LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

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\SFAMVLM051923WMA.M
Title : VOC Analysis

Signal : TIC: VV031142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	69	75	90	rVB	136988	156132	14.79%	2.000%
2	1.529	147	152	168	rVB	111393	141018	13.36%	1.806%
3	2.063	309	318	329	rBV	254927	363003	34.40%	4.649%
4	2.555	469	471	472	rBV2	2529	1166	0.11%	0.015%
5	2.828	554	556	557	rBV2	962	310	0.03%	0.004%
6	3.076	631	633	634	rBV2	1762	657	0.06%	0.008%
7	3.134	647	651	652	rBV4	1616	1164	0.11%	0.015%
8	3.191	666	669	670	rBV3	1540	852	0.08%	0.011%
9	3.211	673	675	676	rBV2	1678	578	0.05%	0.007%
10	3.240	681	684	687	rBV5	1154	985	0.09%	0.013%
11	3.269	691	693	694	rBV2	1473	690	0.07%	0.009%
12	3.429	740	743	744	rBV3	1535	735	0.07%	0.009%
13	3.494	761	763	768	rBV5	2393	2028	0.19%	0.026%
14	3.519	768	771	774	rBV5	1661	1104	0.10%	0.014%
15	3.548	777	780	781	rBV3	1122	631	0.06%	0.008%
16	3.574	787	788	791	rBV3	1094	408	0.04%	0.005%
17	3.706	827	829	830	rBV2	1253	393	0.04%	0.005%
18	3.793	846	856	881	rBV	77034	215480	20.42%	2.760%
19	4.256	990	1000	1024	rVB2	164248	411564	39.00%	5.271%
20	4.551	1090	1092	1094	rBV3	1327	660	0.06%	0.008%
21	4.886	1192	1196	1197	rBV4	1106	695	0.07%	0.009%
22	4.963	1202	1220	1252	rBV2	371441	1055345	100.00%	13.516%
23	5.436	1365	1367	1372	rBV6	2115	2091	0.20%	0.027%
24	5.542	1388	1400	1421	rBV	278392	584437	55.38%	7.485%
25	5.995	1530	1541	1566	rVB	217059	450899	42.73%	5.775%
26	6.490	1693	1695	1696	rBV2	1498	561	0.05%	0.007%
27	6.860	1808	1810	1813	rVB4	2193	923	0.09%	0.012%
28	6.918	1819	1828	1844	rBV	105758	193313	18.32%	2.476%
29	7.249	1921	1931	1945	rBV	413251	712173	67.48%	9.121%
30	7.558	2019	2027	2043	rBV	76780	131275	12.44%	1.681%
31	8.030	2165	2174	2188	rBV	256241	474639	44.97%	6.079%
32	8.792	2400	2411	2434	rBV	435224	721079	68.33%	9.235%
33	8.956	2455	2462	2473	rVB	28030	43793	4.15%	0.561%
34	9.082	2493	2501	2512	rBV	16192	27989	2.65%	0.358%
35	9.265	2553	2558	2561	rBV7	2224	1947	0.18%	0.025%
36	9.310	2569	2572	2574	rBV4	1023	766	0.07%	0.010%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : GBX71

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\SFAMVLM051923WMA.M
Title : VOC Analysis

37	9.391	2595	2597	2599	rBV3	1493	617	0.06%	0.008%
38	9.461	2617	2619	2621	rBV3	2005	1130	0.11%	0.014%
39	9.487	2621	2627	2637	rVV4	8872	17055	1.62%	0.218%
40	9.654	2670	2679	2691	rBV	24759	42685	4.04%	0.547%
41	9.866	2741	2745	2753	rBV9	2194	2830	0.27%	0.036%
42	9.960	2763	2774	2787	rBV2	28728	55779	5.29%	0.714%
43	10.159	2824	2836	2855	rBV	297198	477024	45.20%	6.109%
44	10.333	2881	2890	2902	rVB2	9010	18583	1.76%	0.238%
45	10.384	2902	2906	2907	rBV4	2102	1534	0.15%	0.020%
46	10.519	2944	2948	2949	rBV4	1711	1065	0.10%	0.014%
47	10.603	2970	2974	2978	rBV6	2639	2067	0.20%	0.026%
48	10.644	2985	2987	2989	rBV3	948	586	0.06%	0.008%
49	10.741	3014	3017	3019	rBV4	1346	665	0.06%	0.009%
50	10.751	3019	3020	3022	rBV2	794	343	0.03%	0.004%
51	10.792	3029	3033	3036	rBV6	1039	976	0.09%	0.012%
52	10.821	3040	3042	3043	rBV2	821	310	0.03%	0.004%
53	10.831	3043	3045	3047	rBV3	1212	588	0.06%	0.008%
54	11.191	3146	3157	3173	rBV	401618	629102	59.61%	8.057%
55	11.493	3240	3251	3264	rBV3	50748	109482	10.37%	1.402%
56	11.567	3265	3274	3292	rVB	445704	698186	66.16%	8.942%
57	12.185	3460	3466	3478	rVB4	23687	40256	3.81%	0.516%
58	12.905	3688	3690	3695	rBV6	2054	1583	0.15%	0.020%
59	13.313	3815	3817	3820	rBV4	1883	1392	0.13%	0.018%
60	13.734	3945	3948	3949	rBV3	2455	1239	0.12%	0.016%
61	13.988	4025	4027	4028	rBV2	2000	878	0.08%	0.011%
62	14.168	4081	4083	4084	rBV2	2071	857	0.08%	0.011%

Sum of corrected areas: 7808295

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
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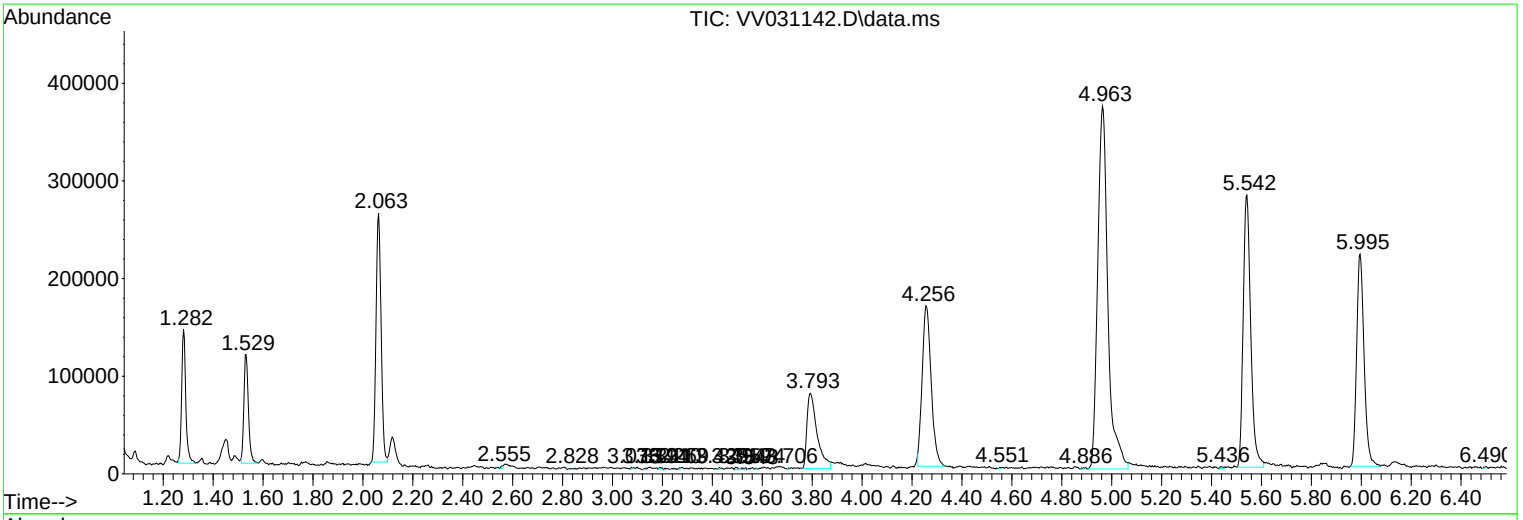
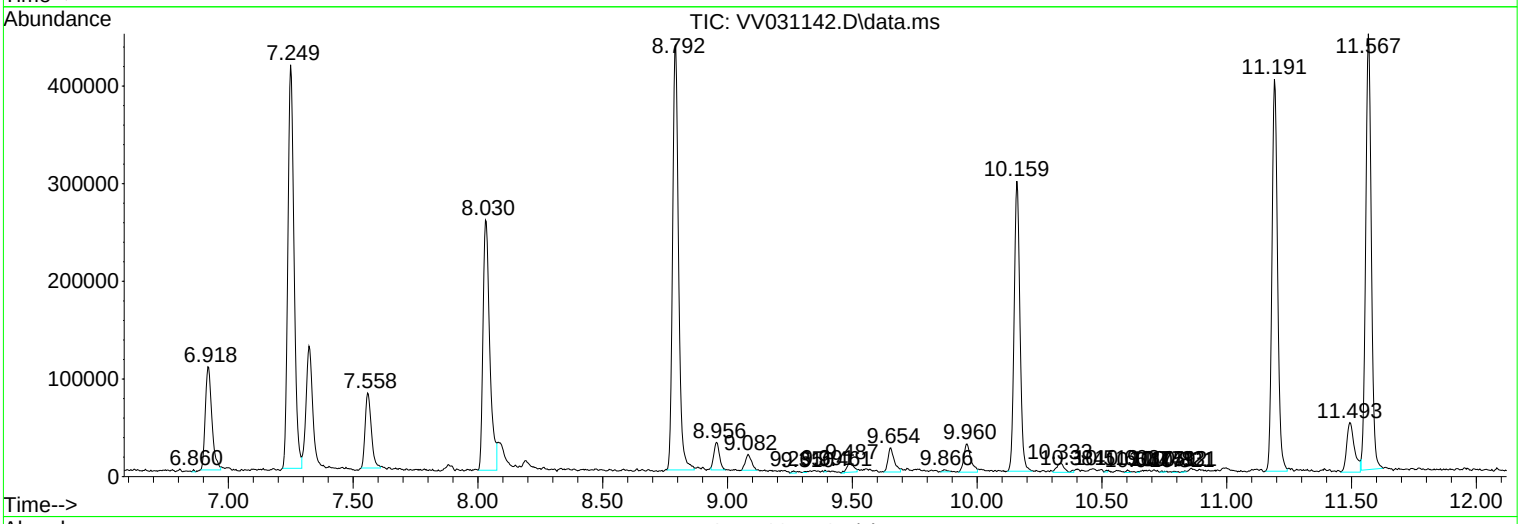
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

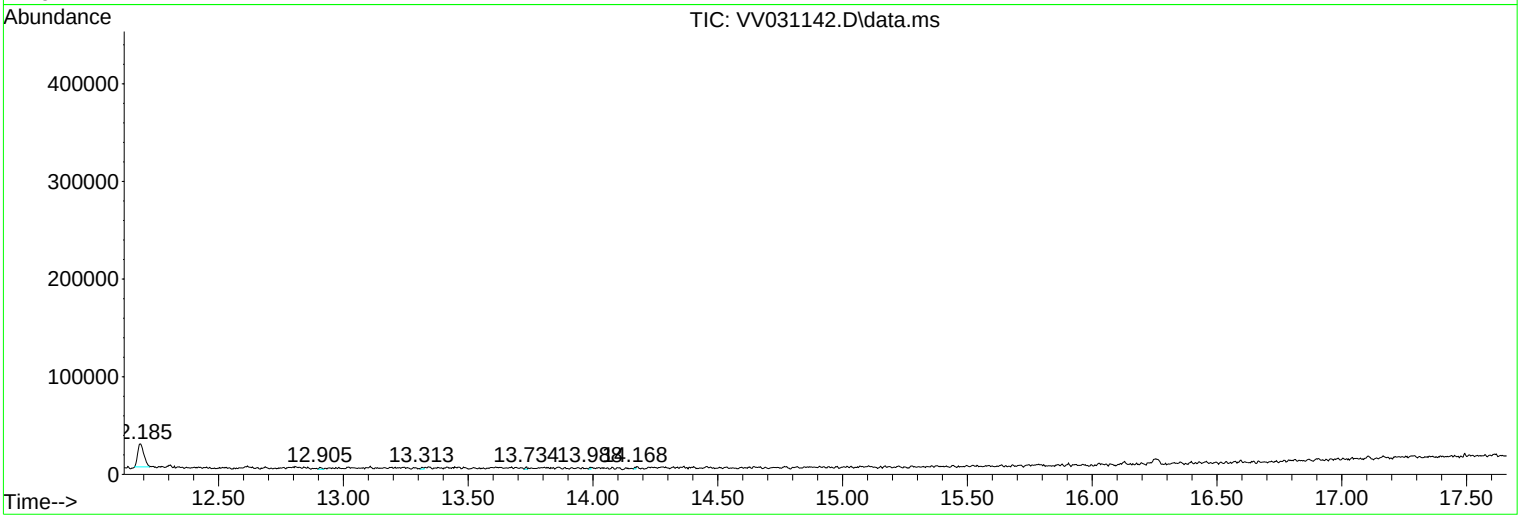
Instrument :
MSVOA_V
ClientSampleId :
GBX71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

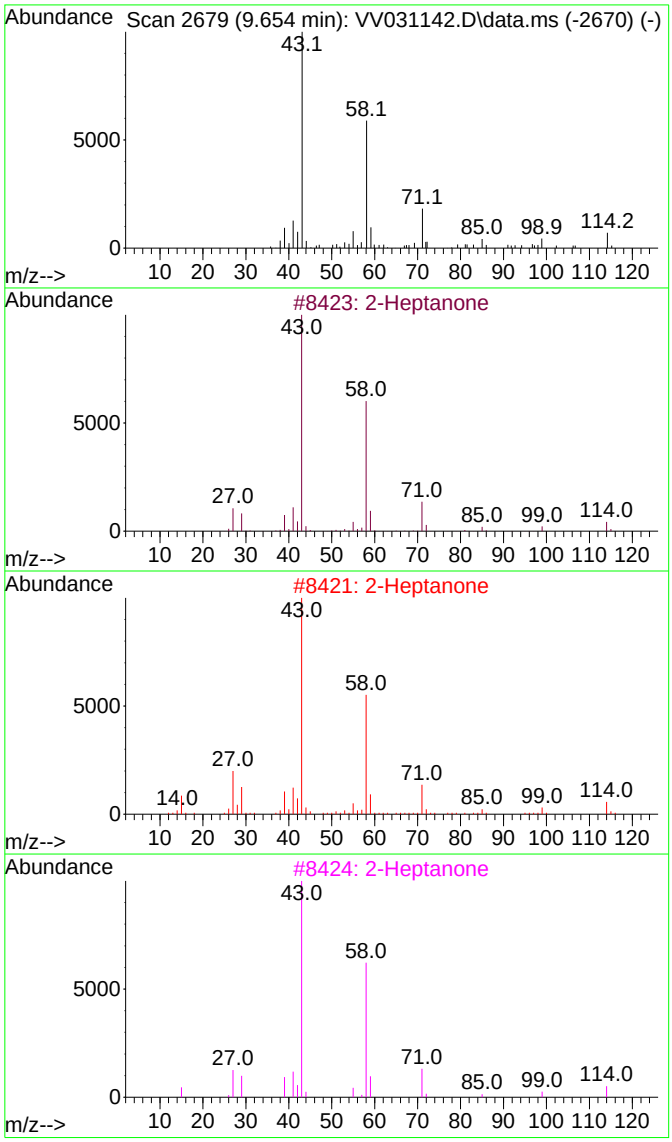
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

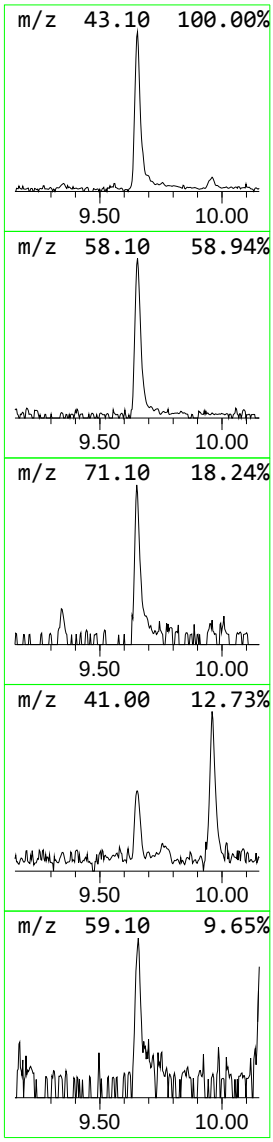
****

Peak Number 2 2-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.654	2.96 ug/L	42685	Chlorobenzene-d5	8.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Heptanone	114	C7H14O	000110-43-0	87
3	2-Heptanone	114	C7H14O	000110-43-0	87
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86
5	2-Heptanone	114	C7H14O	000110-43-0	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

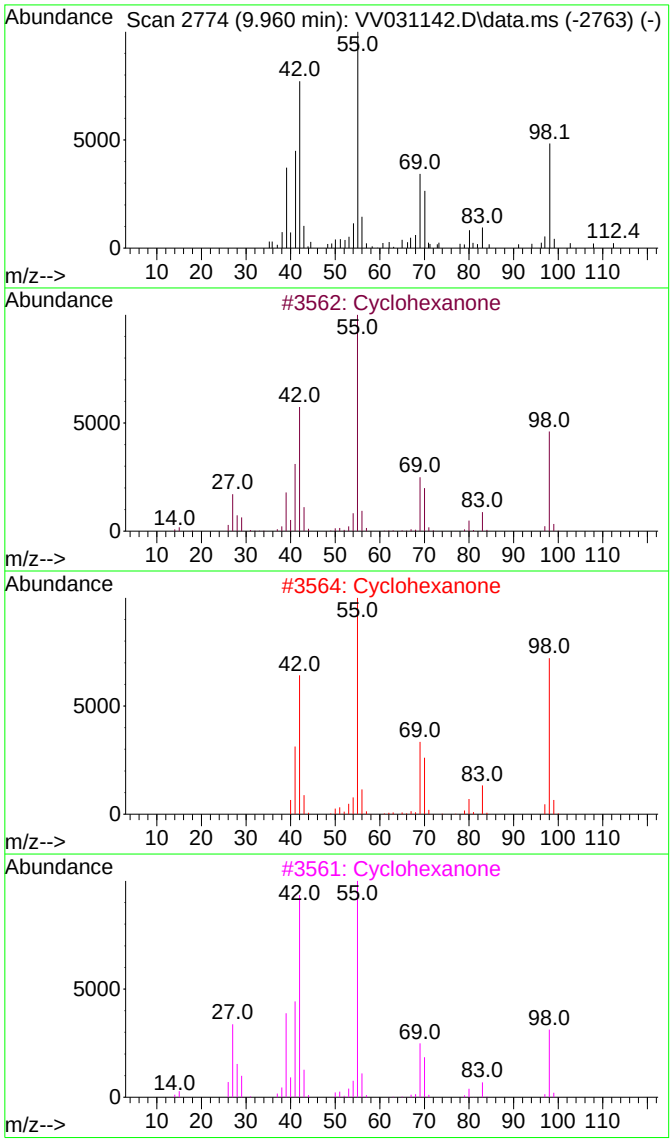
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

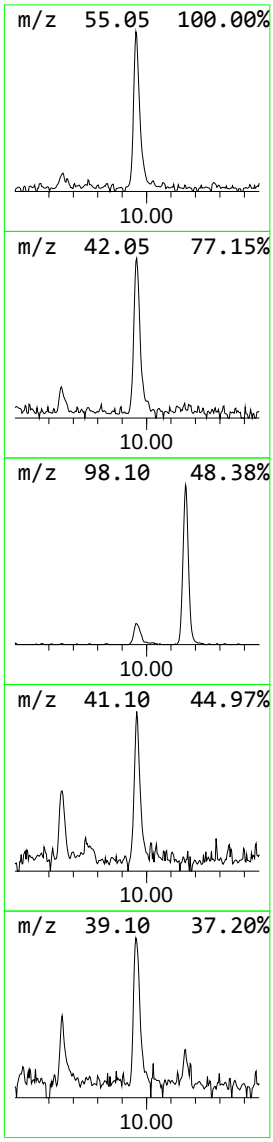
****

Peak Number 3 Cyclohexanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.960	3.87 ug/L	55779	Chlorobenzene-d5	8.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	91
2	Cyclohexanone	98	C6H10O	000108-94-1	91
3	Cyclohexanone	98	C6H10O	000108-94-1	91
4	Cyclohexanone	98	C6H10O	000108-94-1	91
5	Cyclohexanone	98	C6H10O	000108-94-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

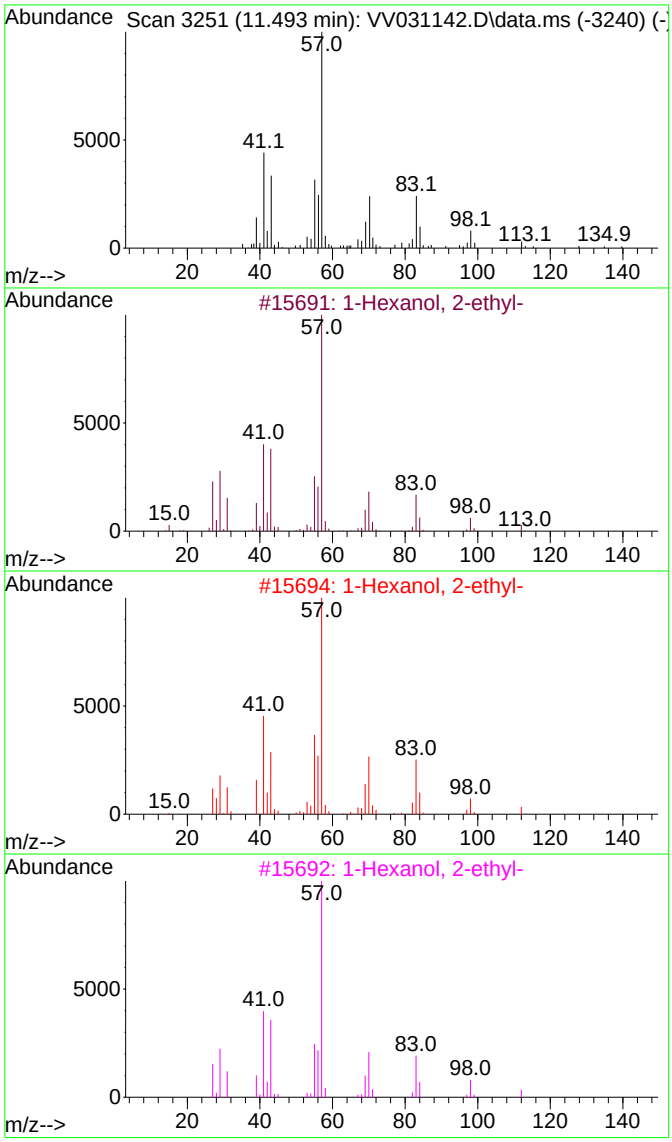
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

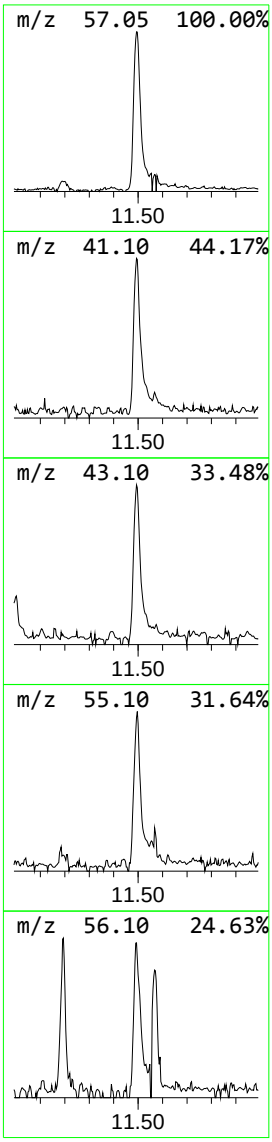
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.493	8.70 ug/L	109482	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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

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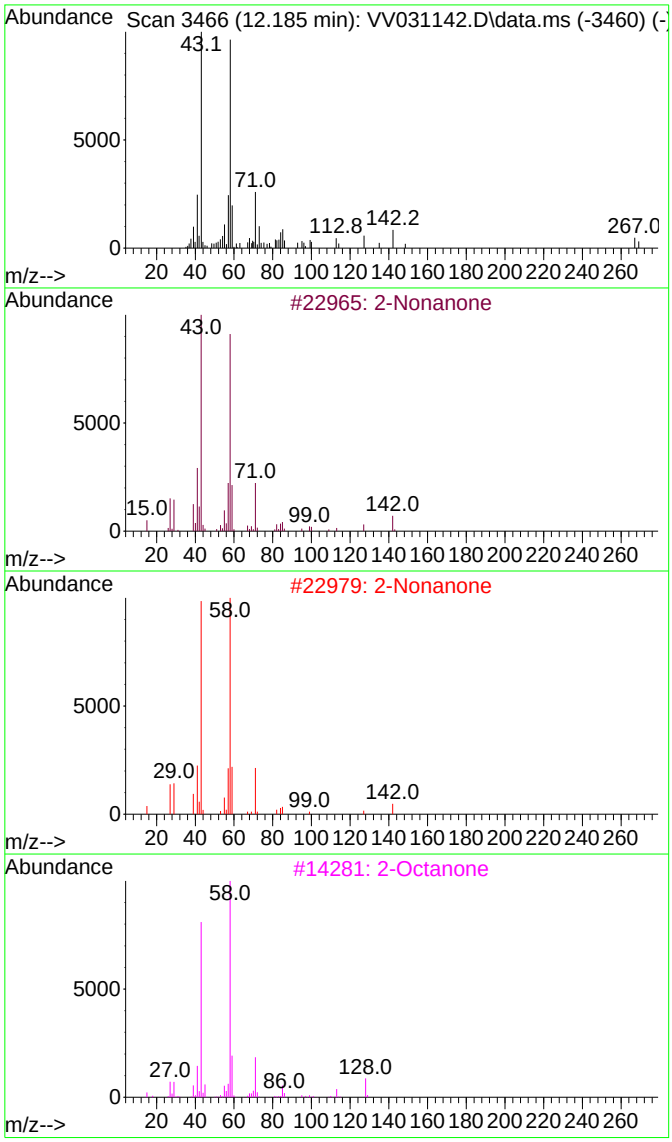
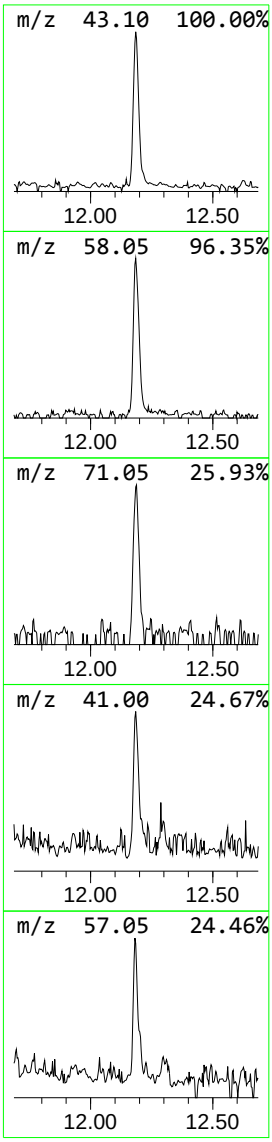
Peak Number 5 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.185	3.20 ug/L	40256	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	80
2	2-Nonanone	142	C9H18O	000821-55-6	74
3	2-Octanone	128	C8H16O	000111-13-7	64
4	2-Octanone	128	C8H16O	000111-13-7	64
5	2-Octanone	128	C8H16O	000111-13-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051923\
Data File : VV031142.D
Acq On : 20 May 2023 06:23
Operator : SY/MD
Sample : 02865-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBX71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Heptanone	9.654	3.0	ug/L	42685	2	8.792	721079	50.0
Cyclohexanone	9.960	3.9	ug/L	55779	2	8.792	721079	50.0
1-Hexanol, 2-et...	11.493	8.7	ug/L	109482	3	11.191	629102	50.0
2-Nonanone	12.185	3.2	ug/L	40256	3	11.191	629102	50.0