	3315	3316	rBV3	1661	1071	0.06%	0.007%
84	11.781	3317	3325	3335	rVV2	14271	21480	1.25%	0.146%
85	11.855	3336	3348	3378	rVV	789851	1325182	77.19%	9.030%
86	12.135	3431	3435	3440	rBV5	705	686	0.04%	0.005%
87	12.475	3531	3541	3555	rVB3	7604	14797	0.86%	0.101%
88	12.572	3562	3571	3581	rBV8	8625	16916	0.99%	0.115%
89	12.774	3624	3634	3645	rVV5	11073	21679	1.26%	0.148%
90	12.829	3649	3651	3654	rVB	1049	578	0.03%	0.004%
91	12.887	3664	3669	3679	rVB4	1316	1887	0.11%	0.013%
92	13.041	3709	3717	3719	rBV7	2019	1985	0.12%	0.014%
93	13.192	3756	3764	3774	rVB7	3631	7107	0.41%	0.048%
94	13.392	3823	3826	3832	rBV4	713	772	0.04%	0.005%
95	13.511	3858	3863	3869	rVB5	1606	1743	0.10%	0.012%
96	13.909	3985	3987	3992	rBV5	571	545	0.03%	0.004%
97	13.938	3994	3996	4000	rBV2	887	721	0.04%	0.005%
98	14.446	4151	4154	4158	rBV2	750	634	0.04%	0.004%
99	14.668	4220	4223	4227	rBV2	714	597	0.03%	0.004%
100	14.906	4294	4297	4302	rBV2	937	858	0.05%	0.006%

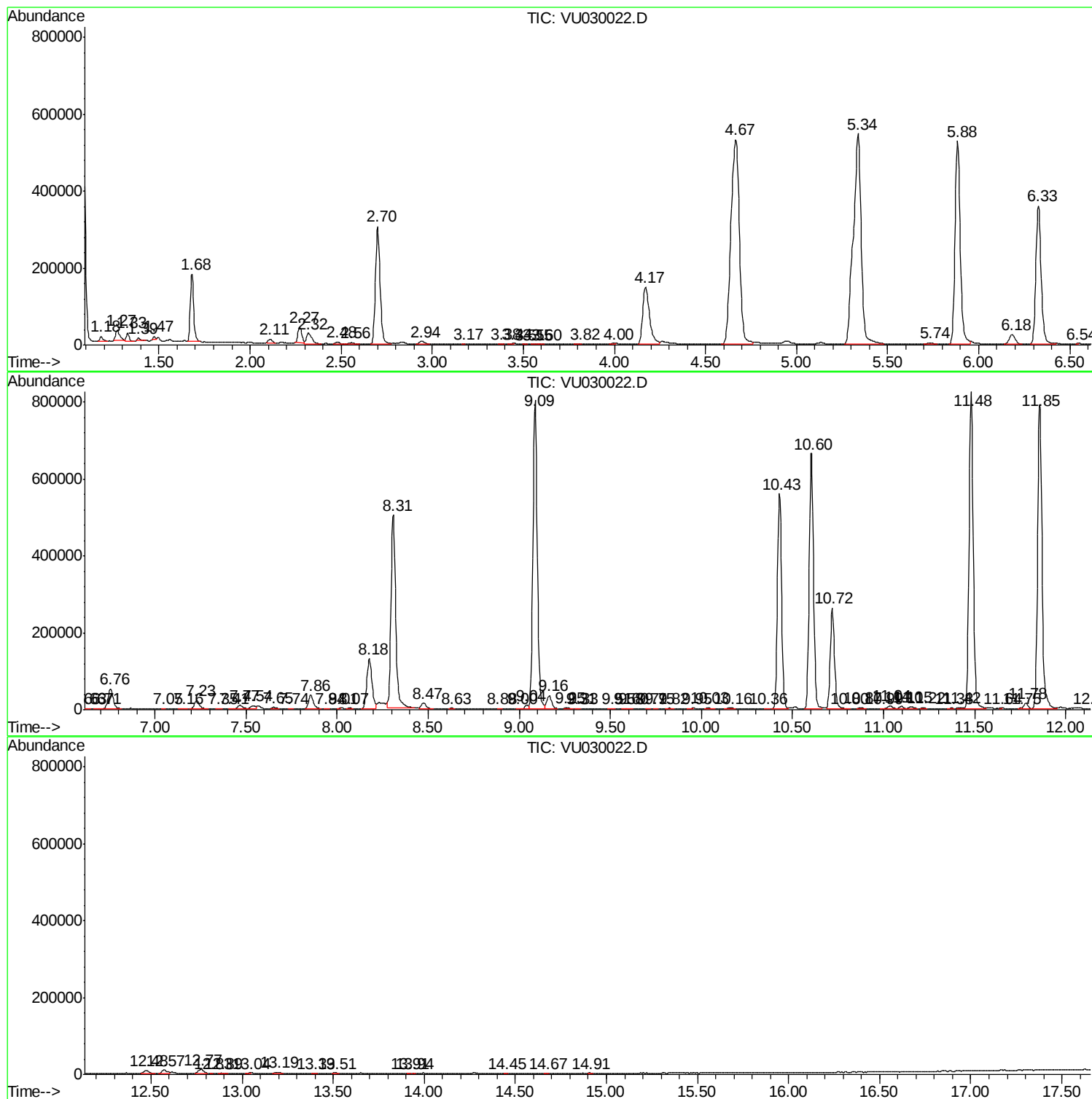
Sum of corrected areas: 14674715

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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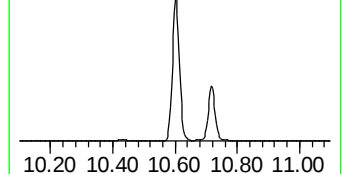
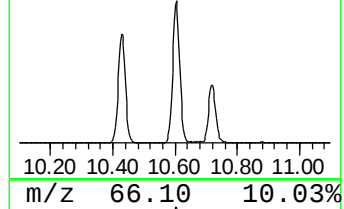
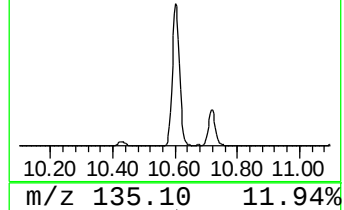
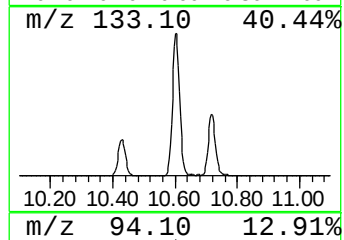
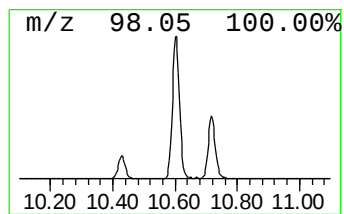
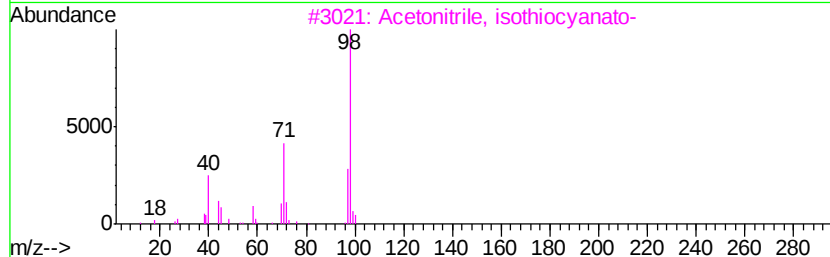
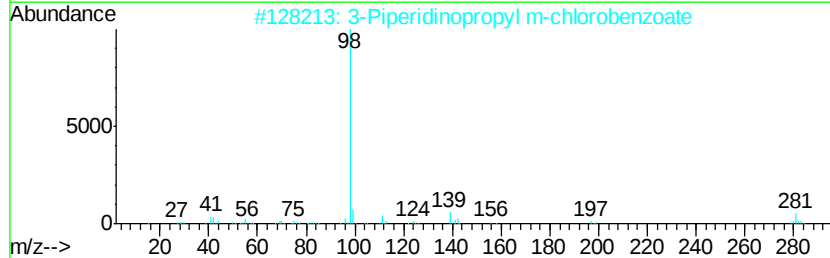
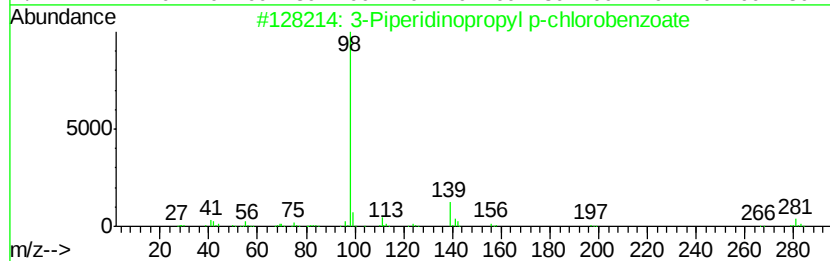
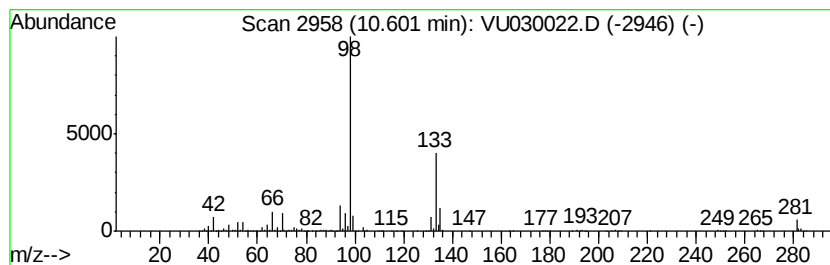
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	41.26 ug/L	1085390	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Piperidinopropyl p-chlorobenzoate	281	C15H20ClN02	1000240-42-7	38
2		3-Piperidinopropyl m-chlorobenzoate	281	C15H20ClN02	1000240-41-2	38
3		Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	32
4		Encainide	352	C22H28N2O2	037612-13-8	32
5		Mepivacaine	246	C15H22N2O	000096-88-8	25



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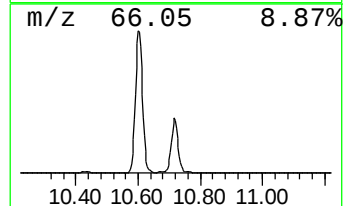
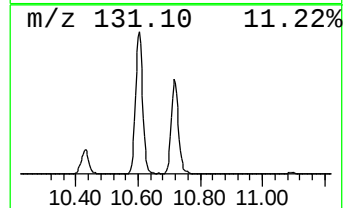
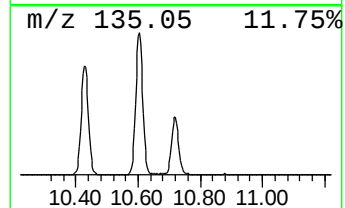
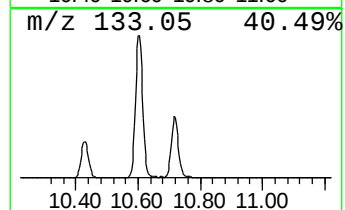
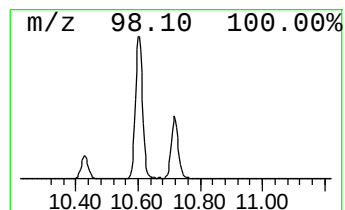
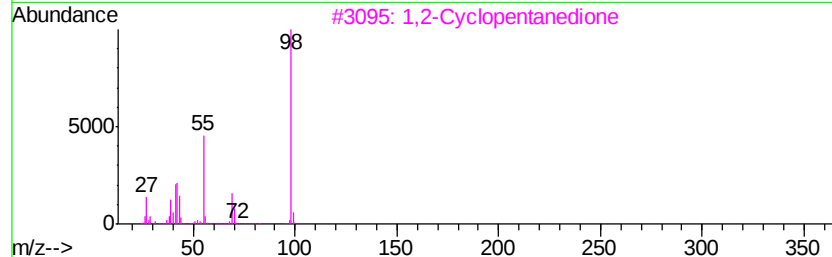
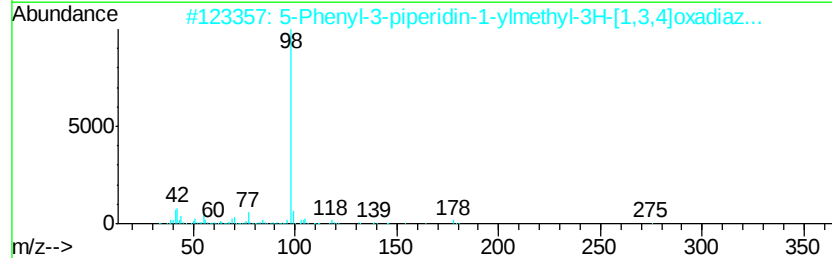
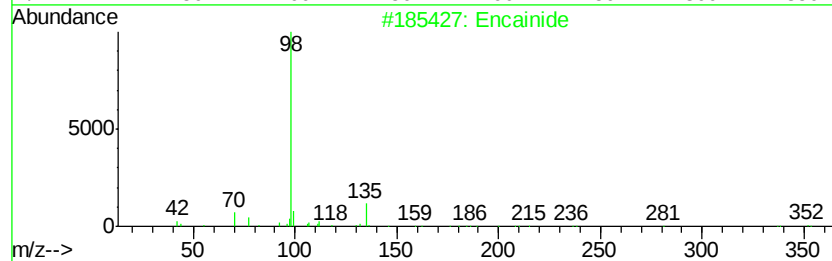
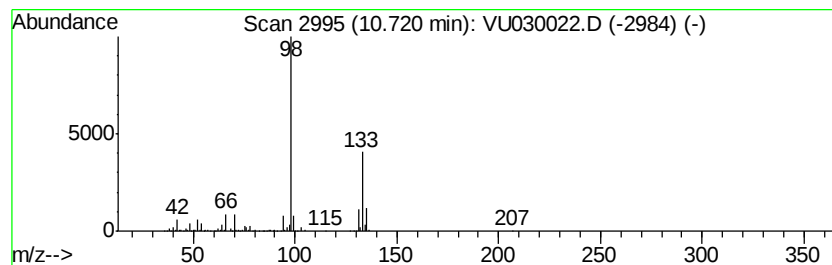
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Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	16.08 ug/L	423007	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Encainide	352 C22H28N2O2	037612-13-8	37
2	5-Phenyl-3-piperidin-1-ylmethyl-...	275 C14H17N3OS	023269-66-1	32
3	1,2-Cyclopentanedione	98 C5H6O2	003008-40-0	32
4	Piperidine, 1,1'-(1,2-ethanediyl...	196 C12H24N2	001932-04-3	23
5	Piperidine, 1-(2-phenylethyl)-	189 C13H19N	000332-14-9	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.60	41.3	ug/L	1085390	3	11.48	1315230	50.0
unknown-02	10.72	16.1	ug/L	423007	3	11.48	1315230	50.0