

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
 Data File : VX028482.D
 Acq On : 02 May 2022 18:45
 Operator : JC/MD
 Sample : N2658-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40818

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_X\Method\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	206	212	222	rBV	31339	53793	2.38%	0.385%
2	5.391	694	706	720	rBV2	271148	788989	34.84%	5.650%
3	5.556	722	733	748	rVB	374142	1051703	46.44%	7.531%
4	5.958	788	799	820	rBV	286045	736871	32.54%	5.276%
5	6.763	922	931	945	rBV	596522	1406235	62.10%	10.070%
6	8.653	1234	1241	1250	rBV	1460322	2264593	100.00%	16.216%
7	10.055	1465	1471	1489	rBV	1355629	1793699	79.21%	12.844%
8	11.085	1634	1640	1646	rBV	1246765	1592812	70.34%	11.406%
9	11.573	1715	1720	1725	rBV	443781	540292	23.86%	3.869%
10	11.756	1745	1750	1755	rVB2	24696	33384	1.47%	0.239%
11	11.829	1755	1762	1767	rBV	88169	127540	5.63%	0.913%
12	11.890	1767	1772	1781	rVV	57873	83495	3.69%	0.598%
13	11.975	1781	1786	1787	rVV	24967	28731	1.27%	0.206%
14	12.024	1787	1794	1801	rVV	1533632	1909647	84.33%	13.674%
15	12.103	1801	1807	1814	rVB3	54591	95862	4.23%	0.686%
16	12.243	1823	1830	1839	rBV3	29293	49392	2.18%	0.354%
17	12.701	1902	1905	1913	rVB2	26136	38924	1.72%	0.279%
18	12.816	1918	1924	1927	rBV5	16714	29466	1.30%	0.211%
19	12.926	1935	1942	1945	rBV	21375	28812	1.27%	0.206%
20	12.963	1945	1948	1954	rVB2	27503	36832	1.63%	0.264%
21	13.170	1973	1982	1984	rBV7	14797	33191	1.47%	0.238%
22	13.292	1997	2002	2007	rVB2	100272	134513	5.94%	0.963%
23	13.420	2019	2023	2030	rVB	44801	63097	2.79%	0.452%
24	13.585	2046	2050	2057	rBV3	50564	90160	3.98%	0.646%
25	13.664	2057	2063	2068	rVB2	31961	64332	2.84%	0.461%
26	13.749	2068	2077	2080	rVB7	15265	26476	1.17%	0.190%
27	13.926	2103	2106	2110	rVV2	25498	32012	1.41%	0.229%
28	13.969	2110	2113	2118	rVB3	20043	27207	1.20%	0.195%
29	14.078	2126	2131	2134	rBV	28142	39013	1.72%	0.279%
30	14.213	2149	2153	2163	rBV4	42868	99461	4.39%	0.712%
31	14.322	2168	2171	2175	rVV3	18459	22756	1.00%	0.163%
32	14.371	2175	2179	2183	rVV	35951	45812	2.02%	0.328%
33	14.481	2192	2197	2202	rBV3	64679	91124	4.02%	0.653%
34	14.615	2210	2219	2226	rBV6	27150	66372	2.93%	0.475%
35	14.676	2226	2229	2233	rVB2	17507	23547	1.04%	0.169%
36	14.779	2241	2246	2251	rBV2	85926	127957	5.65%	0.916%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_X\Method\82X041922W.M
Title : SW846 8260

37	14.908	2261	2267	2273	rBV5	11398	24881	1.10%	0.178%
38	15.188	2308	2313	2319	rVB	32043	55153	2.44%	0.395%
39	15.481	2356	2361	2364	rBV	32750	50408	2.23%	0.361%
40	15.517	2364	2367	2374	rVB6	16195	27415	1.21%	0.196%
41	15.615	2378	2383	2386	rVV	49134	75515	3.33%	0.541%
42	15.651	2386	2389	2397	rVB2	31665	53738	2.37%	0.385%

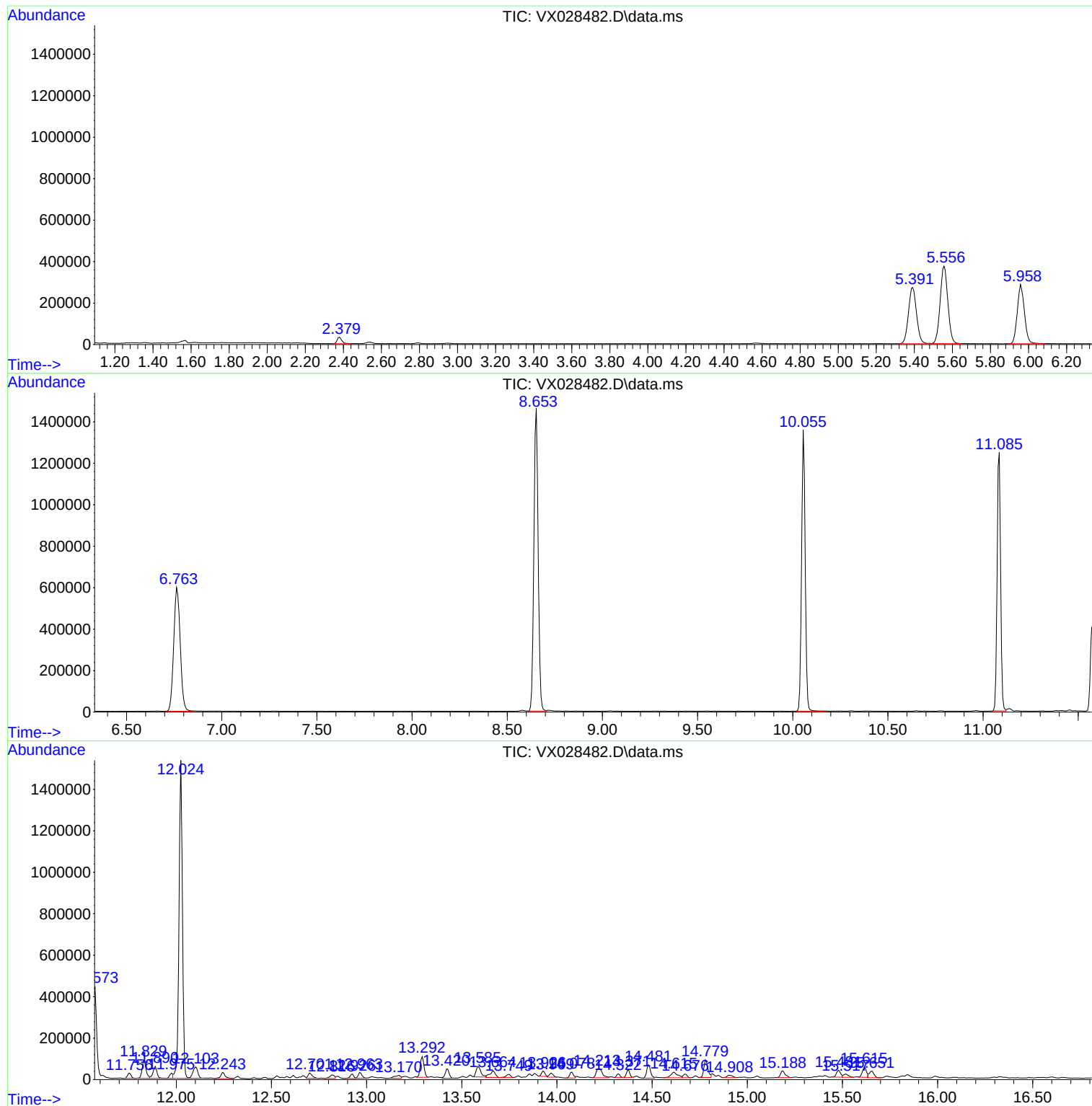
Sum of corrected areas: 13965212

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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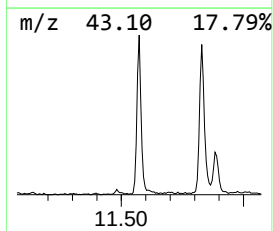
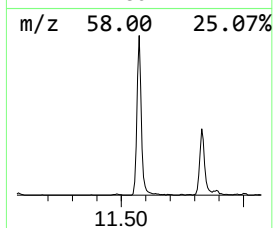
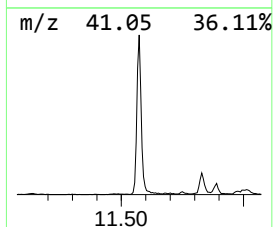
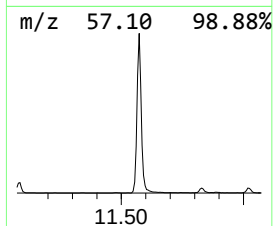
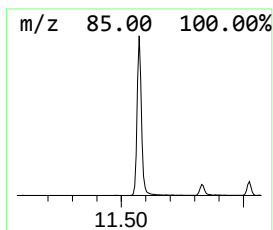
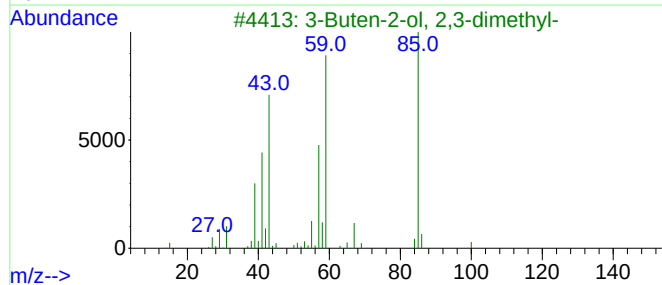
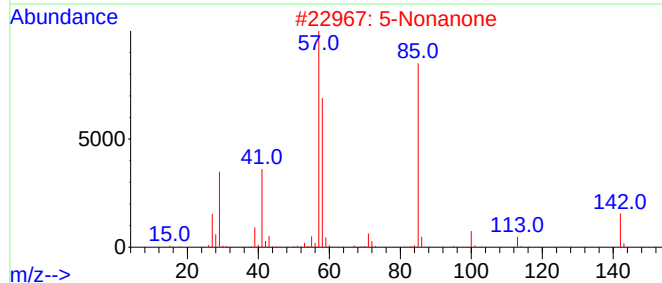
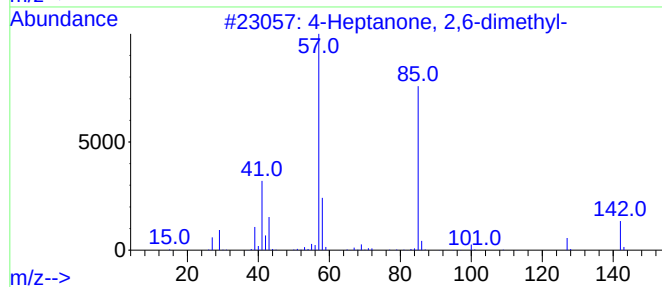
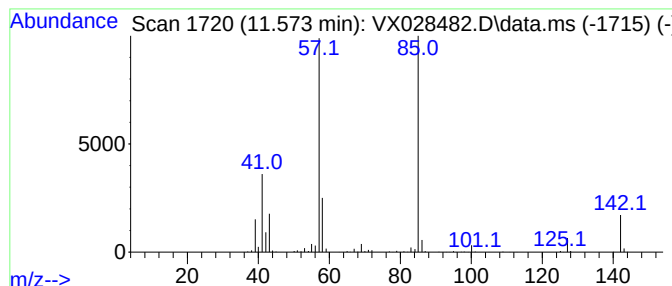
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	14.15 ug/l	540292	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			5-Nonanone	142	C9H18O	000502-56-7	59
3			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
4			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	56
5			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	11.573	14.2	ug/l	540292	4	12.024	1909650	50.0