

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082622\
 Data File : VX030817.D
 Acq On : 26 Aug 2022 12:18
 Operator : JC/MD
 Sample : N4246-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 220817015-02-VOA

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\82X082522W.M
 Title : SW846 8260

Signal : TIC: VX030817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	33	rVB	66998	76889	1.91%	0.442%
2	2.380	205	212	225	rBV2	120246	223246	5.55%	1.282%
3	2.971	298	309	324	rBV	1083379	2396030	59.54%	13.759%
4	4.587	561	574	587	rBV	1230227	4024334	100.00%	23.109%
5	5.013	634	644	671	rVB	420314	1296449	32.22%	7.445%
6	5.391	696	706	722	rVV2	131679	385959	9.59%	2.216%
7	5.556	722	733	748	rVB	244609	689023	17.12%	3.957%
8	5.964	788	800	808	rBV	148775	395840	9.84%	2.273%
9	6.044	808	813	832	rVV2	30195	110832	2.75%	0.636%
10	6.245	834	846	855	rVV3	30913	92419	2.30%	0.531%
11	6.769	920	932	946	rBV	366358	888995	22.09%	5.105%
12	8.580	1220	1229	1234	rVB4	17809	42725	1.06%	0.245%
13	8.653	1234	1241	1248	rBV	760738	1181667	29.36%	6.786%
14	8.720	1248	1252	1260	rVB3	33534	59073	1.47%	0.339%
15	8.805	1261	1266	1271	rBV	28042	46303	1.15%	0.266%
16	9.244	1331	1338	1344	rBV	28398	43800	1.09%	0.252%
17	9.378	1353	1360	1367	rBV	52338	83493	2.07%	0.479%
18	9.494	1373	1379	1384	rVV	42207	61578	1.53%	0.354%
19	10.055	1461	1471	1484	rBV	773636	1113229	27.66%	6.393%
20	10.201	1490	1495	1504	rBV2	50595	97209	2.42%	0.558%
21	10.305	1507	1512	1518	rVV	116644	172970	4.30%	0.993%
22	10.543	1546	1551	1556	rBV2	33192	47236	1.17%	0.271%
23	10.646	1563	1568	1577	rVB	81954	117902	2.93%	0.677%
24	11.085	1634	1640	1646	rBV	587196	782869	19.45%	4.496%
25	11.756	1738	1750	1754	rBV	51462	85466	2.12%	0.491%
26	11.890	1764	1772	1779	rVB2	56337	85539	2.13%	0.491%
27	12.024	1788	1794	1801	rVV	805271	1098084	27.29%	6.306%
28	12.091	1801	1805	1810	rVV	31923	52814	1.31%	0.303%
29	12.146	1810	1814	1824	rVB7	18600	47306	1.18%	0.272%
30	12.244	1825	1830	1840	rBV	65263	106975	2.66%	0.614%
31	12.670	1895	1900	1909	rBV4	21919	45570	1.13%	0.262%
32	12.908	1932	1939	1943	rBV	213965	282500	7.02%	1.622%
33	12.963	1943	1948	1952	rVB6	54458	92326	2.29%	0.530%
34	13.292	1996	2002	2006	rBV4	37085	58801	1.46%	0.338%
35	13.475	2027	2032	2035	rBV	112290	158278	3.93%	0.909%
36	13.512	2035	2038	2046	rVB	207909	279321	6.94%	1.604%

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Instrument :
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ClientSampleId :
220817015-02-VOA

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

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Title : SW846 8260

37	13.591	2046	2051	2055	rBV4	39638	67654	1.68%	0.388%
38	13.780	2077	2082	2087	rVB	188568	242188	6.02%	1.391%
39	13.926	2101	2106	2120	rVB4	49238	124618	3.10%	0.716%
40	14.097	2129	2134	2140	rBV3	42131	59232	1.47%	0.340%
41	14.640	2219	2223	2226	rBV	33784	45475	1.13%	0.261%
42	14.780	2242	2246	2252	rVB2	40147	52142	1.30%	0.299%

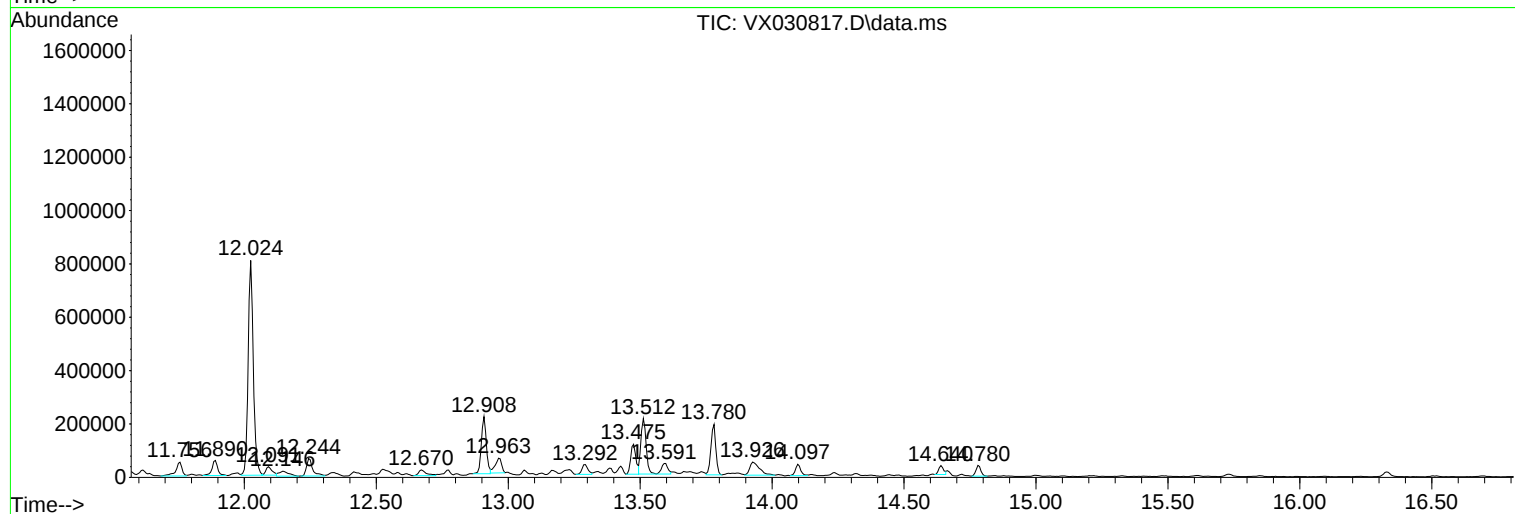
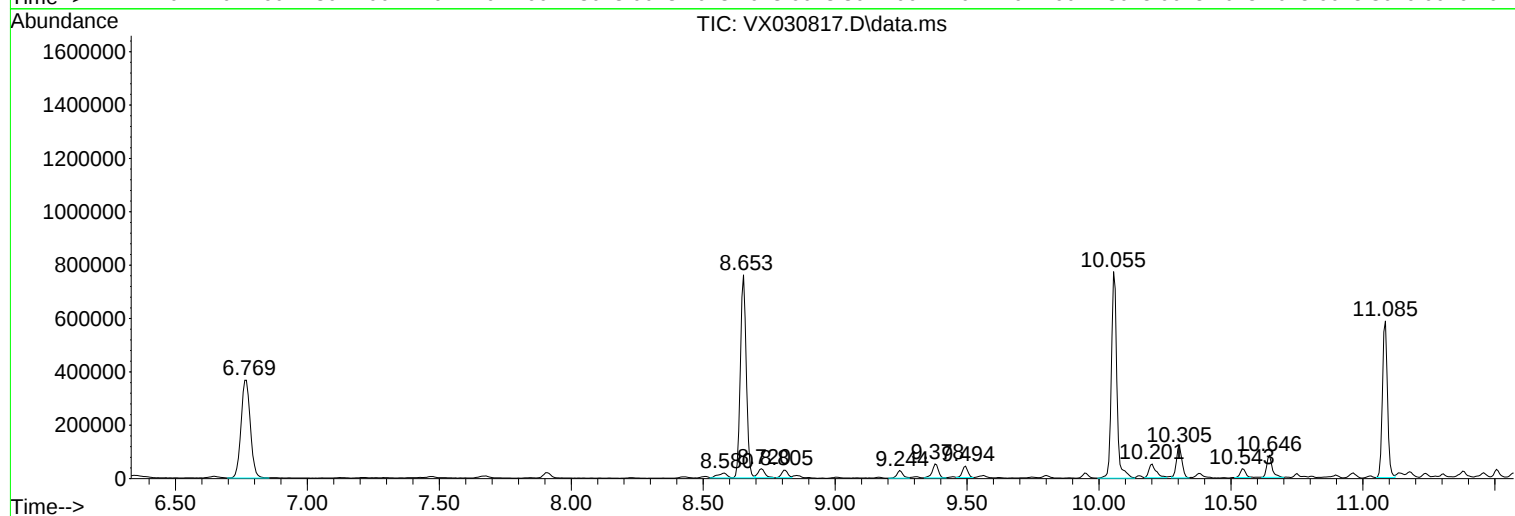
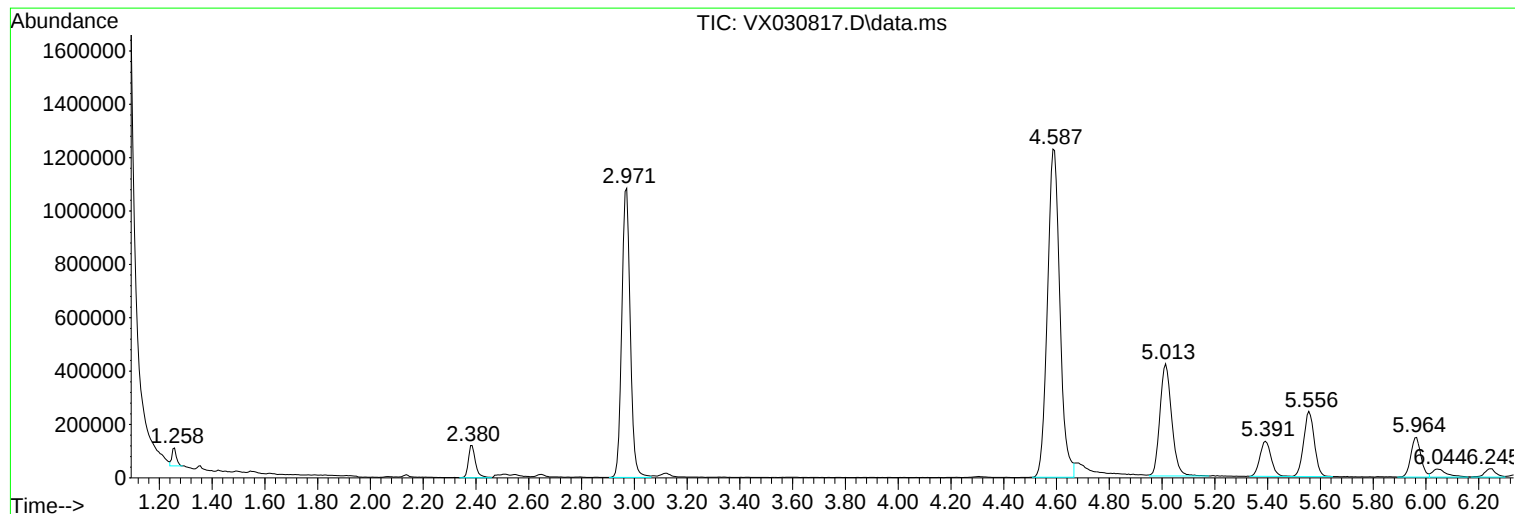
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X082522W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
220817015-02-VOA

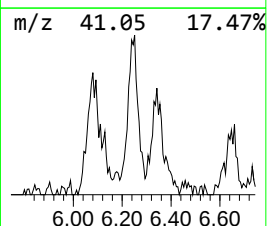
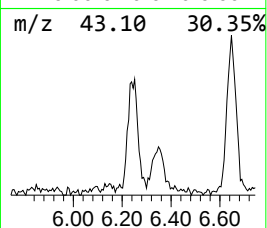
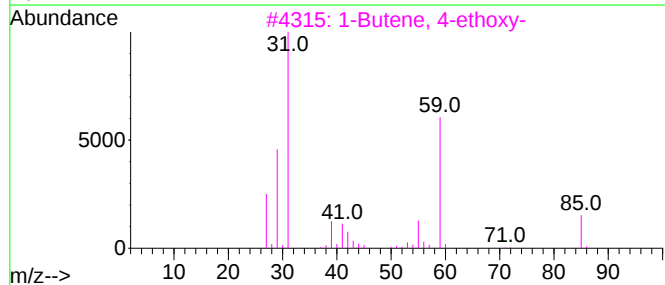
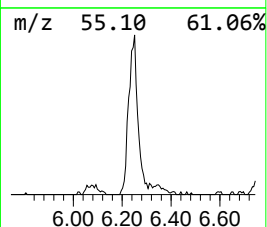
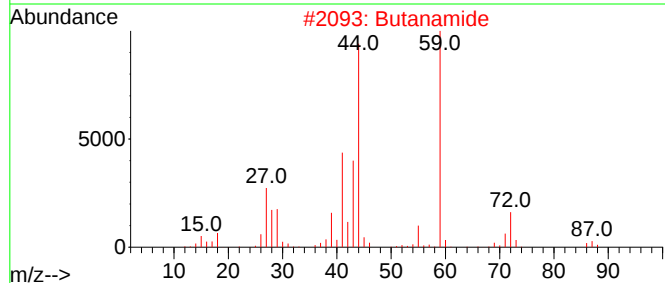
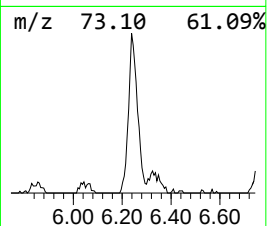
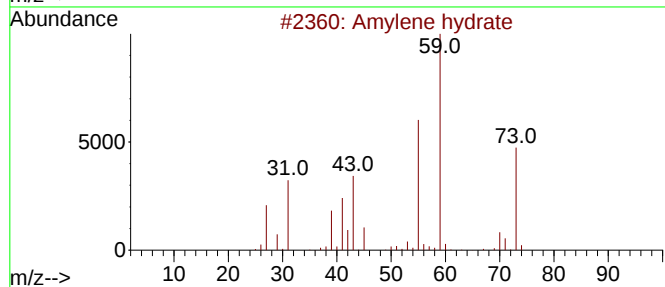
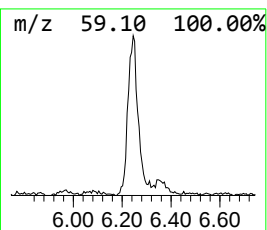
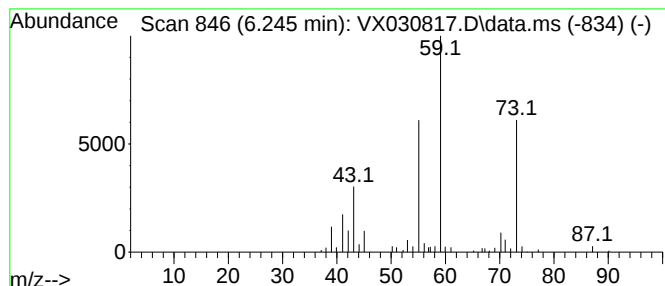
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X082522W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	5.20 ug/l	92419	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	78
2			Butanamide	87	C4H9NO	000541-35-5	53
3			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	40
4			3-Hexanol	102	C6H14O	000623-37-0	39
5			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
220817015-02-VOA

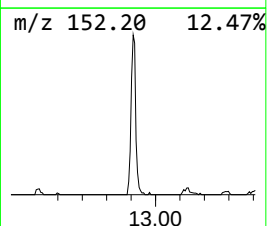
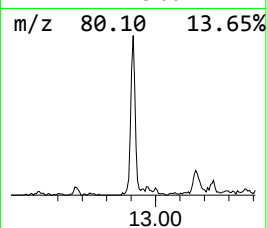
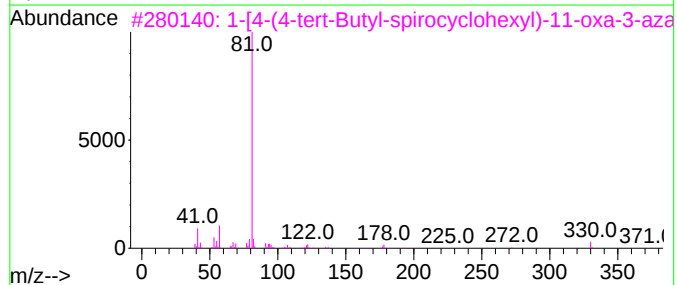
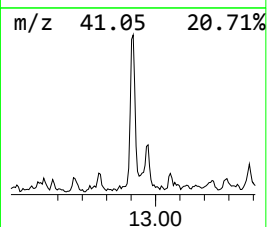
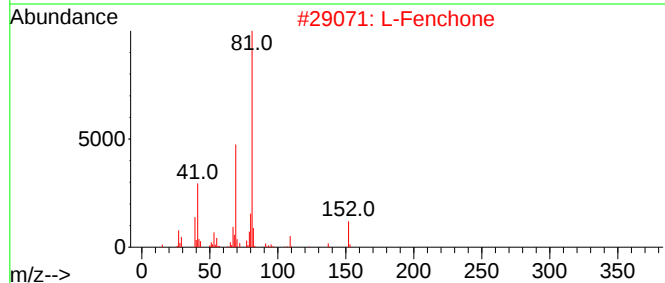
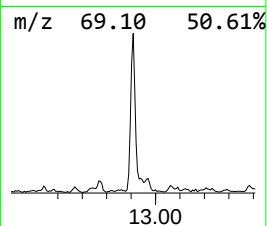
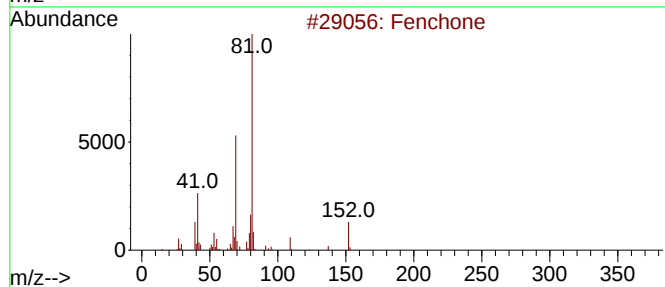
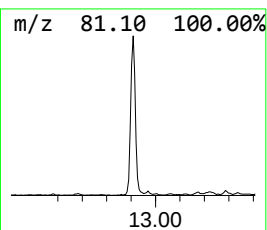
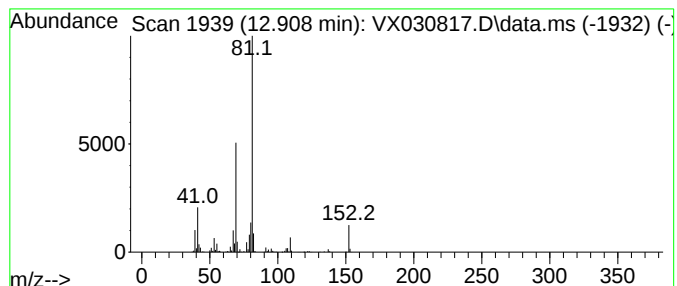
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X082522W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Fenchone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	12.86 ug/l	282500	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	90
3			1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	50
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



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MSVOA_X
ClientSampleId :
220817015-02-VOA

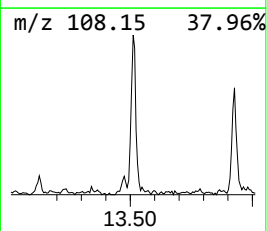
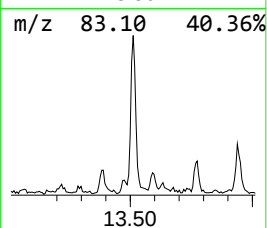
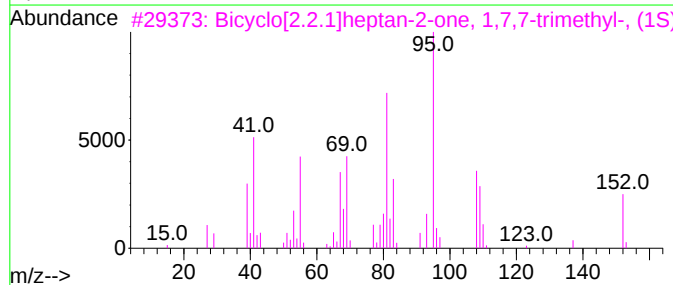
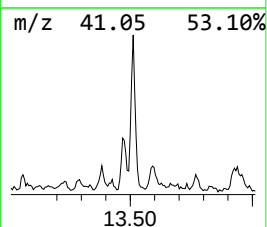
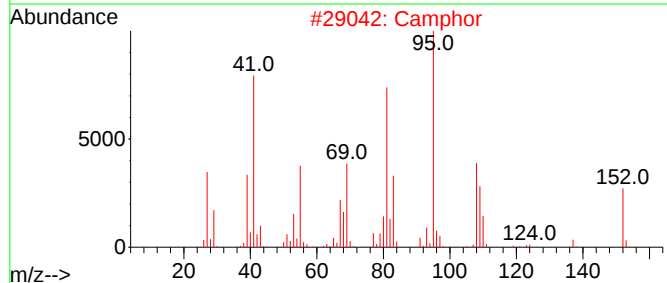
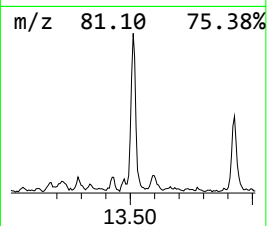
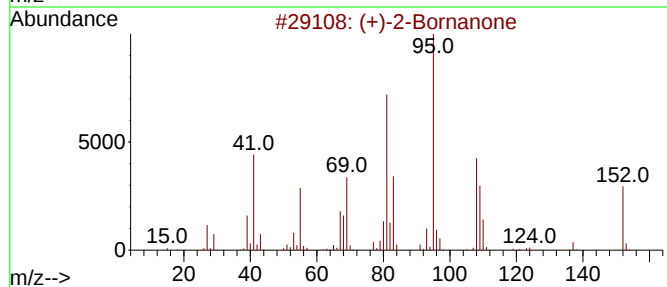
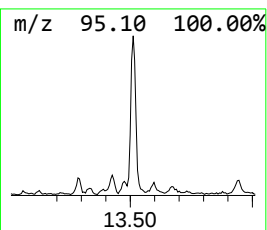
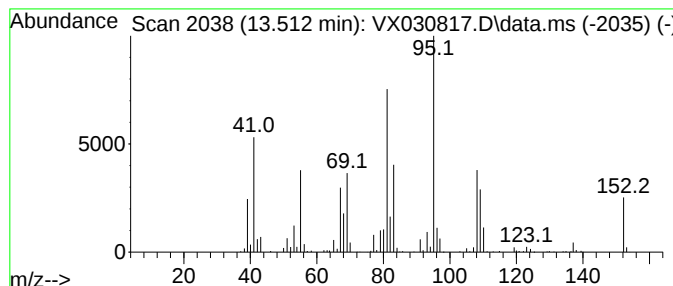
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X082522W.M
Quant Title : SW846 8260

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

Peak Number 5 (+)-2-Bornanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	12.72 ug/l	279321	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
2			Camphor	152	C10H16O	000076-22-2	94
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	43
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	41



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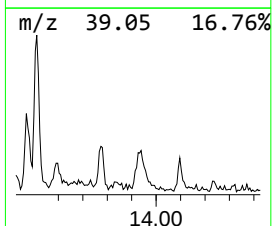
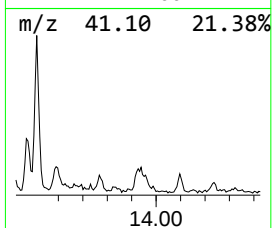
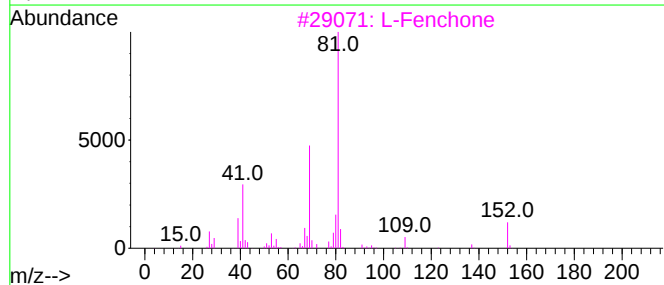
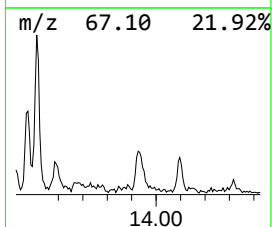
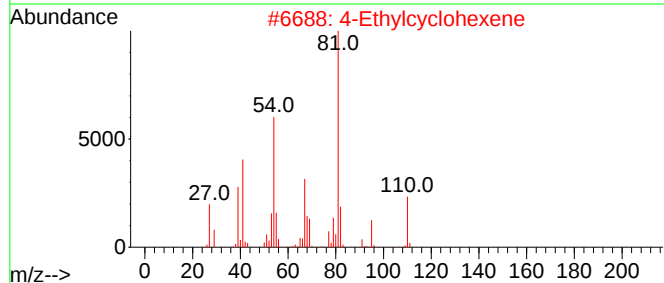
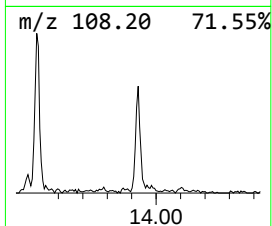
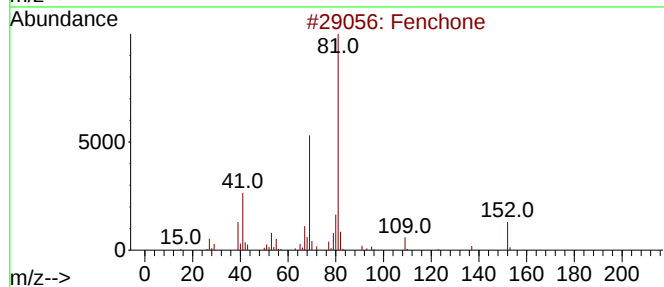
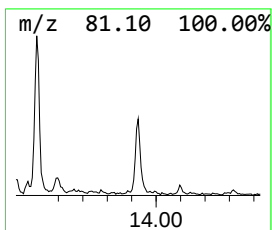
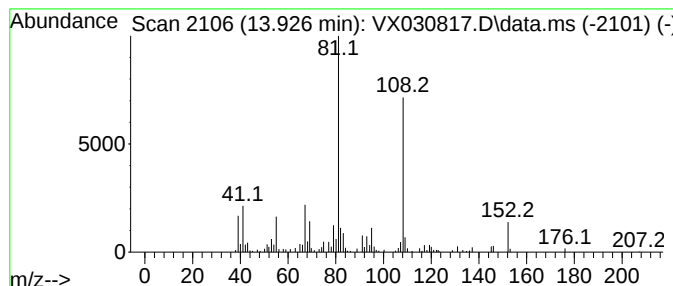
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Quant Title : SW846 8260

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

Peak Number 6 4-Ethylcyclohexene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	5.67 ug/l	124618	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	52
2			4-Ethylcyclohexene	110	C8H14	003742-42-5	50
3			L-Fenchone	152	C10H16O	007787-20-4	49
4			2,4-Nonadienal	138	C9H14O	006750-03-4	47
5			2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	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
Amylene hydrate	6.245	5.2	ug/l	92419	2	6.769	888995	50.0
Fenchone	12.908	12.9	ug/l	282500	4	12.024	1098080	50.0
Bicyclo[2.2.1]h...	13.475	7.2	ug/l	158278	4	12.024	1098080	50.0
(+)-2-Bornanone	13.512	12.7	ug/l	279321	4	12.024	1098080	50.0
4-Ethylcyclohexene	13.926	5.7	ug/l	124618	4	12.024	1098080	50.0