

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090822\
 Data File : VU050680.D
 Acq On : 08 Sep 2022 12:37
 Operator : SY/MD
 Sample : N4475-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVD8

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_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	102	rBV	107209	138660	4.15%	1.164%
2	1.906	168	176	193	rVB	89451	121530	3.64%	1.020%
3	2.437	339	341	342	rBV	339	146	0.00%	0.001%
4	2.475	352	353	357	rBV	326	149	0.00%	0.001%
5	2.565	369	381	395	rBV	227257	367412	10.99%	3.083%
6	2.906	486	487	489	rBV	147	48	0.00%	0.000%
7	2.922	490	492	494	rBV	202	103	0.00%	0.001%
8	3.038	523	528	531	rBV3	916	958	0.03%	0.008%
9	3.375	628	633	641	rVB2	257	290	0.01%	0.002%
10	3.848	775	780	785	rVB2	190	191	0.01%	0.002%
11	3.967	814	817	822	rVB	209	169	0.01%	0.001%
12	3.996	822	826	827	rBV	103	63	0.00%	0.001%
13	4.112	859	862	864	rBV2	137	104	0.00%	0.001%
14	4.231	895	899	903	rBV	286	239	0.01%	0.002%
15	4.330	927	930	933	rVB2	178	116	0.00%	0.001%
16	4.369	941	942	943	rVB	200	39	0.00%	0.000%
17	4.424	955	959	962	rBV2	190	176	0.01%	0.001%
18	4.453	962	968	970	rBV4	856	759	0.02%	0.006%
19	4.620	1008	1020	1057	rBV	106585	299255	8.95%	2.511%
20	5.063	1141	1158	1177	rBV2	226249	501229	15.00%	4.206%
21	5.324	1237	1239	1240	rBV2	175	60	0.00%	0.001%
22	5.362	1248	1251	1253	rBV2	663	418	0.01%	0.004%
23	5.401	1261	1263	1266	rBV	157	72	0.00%	0.001%
24	5.481	1284	1288	1291	rBV2	255	251	0.01%	0.002%
25	5.530	1297	1303	1307	rBV2	295	315	0.01%	0.003%
26	5.649	1338	1340	1342	rBV	71	42	0.00%	0.000%
27	5.726	1342	1364	1388	rBV2	440568	1242033	37.16%	10.422%
28	6.250	1512	1527	1548	rBV	351468	677491	20.27%	5.685%
29	6.382	1567	1568	1569	rBV	748	214	0.01%	0.002%
30	6.481	1596	1599	1602	rBV2	370	292	0.01%	0.002%
31	6.636	1644	1647	1649	rBV2	241	176	0.01%	0.001%
32	6.690	1649	1664	1689	rBV	291466	575210	17.21%	4.827%
33	6.883	1716	1724	1738	rVB4	6794	12653	0.38%	0.106%
34	6.961	1746	1748	1753	rBV	228	165	0.00%	0.001%
35	6.986	1754	1756	1760	rVB	441	282	0.01%	0.002%
36	7.182	1814	1817	1818	rBV2	618	362	0.01%	0.003%

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Integrator: RTE

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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_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	7.253	1838	1839	1840	rBV2	175	61	0.00%	0.001%
38	7.398	1880	1884	1886	rBV2	134	96	0.00%	0.001%
39	7.452	1899	1901	1906	rVB	223	124	0.00%	0.001%
40	7.514	1917	1920	1921	rBV	216	104	0.00%	0.001%
41	7.565	1924	1936	1957	rBV	140192	248500	7.44%	2.085%
42	7.735	1987	1989	1992	rBV2	220	172	0.01%	0.001%
43	7.764	1996	1998	2000	rBV2	125	32	0.00%	0.000%
44	7.777	2000	2002	2003	rBV	276	98	0.00%	0.001%
45	7.790	2003	2006	2010	rVB3	487	387	0.01%	0.003%
46	7.899	2026	2040	2069	rBV	509410	909742	27.22%	7.634%
47	8.179	2116	2127	2147	rBV2	95218	167041	5.00%	1.402%
48	8.475	2217	2219	2222	rVB2	248	112	0.00%	0.001%
49	8.552	2229	2243	2259	rBV	1965463	3342140	100.00%	28.045%
50	8.967	2370	2372	2375	rVB	222	92	0.00%	0.001%
51	8.983	2375	2377	2380	rBV2	313	165	0.00%	0.001%
52	9.028	2390	2391	2393	rVB	317	116	0.00%	0.001%
53	9.044	2393	2396	2398	rBV2	248	157	0.00%	0.001%
54	9.121	2418	2420	2422	rVB	335	155	0.00%	0.001%
55	9.150	2426	2429	2432	rBV	276	225	0.01%	0.002%
56	9.337	2485	2487	2490	rVB2	251	117	0.00%	0.001%
57	9.417	2499	2512	2541	rBV	500823	859697	25.72%	7.214%
58	9.575	2557	2561	2566	rVB4	620	586	0.02%	0.005%
59	9.597	2566	2568	2570	rVB2	309	126	0.00%	0.001%
60	9.694	2594	2598	2602	rBV2	565	567	0.02%	0.005%
61	9.735	2608	2611	2614	rBV2	199	146	0.00%	0.001%
62	9.928	2666	2671	2675	rVB2	331	319	0.01%	0.003%
63	10.102	2722	2725	2726	rBV2	254	134	0.00%	0.001%
64	10.346	2792	2801	2817	rBV3	21623	39980	1.20%	0.335%
65	10.755	2915	2928	2954	rBV	445485	728733	21.80%	6.115%
66	10.902	2972	2974	2975	rBV	192	70	0.00%	0.001%
67	11.044	3016	3018	3020	rBV	239	129	0.00%	0.001%
68	11.086	3028	3031	3032	rBV	394	227	0.01%	0.002%
69	11.111	3037	3039	3043	rBV3	408	313	0.01%	0.003%
70	11.581	3179	3185	3186	rBV2	551	479	0.01%	0.004%
71	11.690	3209	3219	3239	rBV3	60464	110607	3.31%	0.928%
72	11.812	3244	3257	3285	rBV	441417	724749	21.69%	6.082%
73	12.192	3363	3375	3403	rBV	480315	799135	23.91%	6.706%
74	12.388	3433	3436	3439	rBV2	350	300	0.01%	0.003%
75	12.893	3584	3593	3603	rBV3	24425	36552	1.09%	0.307%
76	14.333	4037	4041	4049	rVB4	2472	2747	0.08%	0.023%

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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_U\Method\SFAMULM090222WMA.M
Title : VOC Analysis

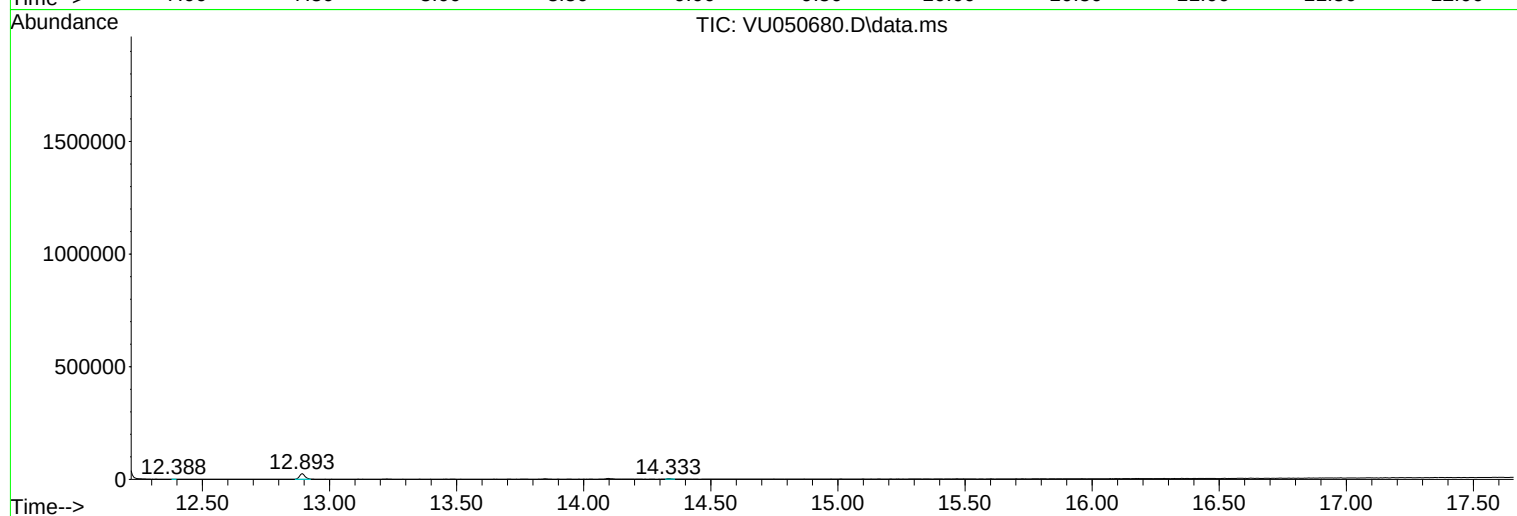
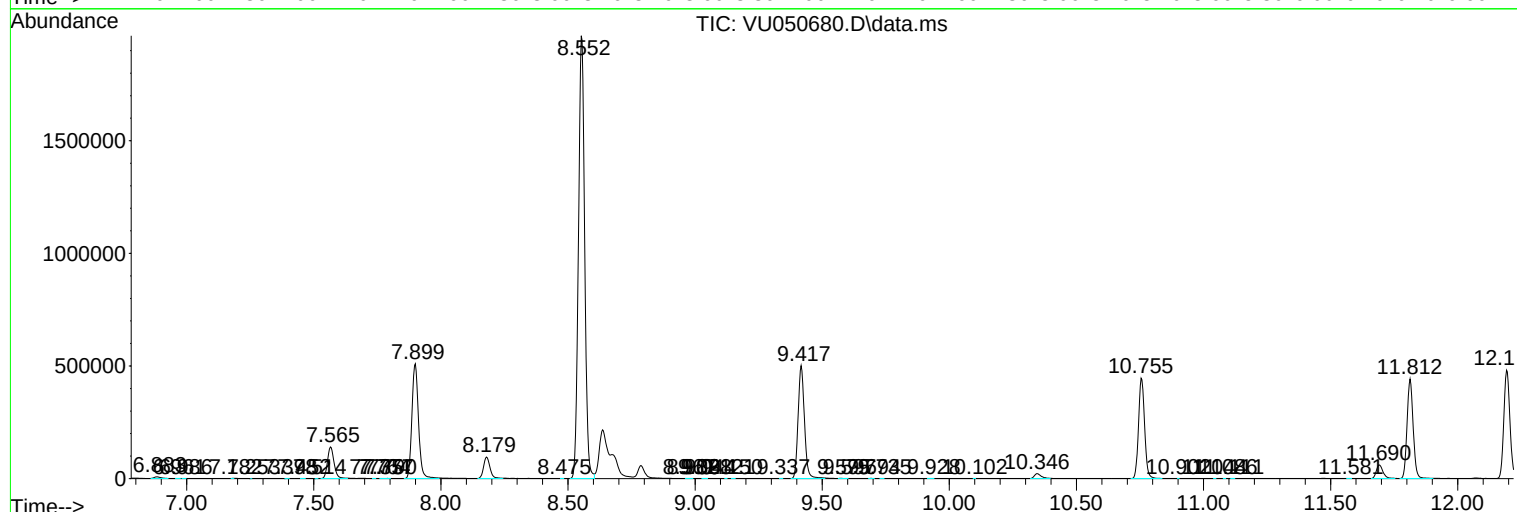
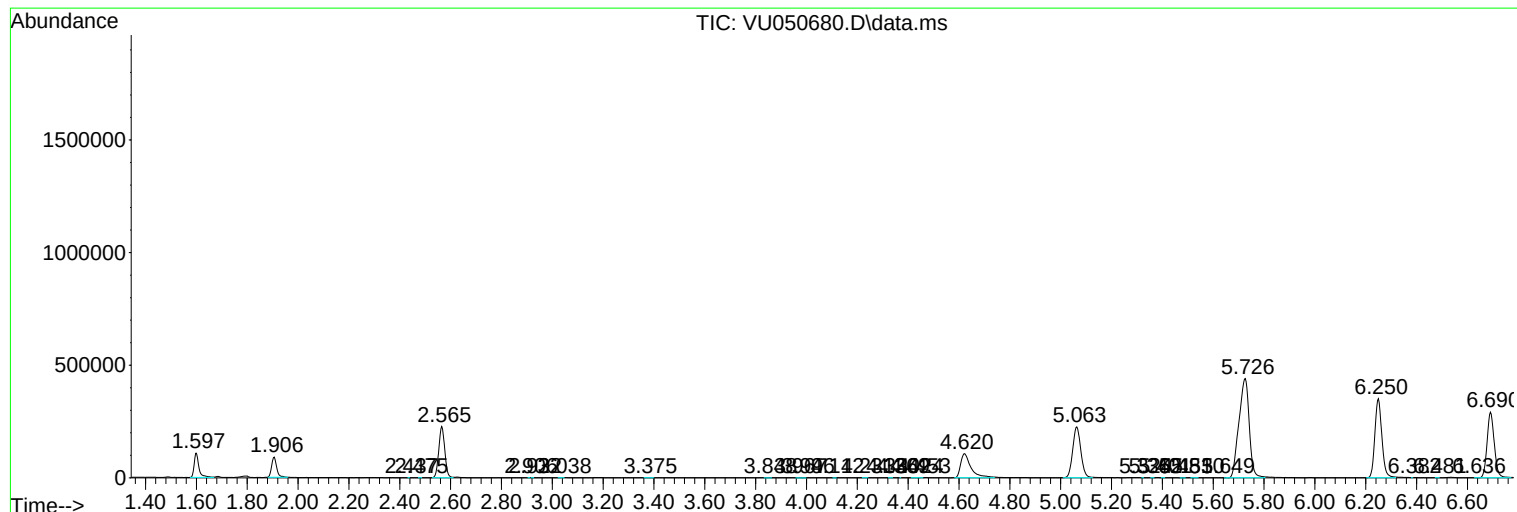
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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Sample : N4475-01
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
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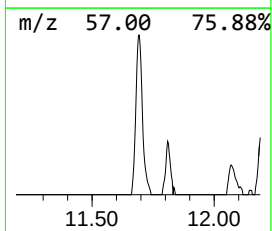
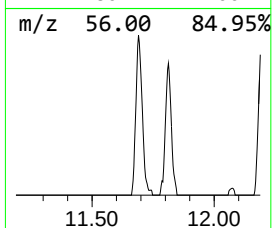
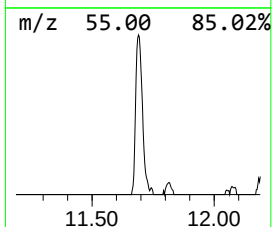
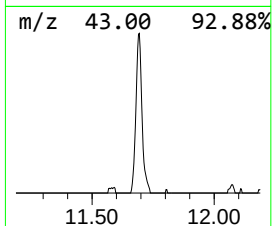
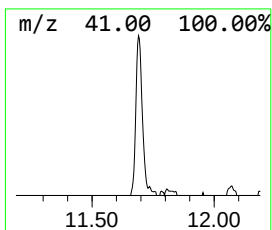
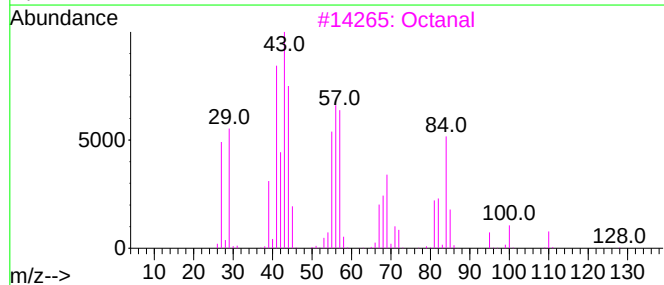
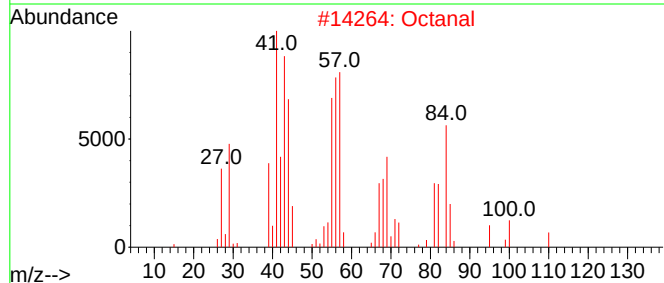
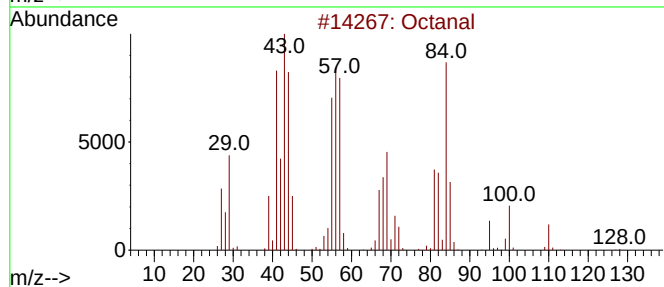
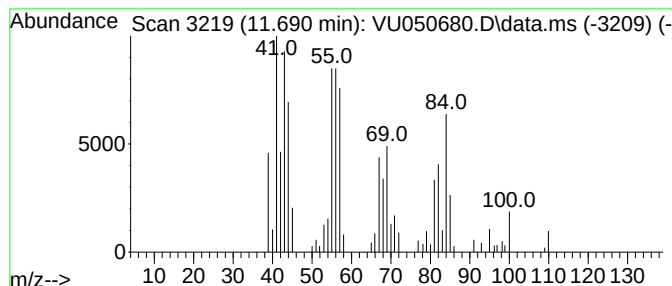
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	7.63 ug/L	110607	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	83
2	Octanal			128	C8H16O	000124-13-0	72
3	Octanal			128	C8H16O	000124-13-0	64
4	Octanal			128	C8H16O	000124-13-0	59
5	Octanal			128	C8H16O	000124-13-0	53



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Instrument :
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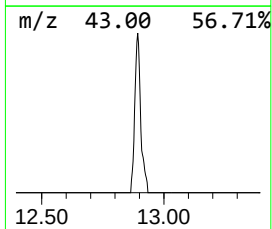
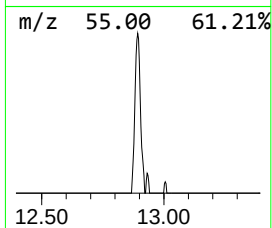
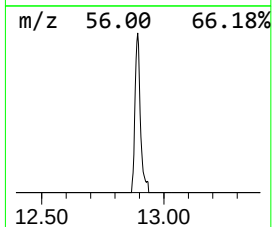
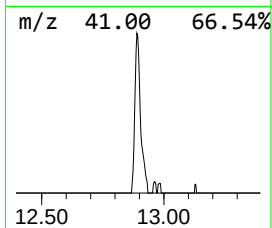
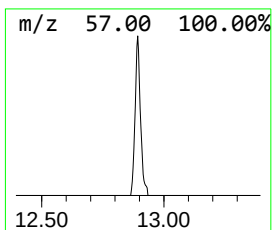
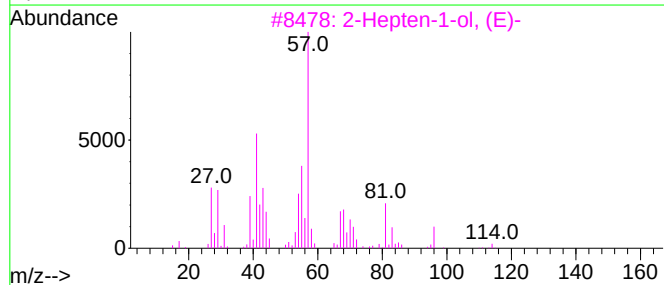
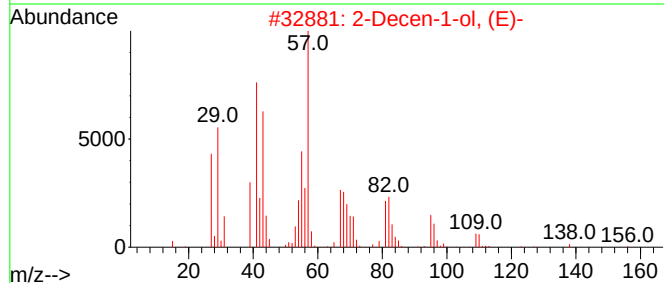
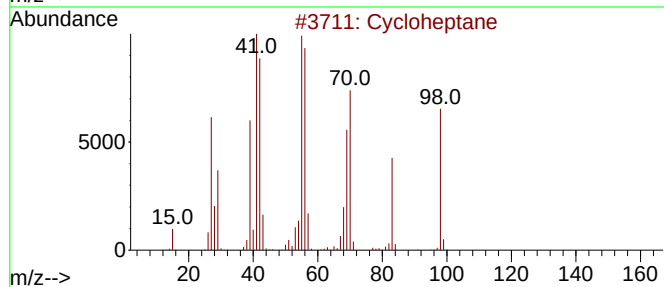
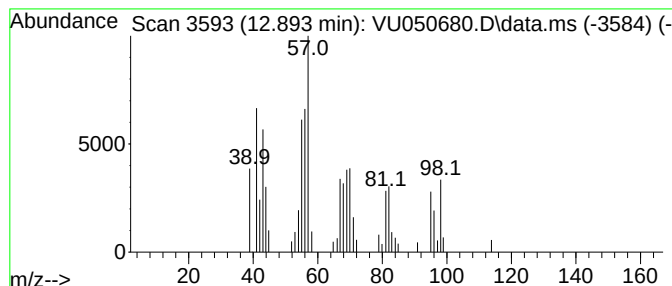
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic12.893 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.893	2.52 ug/L	36552	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane	98	C7H14	000291-64-5	43
2			2-Decen-1-ol, (E)-	156	C10H20O	018409-18-2	38
3			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	30
4			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	30
5			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	25



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octanal	11.690	7.6	ug/L	110607	3	11.812	724749	50.0
(DEL) Alkane: C...	12.893	2.5	ug/L	36552	3	11.812	724749	50.0