

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
 Data File : VV028516.D
 Acq On : 11 Oct 2022 12:18
 Operator : SY/MD
 Sample : N5079-01DL 20X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFYZ8DL

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M

Title : VOC Analysis

Signal : TIC: VV028516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	75	82	100	rVB	158815	168390	12.83%	1.561%
2	1.565	157	163	181	rVB	128139	149679	11.41%	1.388%
3	2.102	321	330	350	rVB	270475	399885	30.48%	3.708%
4	2.401	421	423	426	rBV3	729	403	0.03%	0.004%
5	2.503	446	455	466	rVB4	4055	6931	0.53%	0.064%
6	2.558	466	472	473	rBV2	472	352	0.03%	0.003%
7	2.661	500	504	508	rBV3	513	517	0.04%	0.005%
8	2.989	601	606	607	rBV2	239	227	0.02%	0.002%
9	3.037	615	621	625	rBV3	350	366	0.03%	0.003%
10	3.124	643	648	651	rBV4	534	372	0.03%	0.003%
11	3.185	651	667	684	rBV2	53137	113127	8.62%	1.049%
12	3.355	716	720	723	rVB2	474	354	0.03%	0.003%
13	3.372	723	725	728	rBV	443	295	0.02%	0.003%
14	3.593	789	794	796	rBV2	394	349	0.03%	0.003%
15	3.716	830	832	835	rVV3	352	191	0.01%	0.002%
16	3.767	846	848	852	rVB2	428	278	0.02%	0.003%
17	3.892	877	887	916	rBV2	64307	239740	18.27%	2.223%
18	4.339	1012	1026	1051	rBV	200896	504454	38.45%	4.678%
19	4.600	1091	1107	1129	rBV	264294	656626	50.05%	6.089%
20	4.802	1168	1170	1172	rBV	373	206	0.02%	0.002%
21	5.040	1227	1244	1273	rBV2	508448	1312031	100.00%	12.166%
22	5.368	1343	1346	1348	rBV2	737	474	0.04%	0.004%
23	5.462	1371	1375	1378	rBV3	527	345	0.03%	0.003%
24	5.532	1394	1397	1400	rBV3	379	242	0.02%	0.002%
25	5.613	1406	1422	1444	rBV	342220	703830	53.64%	6.526%
26	5.912	1506	1515	1527	rVB10	3087	6446	0.49%	0.060%
27	6.005	1540	1544	1549	rBV4	501	640	0.05%	0.006%
28	6.063	1549	1562	1592	rBV	283641	590320	44.99%	5.474%
29	6.314	1630	1640	1653	rVB	12547	24265	1.85%	0.225%
30	6.381	1659	1661	1663	rVB2	563	187	0.01%	0.002%
31	6.506	1696	1700	1706	rBV3	611	665	0.05%	0.006%
32	6.677	1749	1753	1755	rBV2	269	199	0.02%	0.002%
33	6.844	1800	1805	1806	rBV2	335	249	0.02%	0.002%
34	6.931	1822	1832	1837	rBV7	4579	7705	0.59%	0.071%
35	6.982	1838	1848	1874	rVB	177150	324580	24.74%	3.010%
36	7.133	1886	1895	1908	rVV4	9874	19523	1.49%	0.181%

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 Title : VOC Analysis

37	7.201	1912	1916	1919	rBV4	538	542	0.04%	0.005%
38	7.243	1926	1929	1931	rBV2	504	338	0.03%	0.003%
39	7.310	1938	1950	1981	rBV	613691	1076507	82.05%	9.982%
40	7.616	2035	2045	2070	rBV	121381	219709	16.75%	2.037%
41	7.825	2108	2110	2113	rBV3	503	264	0.02%	0.002%
42	7.889	2127	2130	2132	rBV	289	192	0.01%	0.002%
43	7.989	2159	2161	2164	rBV2	330	189	0.01%	0.002%
44	8.024	2169	2172	2176	rBV3	616	413	0.03%	0.004%
45	8.085	2181	2191	2232	rBV	324881	663304	50.56%	6.151%
46	8.500	2318	2320	2321	rBV2	612	302	0.02%	0.003%
47	8.613	2353	2355	2358	rBV	511	347	0.03%	0.003%
48	8.735	2390	2393	2396	rVB4	294	212	0.02%	0.002%
49	8.754	2396	2399	2401	rBV2	641	372	0.03%	0.003%
50	8.847	2416	2428	2448	rBV	499661	821856	62.64%	7.621%
51	9.059	2490	2494	2496	rBV2	500	423	0.03%	0.004%
52	9.104	2505	2508	2511	rVB2	408	293	0.02%	0.003%
53	9.121	2511	2513	2515	rBV	426	234	0.02%	0.002%
54	9.175	2525	2530	2535	rBV4	663	587	0.04%	0.005%
55	9.294	2563	2567	2571	rBV2	416	272	0.02%	0.003%
56	9.339	2577	2581	2583	rBV	349	235	0.02%	0.002%
57	9.358	2583	2587	2591	rVB3	379	304	0.02%	0.003%
58	9.391	2591	2597	2599	rBV3	349	351	0.03%	0.003%
59	9.500	2630	2631	2635	rVB2	476	279	0.02%	0.003%
60	9.522	2635	2638	2639	rBV	366	189	0.01%	0.002%
61	9.728	2692	2702	2728	rVV	83637	156718	11.94%	1.453%
62	9.902	2754	2756	2758	rVB2	402	207	0.02%	0.002%
63	9.918	2758	2761	2763	rBV2	494	367	0.03%	0.003%
64	9.947	2767	2770	2772	rBV4	680	393	0.03%	0.004%
65	9.995	2782	2785	2786	rBV2	503	289	0.02%	0.003%
66	10.211	2838	2852	2877	rVV	366793	589452	44.93%	5.466%
67	10.362	2895	2899	2901	rVB3	777	538	0.04%	0.005%
68	10.374	2901	2903	2905	rBV	545	265	0.02%	0.002%
69	10.474	2922	2934	2951	rBV2	152888	256588	19.56%	2.379%
70	10.683	2994	2999	3002	rVB3	513	411	0.03%	0.004%
71	10.702	3002	3005	3010	rBV2	350	200	0.02%	0.002%
72	10.735	3010	3015	3016	rBV	387	258	0.02%	0.002%
73	10.866	3054	3056	3059	rVB	381	188	0.01%	0.002%
74	10.915	3067	3071	3075	rBV3	713	601	0.05%	0.006%
75	10.934	3075	3077	3081	rVB2	705	340	0.03%	0.003%
76	11.005	3096	3099	3100	rBV2	519	243	0.02%	0.002%

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77	11.088	3122	3125	3129	rBV5	690	516	0.04%	0.005%
78	11.239	3161	3172	3196	rBV	523930	822119	62.66%	7.623%
79	11.455	3235	3239	3241	rVB4	417	302	0.02%	0.003%
80	11.503	3249	3254	3255	rBV2	540	473	0.04%	0.004%
81	11.522	3255	3260	3267	rVV5	5194	7290	0.56%	0.068%
82	11.616	3277	3289	3312	rBV	588014	915970	69.81%	8.493%
83	11.812	3347	3350	3351	rBV	344	189	0.01%	0.002%
84	12.005	3408	3410	3413	rBV	474	286	0.02%	0.003%
85	12.114	3439	3444	3445	rBV	325	262	0.02%	0.002%
86	12.317	3498	3507	3514	rBV7	2399	3733	0.28%	0.035%
87	12.513	3564	3568	3571	rBV2	440	360	0.03%	0.003%
88	12.596	3590	3594	3596	rBV	364	204	0.02%	0.002%
89	12.616	3596	3600	3604	rVB2	308	297	0.02%	0.003%
90	12.644	3604	3609	3610	rBV2	844	525	0.04%	0.005%
91	12.715	3627	3631	3633	rBV3	391	297	0.02%	0.003%
92	12.966	3707	3709	3711	rBV2	341	210	0.02%	0.002%
93	13.053	3734	3736	3739	rBV	391	229	0.02%	0.002%
94	13.140	3761	3763	3766	rVB	263	187	0.01%	0.002%
95	13.159	3766	3769	3775	rBV2	428	385	0.03%	0.004%
96	13.249	3795	3797	3799	rBV	648	273	0.02%	0.003%
97	13.792	3964	3966	3970	rVB	566	271	0.02%	0.003%
98	13.915	4002	4004	4007	rBV2	395	258	0.02%	0.002%
99	14.114	4060	4066	4068	rBV3	517	392	0.03%	0.004%
100	14.477	4177	4179	4181	rBV	518	272	0.02%	0.003%

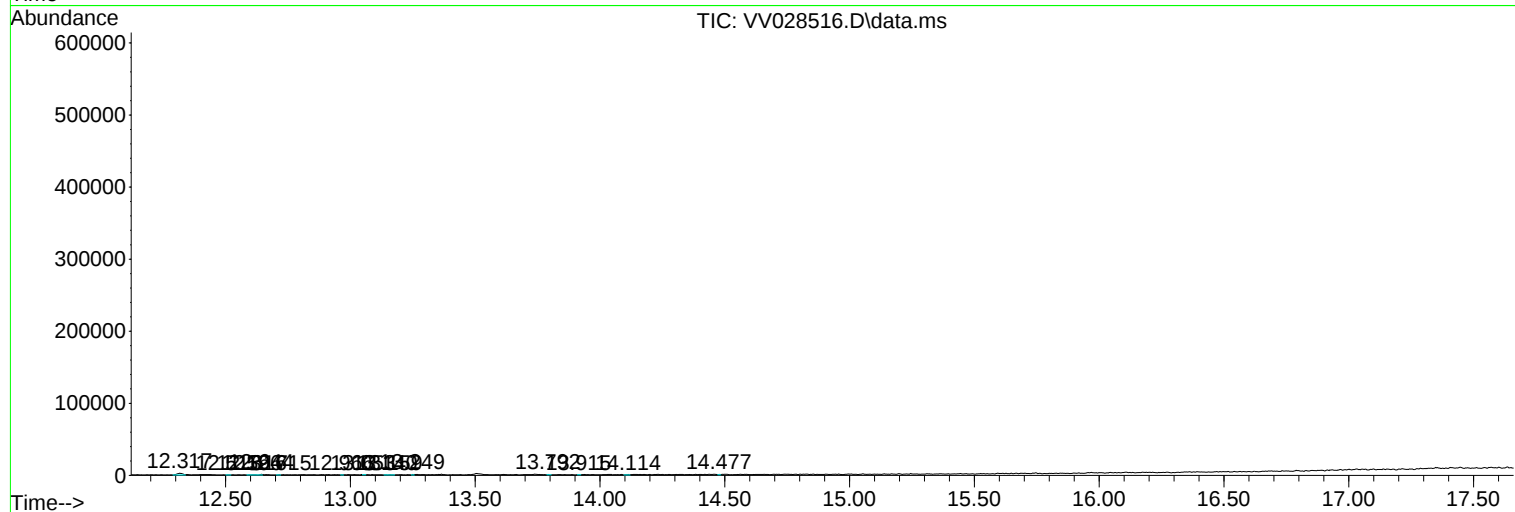
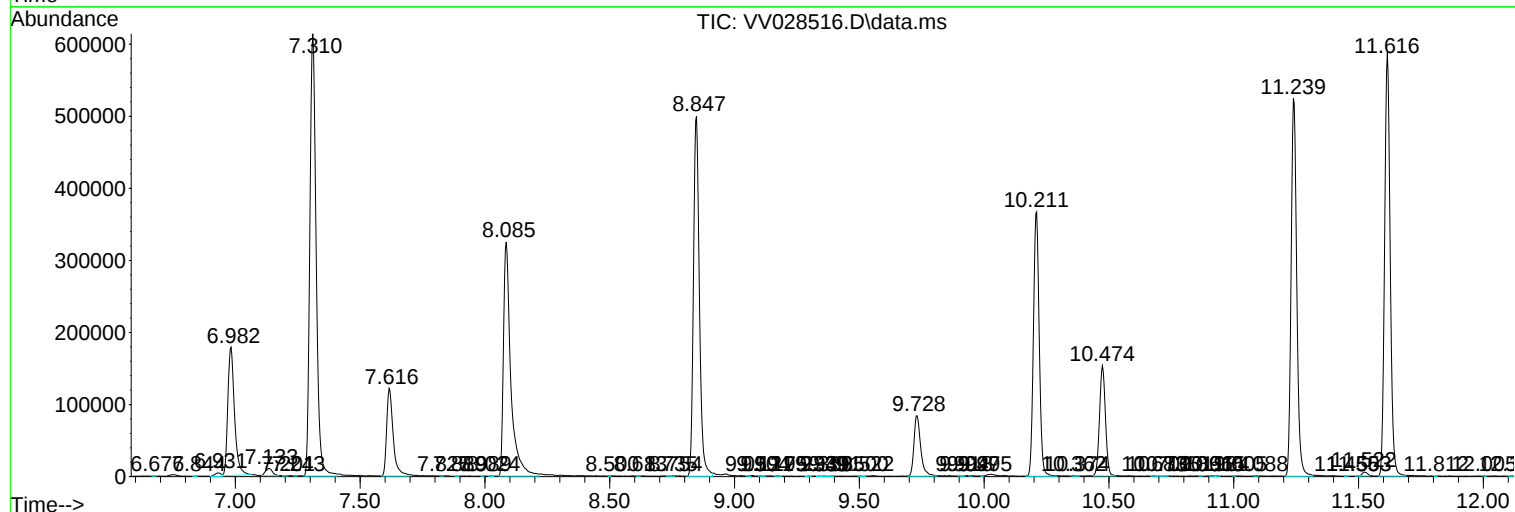
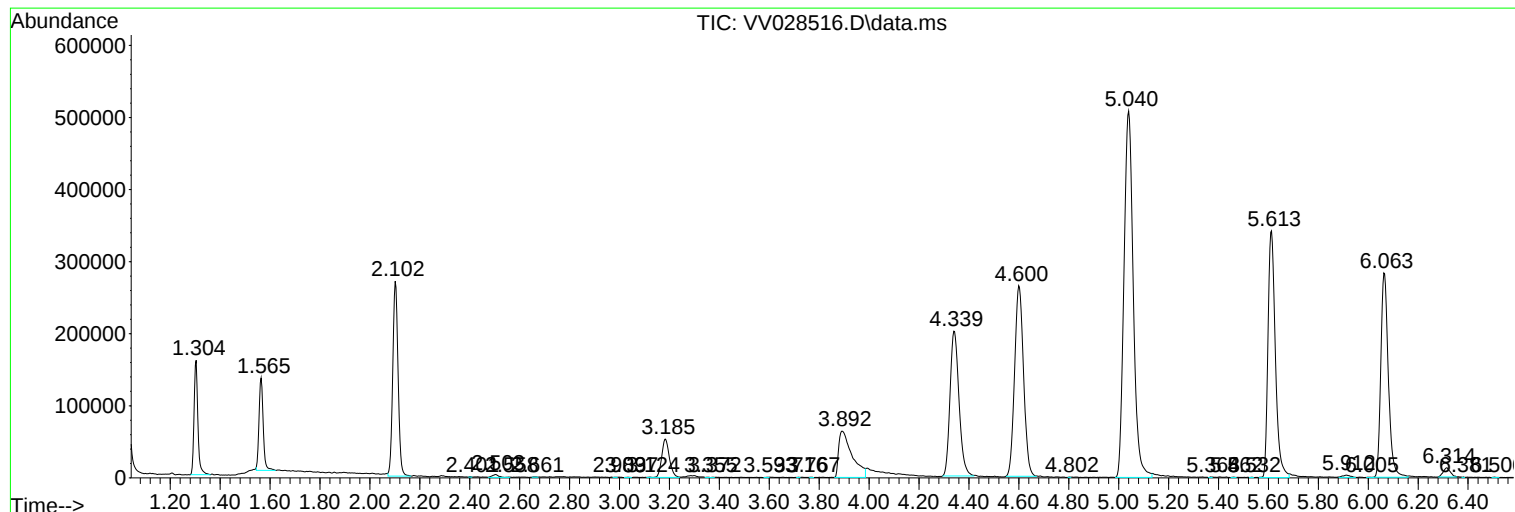
Sum of corrected areas: 10784515

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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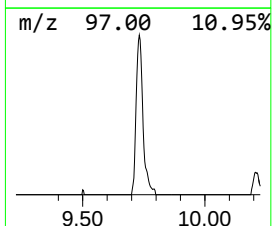
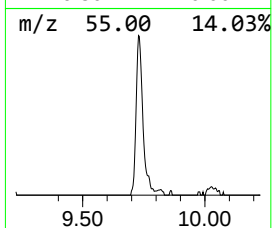
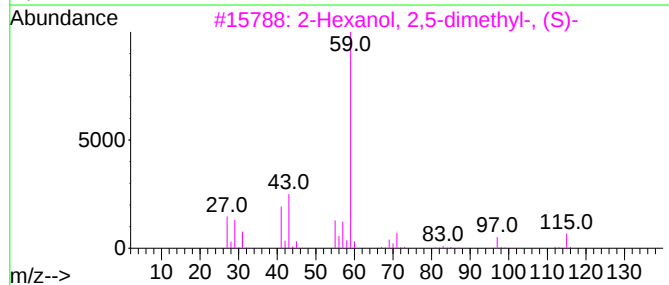
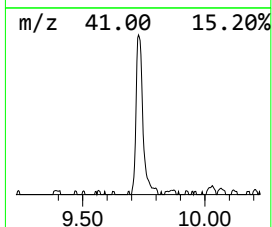
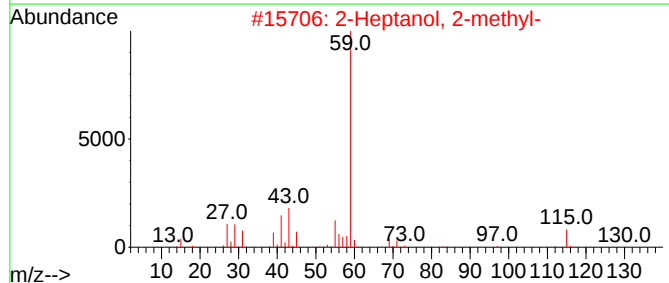
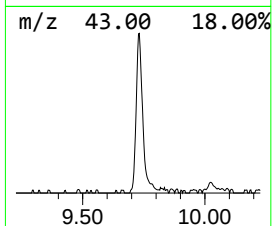
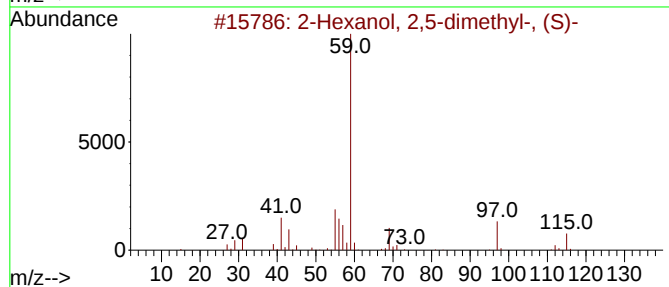
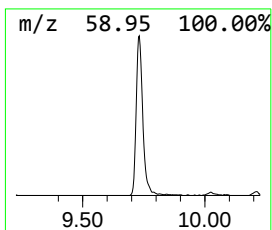
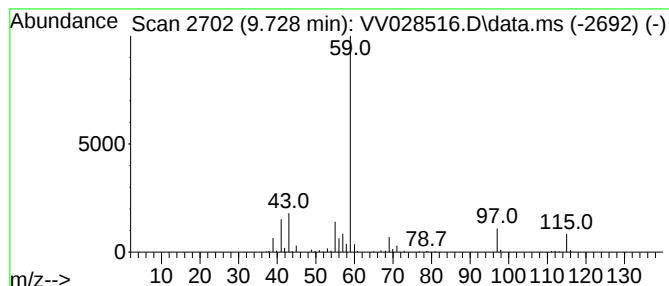
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	9.53 ug/L	156718	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	74
2			2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	64
3			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	64
5			2-Decanol, methyl ether	172	C11H24O	1000333-83-9	64



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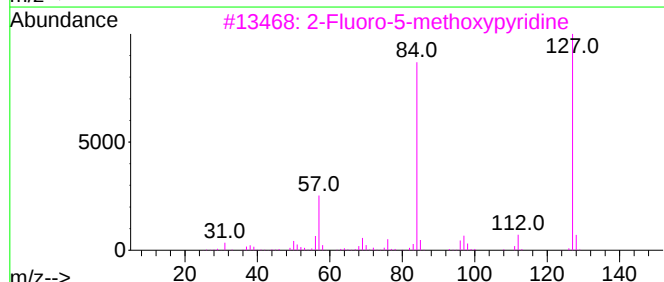
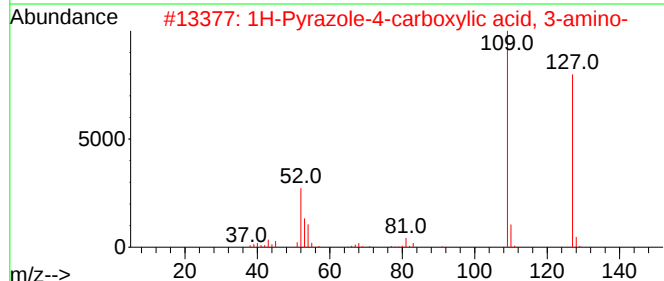
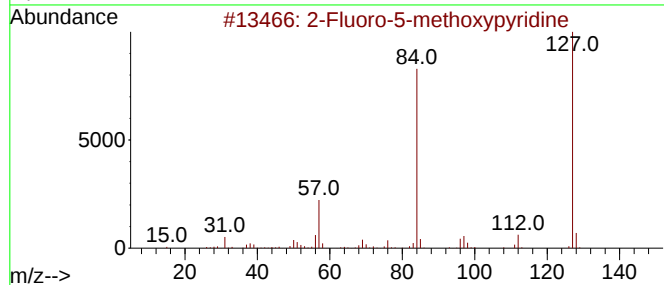
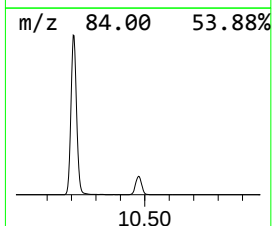
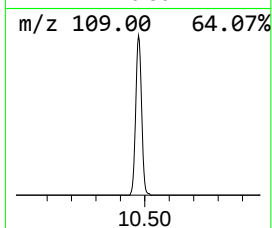
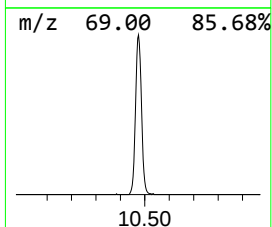
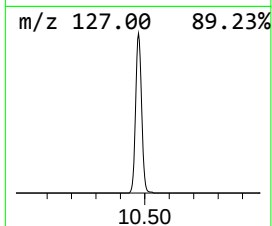
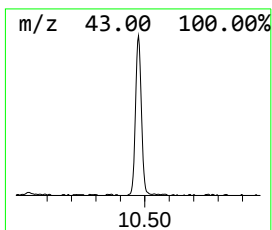
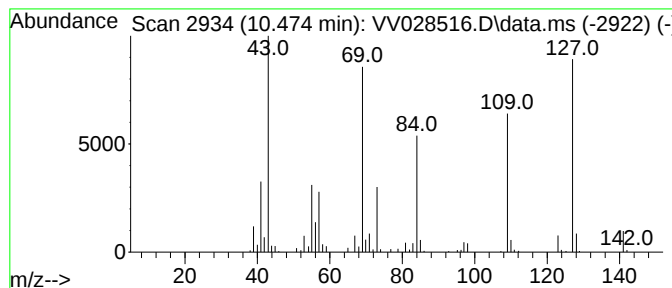
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.474	15.61 ug/L	256588	1,4-Dichlorobenzene-d4	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoro-5-methoxypyridine		127	C6H6FNO	136888-79-4	38	
2	1H-Pyrazole-4-carboxylic acid, 3...		127	C4H5N3O2	041680-34-6	35	
3	2-Fluoro-5-methoxypyridine		127	C6H6FNO	136888-79-4	35	
4	Pentane, 3-methylene-		84	C6H12	000760-21-4	27	
5	3-Methylpentyl methacrylate		170	C10H18O2	113615-00-2	27	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2,5-...	9.728	9.5	ug/L	156718	2	8.847	821856	50.0
unknown-01	10.474	15.6	ug/L	256588	3	11.239	822119	50.0