

Data Path : Z:\VOASRV\HPCHEM1\MSVOA F\DATA\VF062718\
 Data File : VF059340.D
 Acq On : 27 Jun 2018 15:46
 Operator : VA/AP
 Sample : J3629-16
 Misc : 6.95g/5mL/MSVOA-F/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_F
 ClientSampleId :
 A0C22-02

Integration Parameters: RTEINT.P

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

Filtering: 5
 Min Area: 3 % 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_F\METHODS\82F062518S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.088	55	56	59	rVB	9988	9151	4.52%	0.824%
2	1.167	61	64	65	rBV2	2163	3459	1.71%	0.311%
3	1.206	65	68	70	rVV4	2914	4558	2.25%	0.410%
4	1.255	70	73	74	rVV3	2345	4194	2.07%	0.377%
5	1.324	79	80	82	rVV2	2949	3558	1.76%	0.320%
6	1.413	86	89	91	rVV3	3103	5652	2.79%	0.509%
7	1.482	93	96	100	rVB7	3040	8722	4.31%	0.785%
8	1.748	121	123	126	rBV3	2597	5269	2.60%	0.474%
9	2.004	147	149	153	rVB2	1234	2171	1.07%	0.195%
10	2.083	155	157	160	rVB2	1621	2554	1.26%	0.230%
11	2.142	160	163	165	rBV2	1811	3551	1.75%	0.320%
12	2.221	169	171	173	rVV2	1266	2095	1.03%	0.189%
13	2.271	173	176	182	rVB4	6954	16885	8.34%	1.520%
14	2.478	192	197	202	rVV3	8434	19595	9.68%	1.763%
15	2.616	207	211	212	rVB2	1872	2608	1.29%	0.235%
16	2.645	212	214	216	rBV	1580	2444	1.21%	0.220%
17	2.704	216	220	221	rBV2	1092	2092	1.03%	0.188%
18	2.842	232	234	239	rVB2	969	2178	1.08%	0.196%
19	2.970	245	247	248	rVB	2028	2256	1.11%	0.203%
20	3.552	301	306	308	rBV2	1696	3460	1.71%	0.311%
21	4.084	357	360	363	rBV2	1283	2100	1.04%	0.189%
22	4.193	366	371	374	rVV2	1670	4293	2.12%	0.386%
23	4.281	377	380	381	rVV2	1426	2180	1.08%	0.196%
24	4.528	400	405	410	rVV3	1209	4200	2.07%	0.378%
25	4.617	410	414	415	rVV3	1047	2171	1.07%	0.195%
26	4.695	421	422	426	rVB	1741	2620	1.29%	0.236%
27	4.755	426	428	430	rBV2	1099	2095	1.03%	0.189%
28	4.833	432	436	441	rVV4	3169	8146	4.02%	0.733%
29	4.922	443	445	448	rBV2	1127	2421	1.20%	0.218%
30	5.021	448	455	464	rVV	68944	198522	98.06%	17.866%
31	5.159	466	469	472	rVB4	1557	2821	1.39%	0.254%
32	5.228	472	476	478	rBV	2059	4368	2.16%	0.393%
33	5.750	523	529	536	rBV	76708	200311	98.94%	18.027%
34	6.006	552	555	558	rVV3	1046	2370	1.17%	0.213%

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35	6.233	574	578	580	rVB3	1688	2147	1.06%	0.193%
36	6.351	585	590	591	rBV	1762	2575	1.27%	0.232%
37	6.529	606	608	611	rVV	1935	2214	1.09%	0.199%
38	7.170	671	673	676	rVB4	1605	2185	1.08%	0.197%
39	7.327	688	689	693	rVB2	1370	2385	1.18%	0.215%
40	7.485	701	705	706	rBV2	1702	3192	1.58%	0.287%
41	7.702	722	727	730	rBV4	2407	5803	2.87%	0.522%
42	7.968	750	754	759	rVB4	1204	2816	1.39%	0.253%
43	8.461	799	804	805	rBV	1035	2082	1.03%	0.187%
44	8.619	814	820	824	rVB3	1375	4550	2.25%	0.409%
45	8.816	839	840	843	rBV2	1970	2299	1.14%	0.207%
46	8.905	846	849	850	rBV2	1745	2333	1.15%	0.210%
47	9.043	861	863	868	rVB3	1472	2108	1.04%	0.190%
48	9.309	888	890	892	rVV2	1598	2164	1.07%	0.195%
49	9.673	924	927	929	rBV	1621	2390	1.18%	0.215%
50	9.900	943	950	957	rBV	84419	202458	100.00%	18.221%
51	9.979	957	958	963	rVV5	1382	3414	1.69%	0.307%
52	10.166	973	977	979	rVB2	1238	2321	1.15%	0.209%
53	10.363	995	997	1000	rVB2	1242	2205	1.09%	0.198%
54	10.423	1000	1003	1004	rVB2	1482	2084	1.03%	0.188%
55	10.442	1004	1005	1009	rBV	1278	2427	1.20%	0.218%
56	10.521	1009	1013	1015	rBV3	1455	3407	1.68%	0.307%
57	10.620	1021	1023	1027	rBV2	1690	3020	1.49%	0.272%
58	10.738	1029	1035	1036	rBV3	937	2100	1.04%	0.189%
59	10.886	1048	1050	1052	rBV	43577	29591	14.62%	2.663%
60	11.270	1085	1089	1092	rBV3	2293	5850	2.89%	0.526%
61	11.418	1101	1104	1105	rBV2	1923	2549	1.26%	0.229%
62	11.507	1110	1113	1115	rVV3	4466	5600	2.77%	0.504%
63	11.645	1123	1127	1131	rVB5	2742	7985	3.94%	0.719%
64	11.743	1134	1137	1139	rVB2	3177	5133	2.54%	0.462%
65	12.256	1186	1189	1192	rBV3	1671	3569	1.76%	0.321%
66	12.562	1217	1220	1222	rBV2	1814	2804	1.38%	0.252%
67	12.621	1222	1226	1230	rBV	93696	146905	72.56%	13.221%
68	12.818	1242	1246	1248	rBV3	1164	2099	1.04%	0.189%
69	12.966	1260	1261	1264	rVB2	1996	2341	1.16%	0.211%
70	13.311	1293	1296	1297	rBV	2418	3723	1.84%	0.335%
71	13.340	1297	1299	1303	rVB3	1632	2799	1.38%	0.252%

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72	13.449	1307	1310	1311	rVB	2020	2897	1.43%	0.261%
73	13.478	1311	1313	1315	rBV2	2729	4889	2.41%	0.440%
74	13.656	1329	1331	1333	rBV2	1744	2699	1.33%	0.243%
75	13.764	1336	1342	1347	rBV5	5116	12188	6.02%	1.097%
76	14.011	1364	1367	1368	rVV3	1321	2061	1.02%	0.185%
77	14.119	1377	1378	1381	rBV2	1829	2597	1.28%	0.234%
78	14.218	1385	1388	1389	rBV2	3643	6241	3.08%	0.562%
79	14.316	1396	1398	1400	rBV2	2045	3108	1.54%	0.280%
80	14.513	1417	1418	1423	rVB2	2217	3618	1.79%	0.326%
81	14.622	1426	1429	1431	rBV2	1791	4398	2.17%	0.396%
82	14.710	1436	1438	1439	rBV2	1908	2530	1.25%	0.228%
83	14.878	1453	1455	1458	rVB2	1659	2264	1.12%	0.204%
84	15.115	1476	1479	1482	rVB	1984	4097	2.02%	0.369%
85	15.174	1482	1485	1486	rBV3	2681	4762	2.35%	0.429%
86	15.322	1498	1500	1501	rVV	3396	3482	1.72%	0.313%
87	15.371	1503	1505	1507	rVB2	2272	3269	1.61%	0.294%
88	15.450	1510	1513	1516	rBV4	1882	4079	2.01%	0.367%
89	15.696	1536	1538	1541	rVB3	2231	2284	1.13%	0.206%
90	15.814	1549	1550	1552	rBV2	3454	4576	2.26%	0.412%
91	15.923	1560	1561	1565	rBV3	2564	4409	2.18%	0.397%

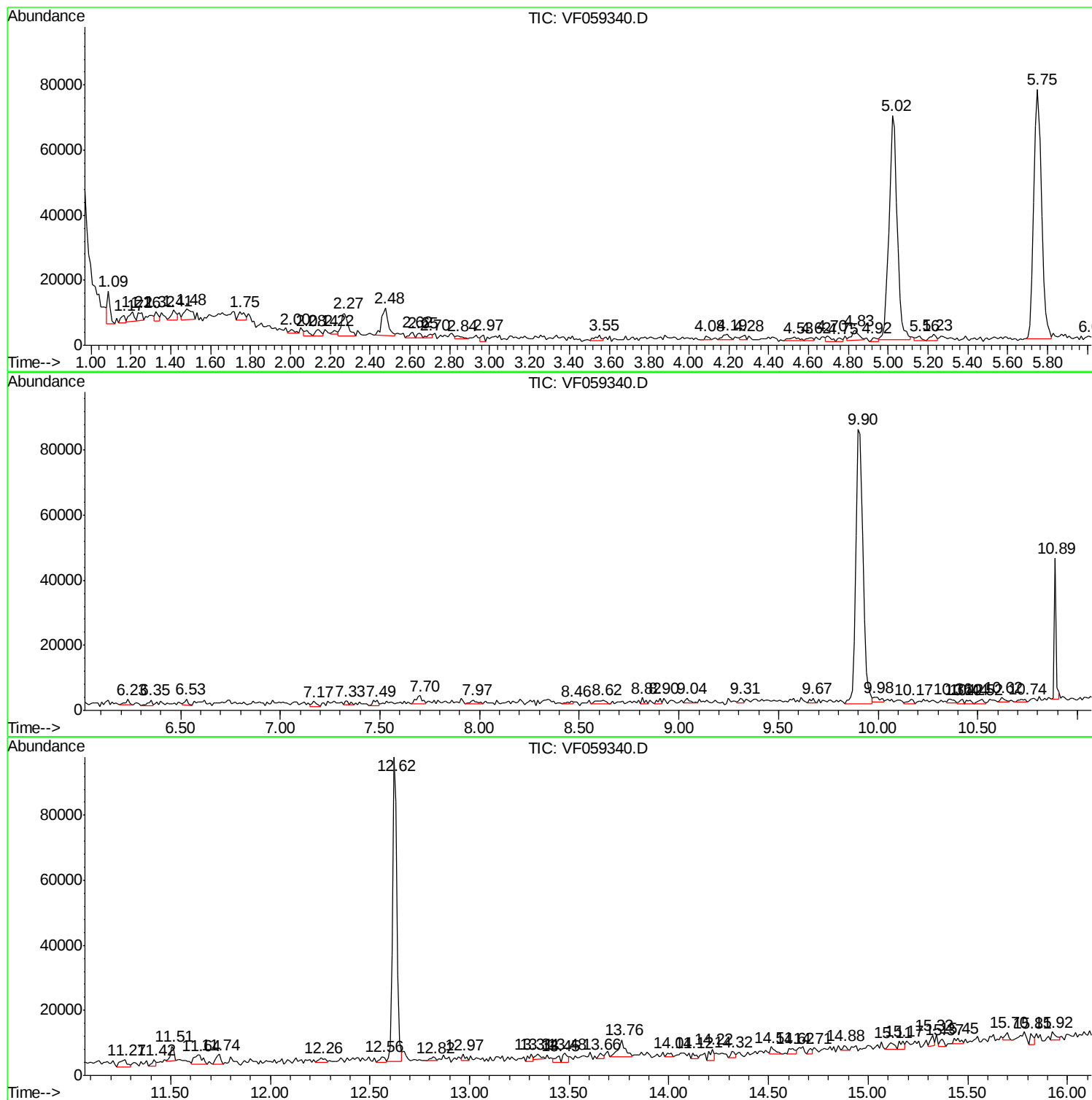
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_F\METHODS\82F062518S.M
Quant Title : SW846 8260

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



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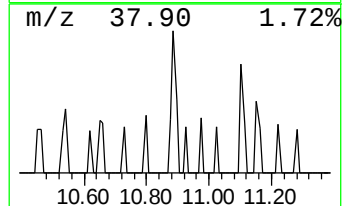
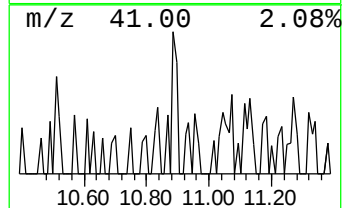
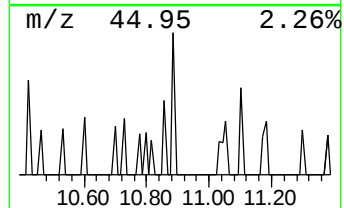
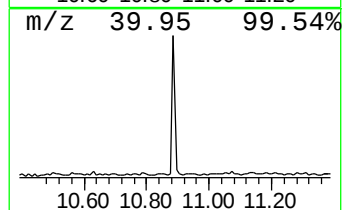
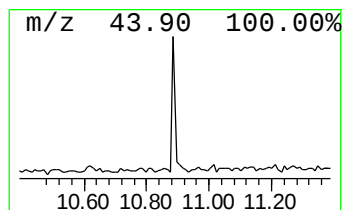
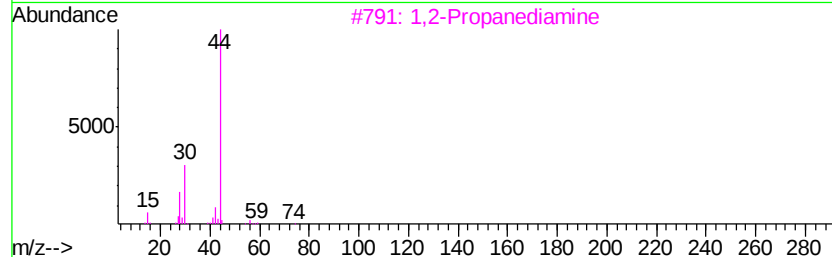
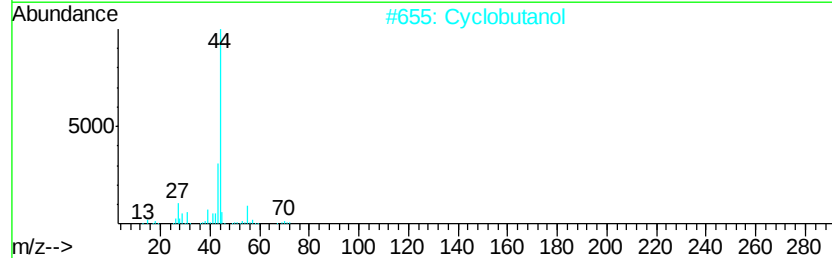
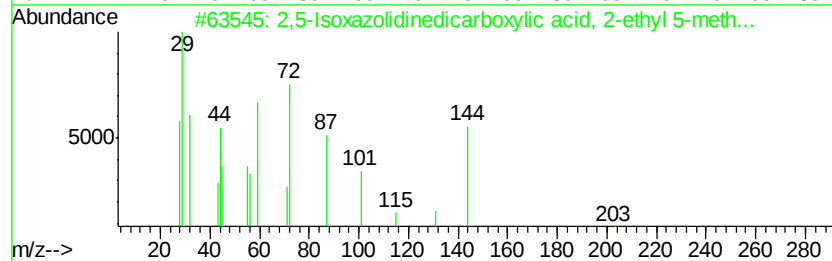
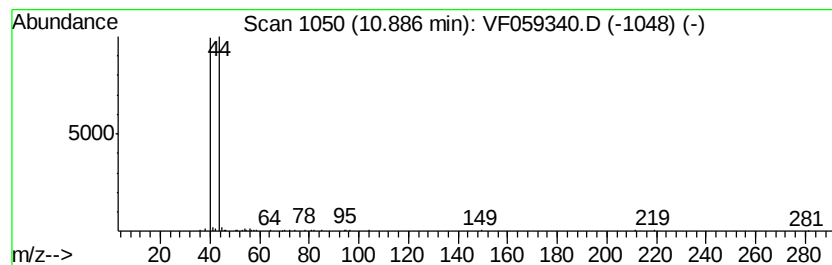
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_F\METHODS\82F062518S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown10.89 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	7.31 ug/l	29591	Chlorobenzene-d5	9.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Isoxazolidinedicarboxylic ac...	203	C8H13N05	015166-62-8	12
2		Cyclobutanol	72	C4H8O	002919-23-5	9
3		1,2-Propanediamine	74	C3H10N2	000078-90-0	5
4		Heptadecanenitrile, 6-aza-2-(4-h...	276	C16H24N2O2	1000150-02-8	4
5		dl-Alanyl-dl-leucine	202	C9H18N2O3	001999-42-4	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown10.89	10.89	7.3	ug/l	29591	3	9.91	202458	50.0