

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
 Data File : VX028481.D
 Acq On : 02 May 2022 18:22
 Operator : JC/MD
 Sample : N2658-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40817

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: VX028481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	207	212	219	rBV	23059	38678	1.65%	0.280%
2	2.532	230	237	246	rBV	16736	31944	1.36%	0.231%
3	5.391	694	706	722	rBV	278974	818131	34.80%	5.926%
4	5.556	722	733	751	rVB2	380936	1080751	45.97%	7.829%
5	5.958	786	799	818	rBV	289122	766823	32.62%	5.555%
6	6.763	921	931	947	rBV	606651	1454509	61.87%	10.536%
7	8.653	1234	1241	1249	rBV	1495692	2351046	100.00%	17.030%
8	10.055	1465	1471	1491	rBV	1420942	1880522	79.99%	13.622%
9	11.085	1634	1640	1651	rBV	1288928	1669687	71.02%	12.095%
10	11.573	1715	1720	1737	rBV	441457	561736	23.89%	4.069%
11	11.829	1755	1762	1768	rBV	87494	127977	5.44%	0.927%
12	11.890	1768	1772	1782	rVB2	42122	59054	2.51%	0.428%
13	12.024	1788	1794	1801	rBV	1576204	1899418	80.79%	13.759%
14	12.103	1801	1807	1813	rVB3	42195	78399	3.33%	0.568%
15	12.244	1824	1830	1838	rVB2	26722	42877	1.82%	0.311%
16	12.701	1901	1905	1912	rVB2	24654	38751	1.65%	0.281%
17	12.920	1934	1941	1945	rBV	21163	28880	1.23%	0.209%
18	12.963	1945	1948	1955	rVB2	24637	33752	1.44%	0.244%
19	13.292	1997	2002	2008	rVB2	89148	122682	5.22%	0.889%
20	13.420	2018	2023	2031	rVB	41280	57450	2.44%	0.416%
21	13.585	2046	2050	2055	rVB3	20896	29974	1.27%	0.217%
22	13.664	2060	2063	2068	rVB2	26862	40785	1.73%	0.295%
23	13.926	2099	2106	2110	rBV2	25867	39619	1.69%	0.287%
24	14.079	2126	2131	2135	rBV	21203	29930	1.27%	0.217%
25	14.231	2148	2156	2163	rBV3	49794	98782	4.20%	0.716%
26	14.371	2175	2179	2184	rVB	28132	34971	1.49%	0.253%
27	14.481	2192	2197	2203	rBV2	50927	68638	2.92%	0.497%
28	14.615	2211	2219	2225	rBV6	21169	50598	2.15%	0.367%
29	14.780	2242	2246	2250	rBV2	53770	77848	3.31%	0.564%
30	15.188	2308	2313	2320	rVB2	23268	42663	1.81%	0.309%
31	15.481	2353	2361	2364	rBV3	22786	38690	1.65%	0.280%
32	15.517	2364	2367	2374	rVV7	13888	25501	1.08%	0.185%
33	15.615	2378	2383	2386	rVV	30280	48315	2.06%	0.350%
34	15.652	2386	2389	2396	rVB3	21332	35609	1.51%	0.258%

Sum of corrected areas: 13804990

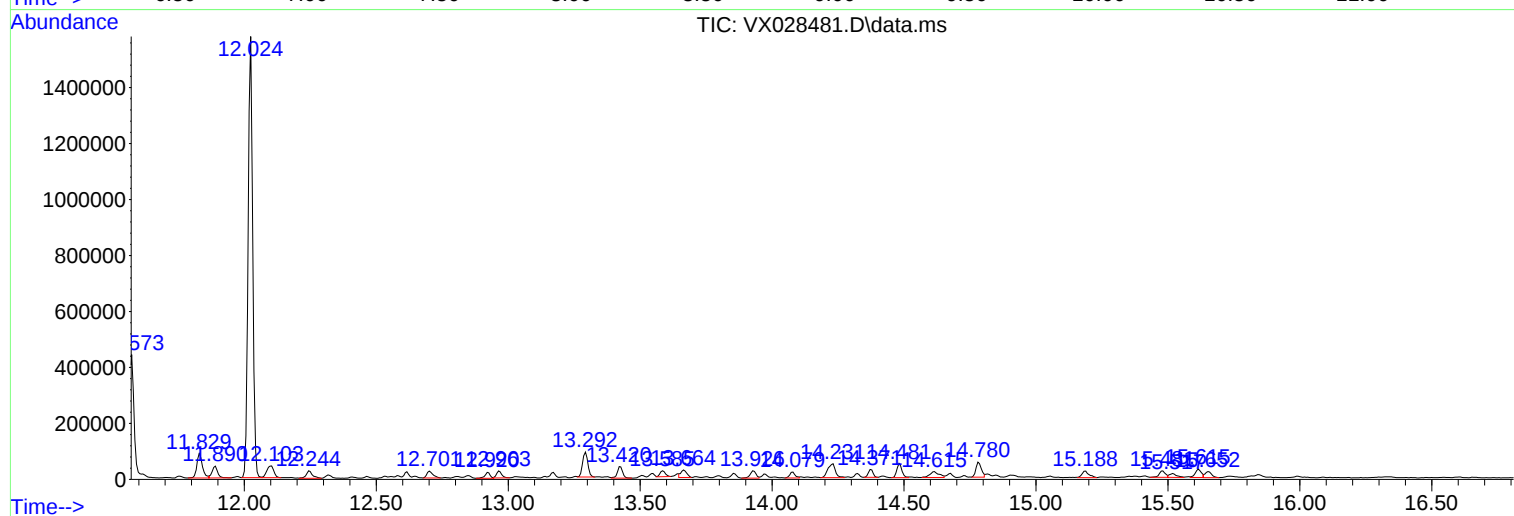
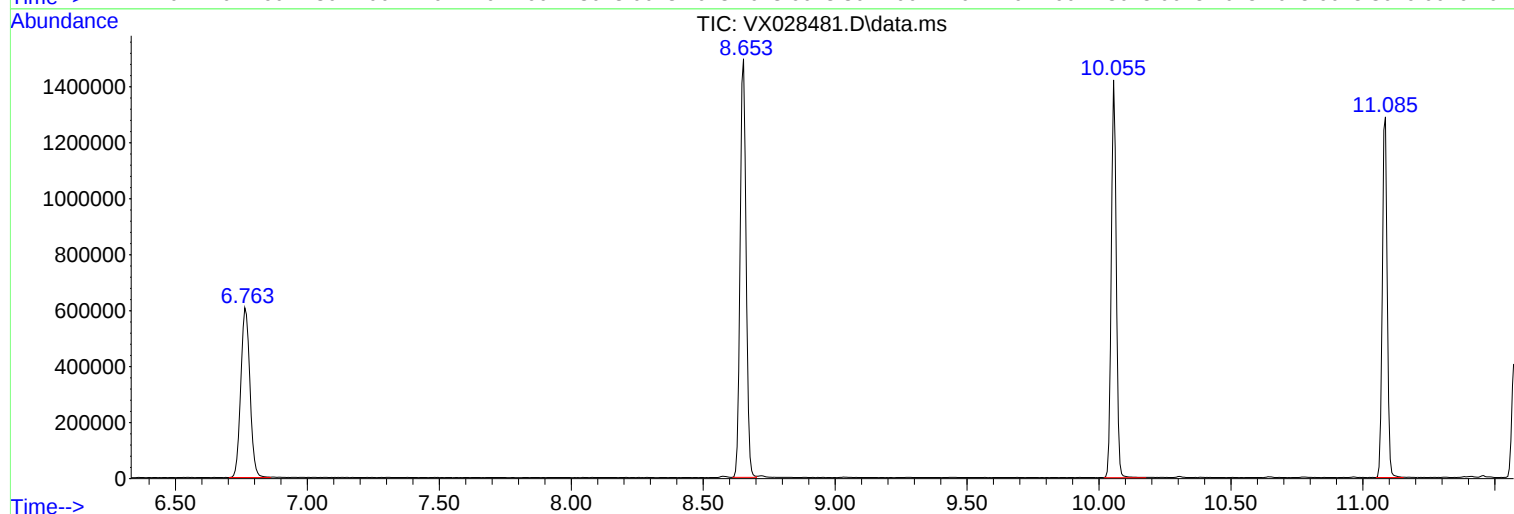
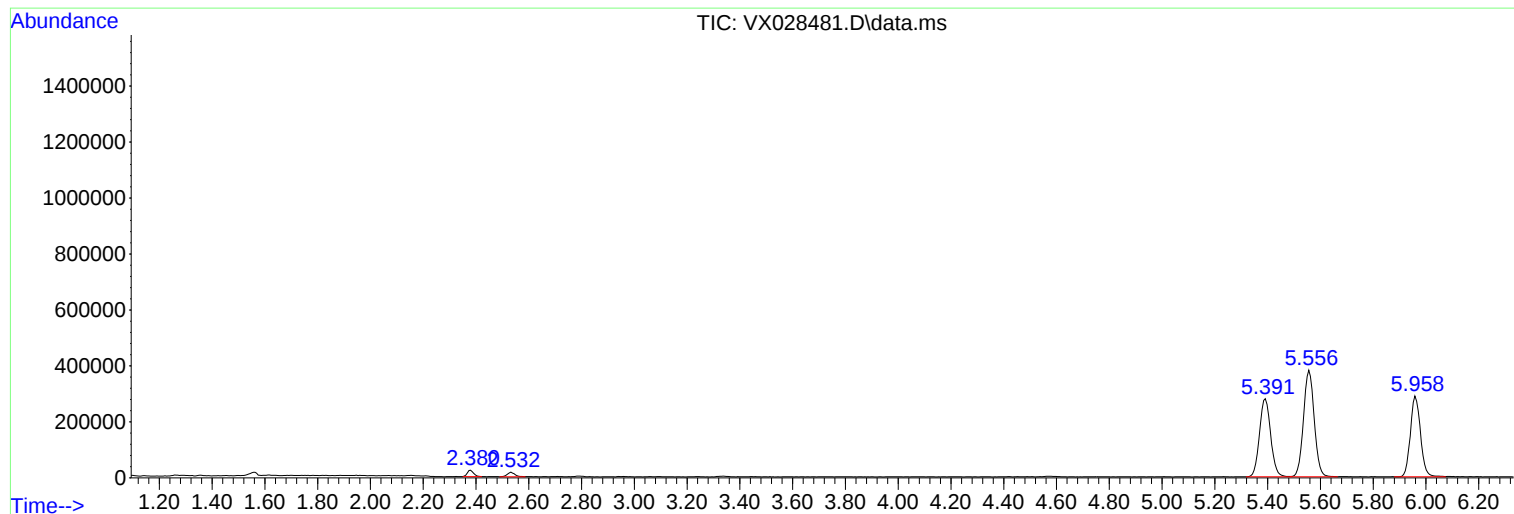
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Quant Title : SW846 8260

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



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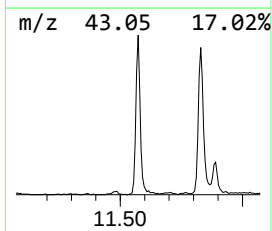
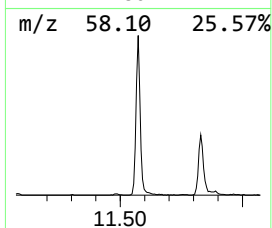
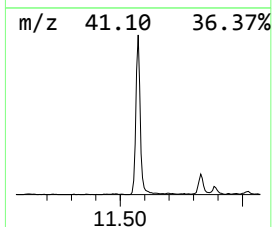
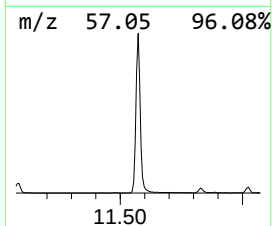
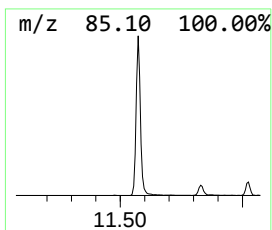
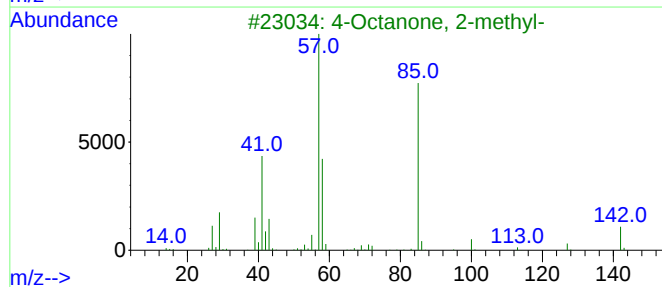
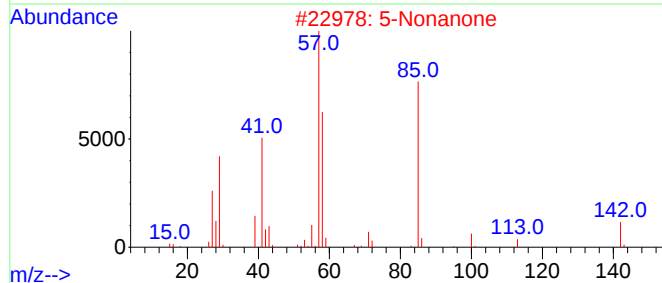
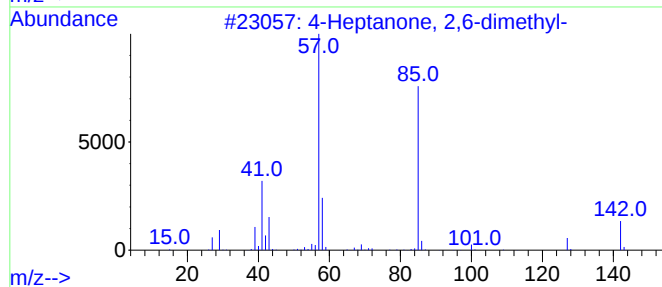
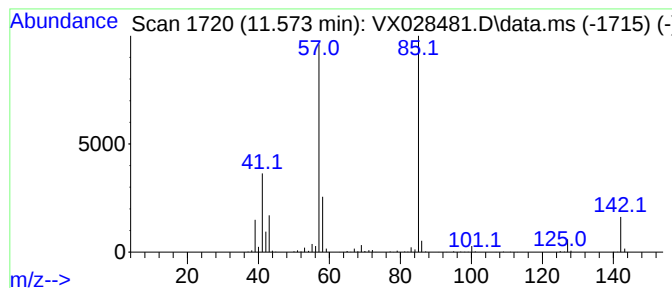
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Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	14.79 ug/l	561736	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	64
3			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	56
4			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
5			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	11.573	14.8	ug/l	561736	4	12.024	1899420	50.0