

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
 Data File : VX046506.D
 Acq On : 04 Jun 2025 17:25
 Operator : JC/MD
 Sample : Q2198-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-202-GW01

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	37	rBV	12729	24218	5.84%	0.885%
2	1.587	73	82	83	rBV5	3400	8135	1.96%	0.297%
3	2.386	205	213	220	rVB	3226	5261	1.27%	0.192%
4	2.947	299	305	319	rBV4	2265	6802	1.64%	0.249%
5	5.385	695	705	721	rBV2	48223	145454	35.05%	5.316%
6	5.550	721	732	745	rVV2	68101	196943	47.46%	7.197%
7	5.958	789	799	815	rBV	55452	153275	36.93%	5.601%
8	6.757	920	930	953	rBV	120604	301970	72.76%	11.035%
9	8.647	1234	1240	1249	rBV	268423	414997	100.00%	15.166%
10	8.720	1249	1252	1259	rVB	6280	10822	2.61%	0.395%
11	10.055	1465	1471	1481	rBV	270152	376501	90.72%	13.759%
12	10.299	1506	1511	1519	rBV	13316	19298	4.65%	0.705%
13	11.079	1634	1639	1651	rBV	223561	288140	69.43%	10.530%
14	12.018	1788	1793	1801	rBV	255729	331799	79.95%	12.126%
15	12.085	1801	1804	1810	rVB2	3484	5343	1.29%	0.195%
16	12.244	1827	1830	1832	rVV3	4890	7096	1.71%	0.259%
17	12.268	1832	1834	1838	rVV	6614	7383	1.78%	0.270%
18	12.317	1838	1842	1853	rVB	13474	20251	4.88%	0.740%
19	12.463	1862	1866	1872	rVV	5122	6153	1.48%	0.225%
20	12.530	1872	1877	1879	rVV	13729	17268	4.16%	0.631%
21	12.555	1879	1881	1886	rVV	14612	16549	3.99%	0.605%
22	12.610	1886	1890	1901	rVV	27682	36951	8.90%	1.350%
23	12.713	1901	1907	1914	rVB5	4381	9825	2.37%	0.359%
24	12.847	1925	1929	1935	rBV	10495	14522	3.50%	0.531%
25	12.921	1935	1941	1944	rVV	30189	36764	8.86%	1.344%
26	12.963	1944	1948	1955	rVV	48390	61618	14.85%	2.252%
27	13.024	1955	1958	1960	rVV4	3152	4621	1.11%	0.169%
28	13.073	1963	1966	1970	rVB2	4005	5074	1.22%	0.185%
29	13.164	1975	1981	1986	rVV2	13819	18297	4.41%	0.669%
30	13.256	1991	1996	1997	rVV2	5246	6538	1.58%	0.239%
31	13.286	1997	2001	2011	rVV2	35852	59341	14.30%	2.169%
32	13.372	2011	2015	2020	rVB2	5039	6794	1.64%	0.248%
33	13.573	2044	2048	2051	rBV2	9890	14292	3.44%	0.522%
34	13.676	2061	2065	2070	rVB2	5721	7260	1.75%	0.265%
35	13.774	2076	2081	2089	rBV	45026	62148	14.98%	2.271%
36	14.073	2125	2130	2135	rBV2	3290	4191	1.01%	0.153%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

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\82X050525W.M
Title : SW846 8260

37	14.213	2149	2153	2159	rBV5	2727	4313	1.04%	0.158%
38	14.317	2166	2170	2176	rVB	4004	5056	1.22%	0.185%
39	14.640	2219	2223	2230	rBV	7024	9068	2.19%	0.331%
40	14.780	2241	2246	2252	rBV2	4343	6030	1.45%	0.220%

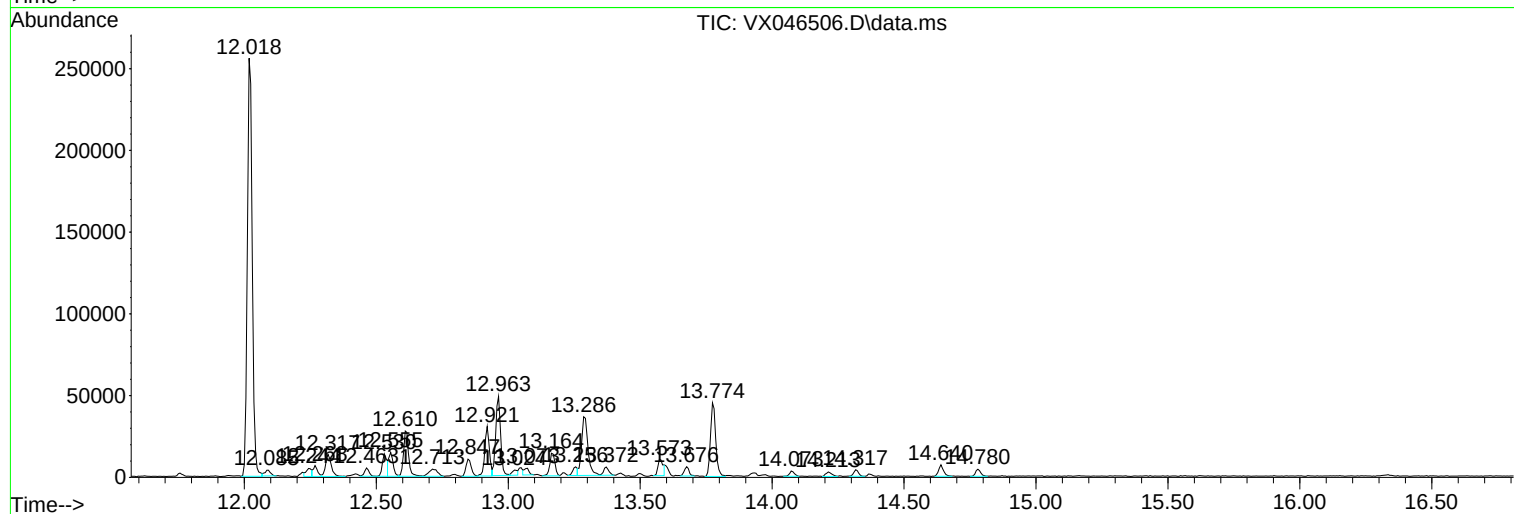
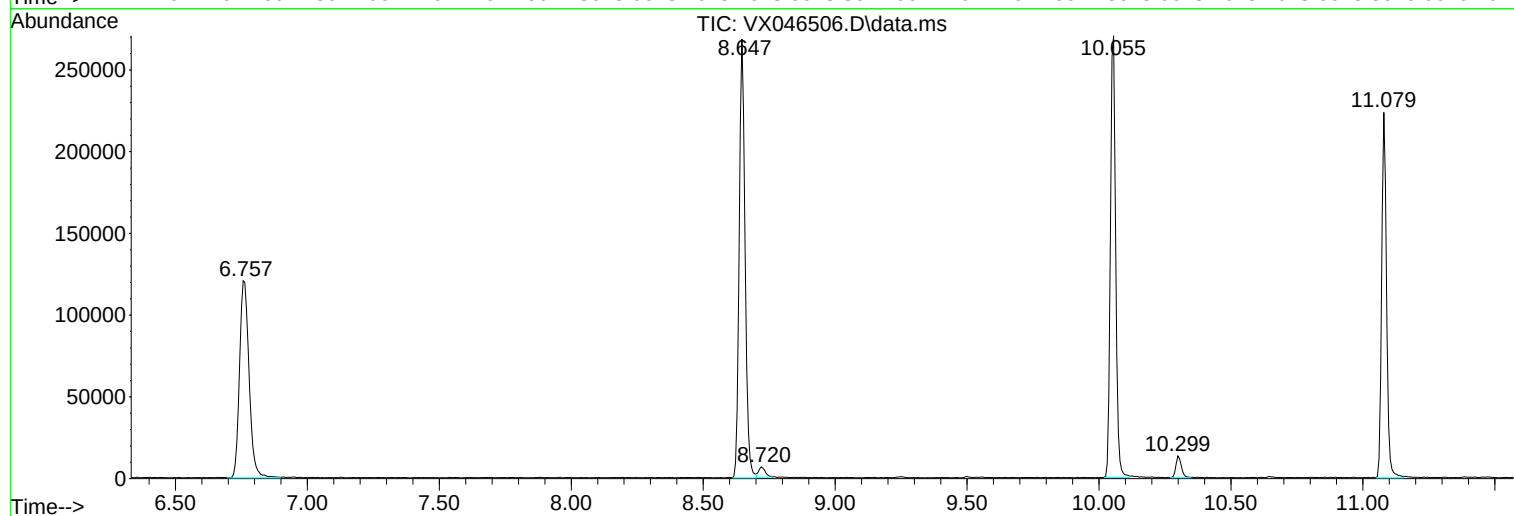
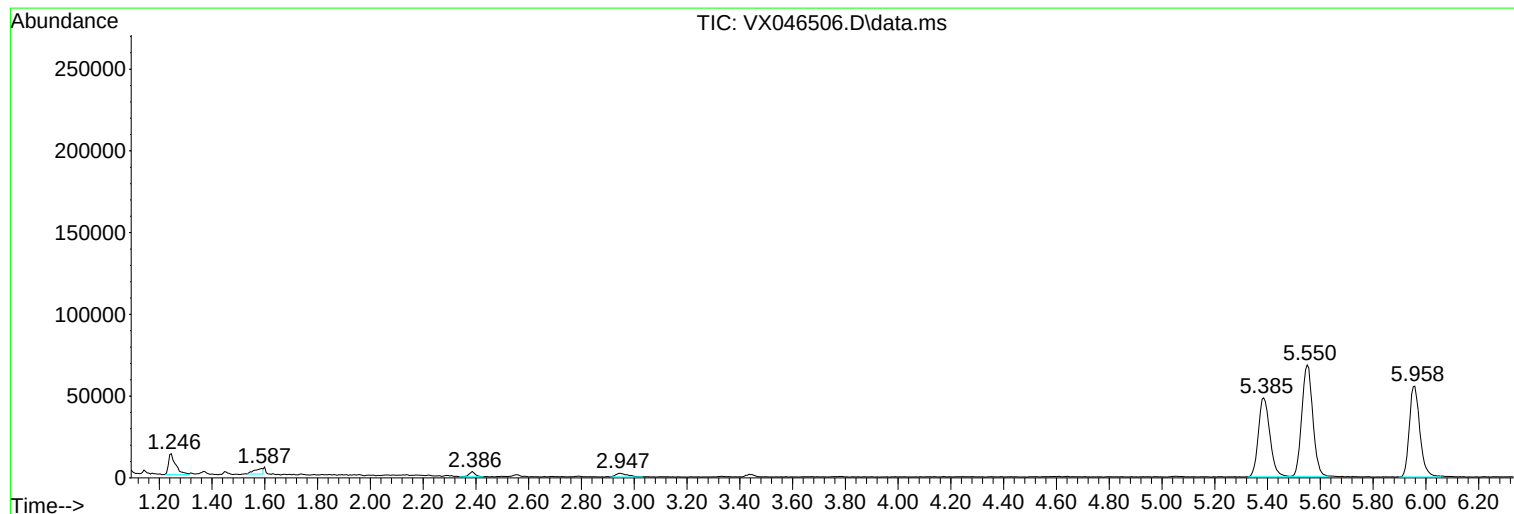
Sum of corrected areas: 2736361

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

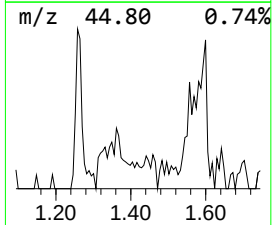
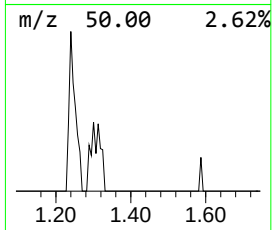
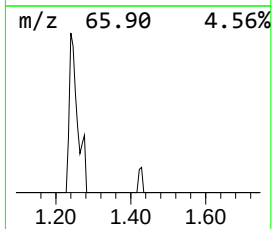
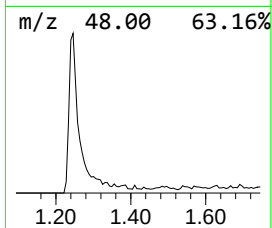
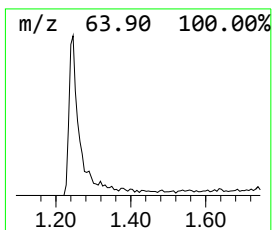
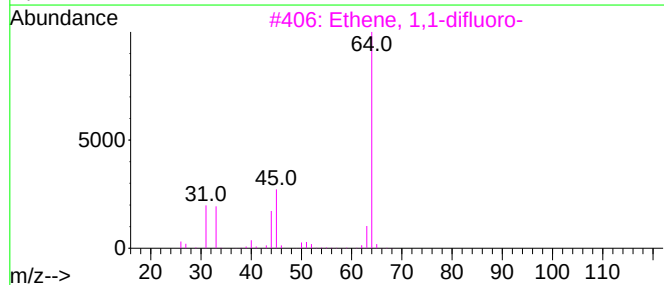
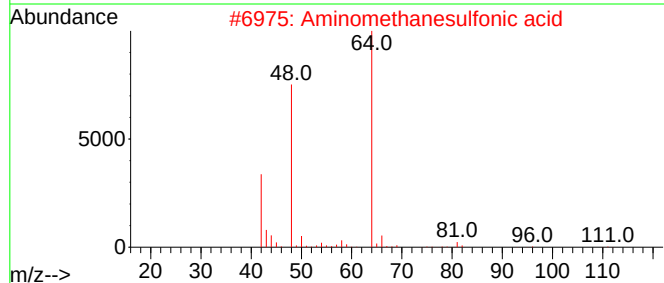
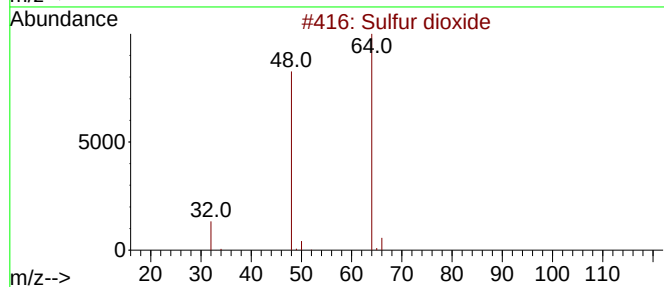
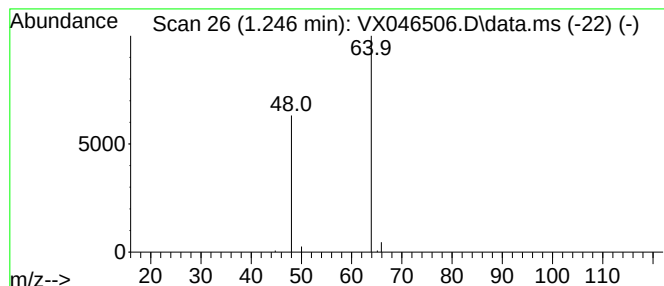
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	6.15 ug/l	24218	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

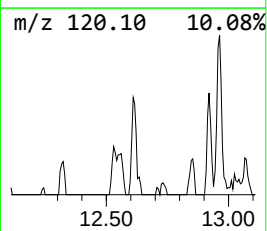
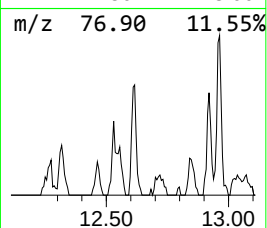
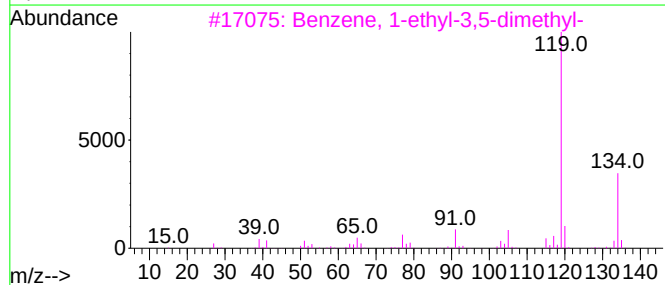
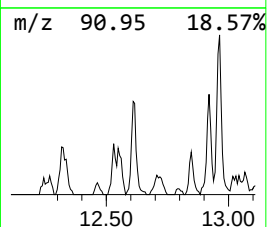
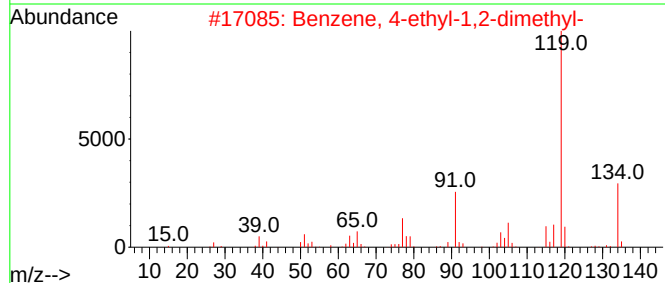
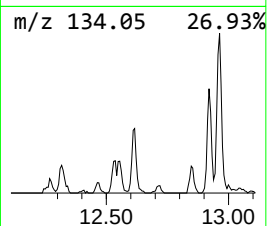
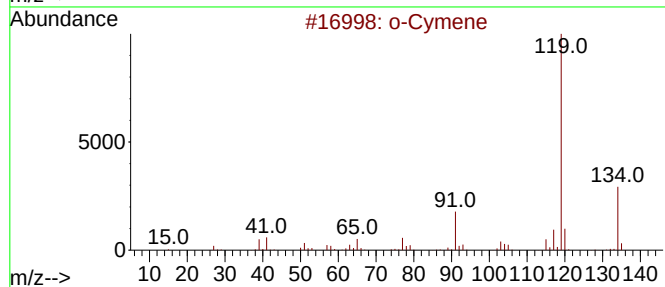
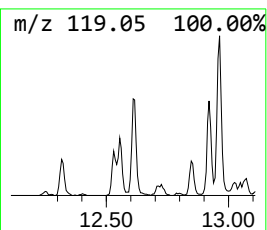
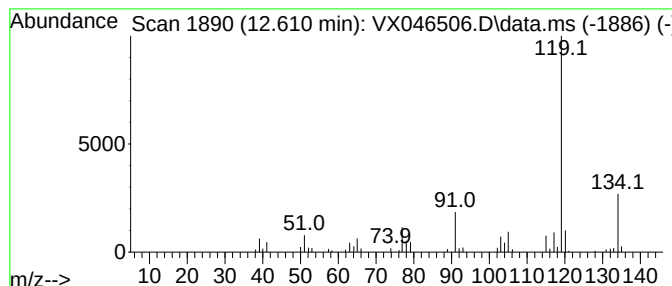
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	5.57 ug/l	36951	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

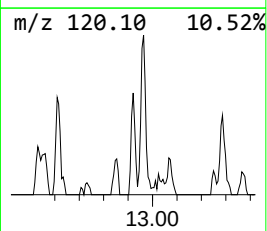
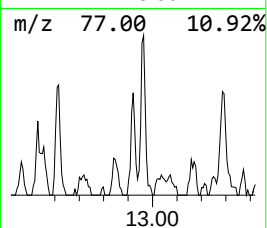
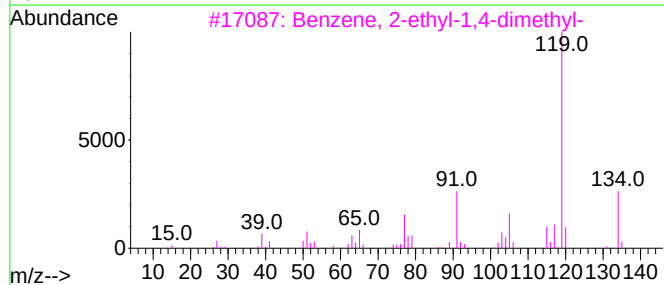
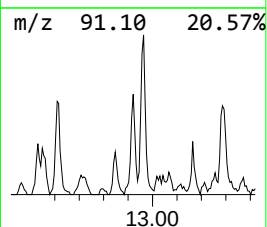
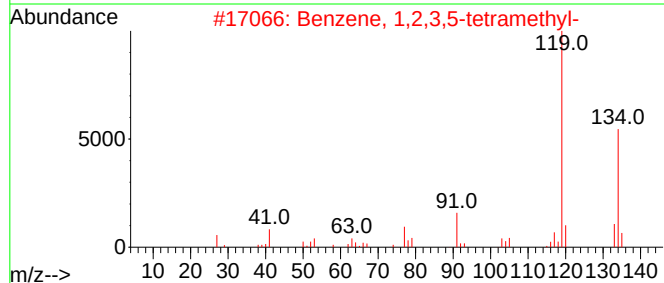
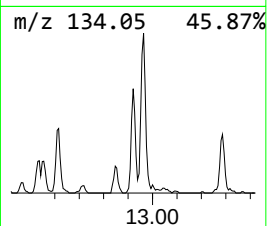
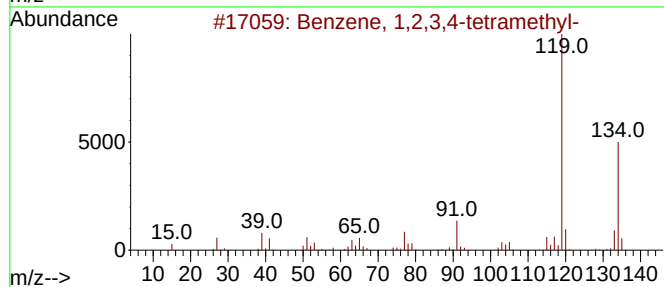
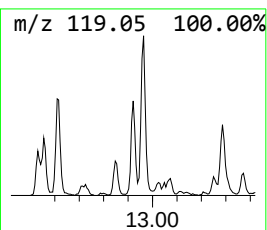
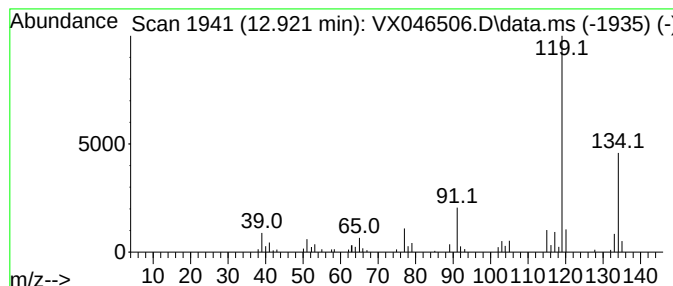
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	5.54 ug/l	36764	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

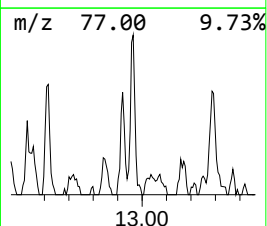
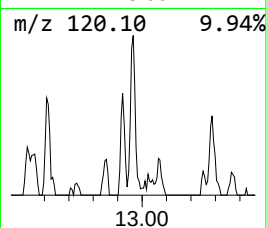
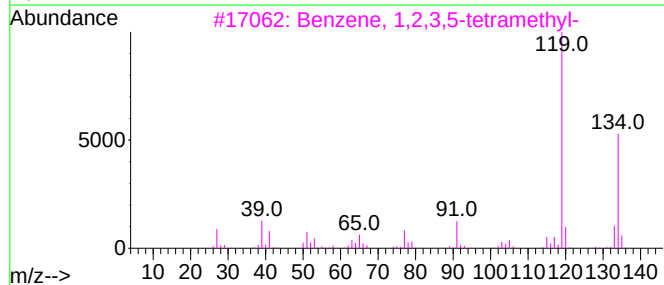
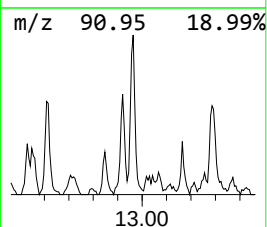
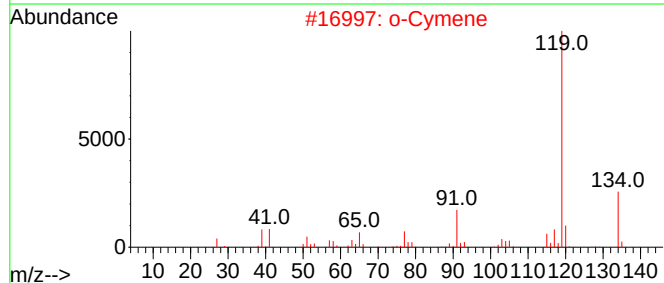
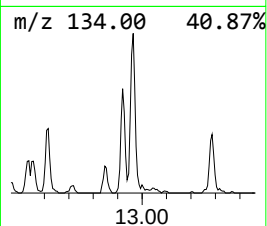
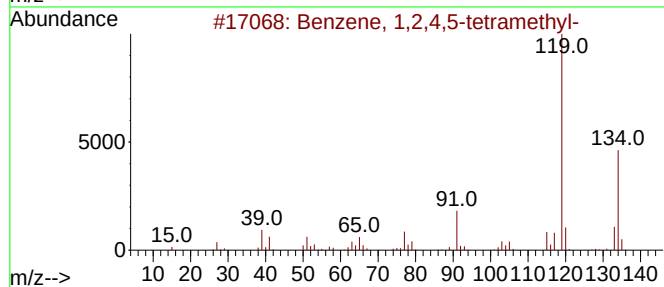
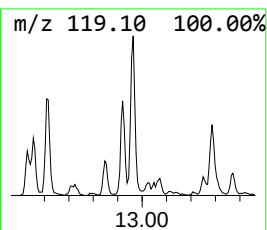
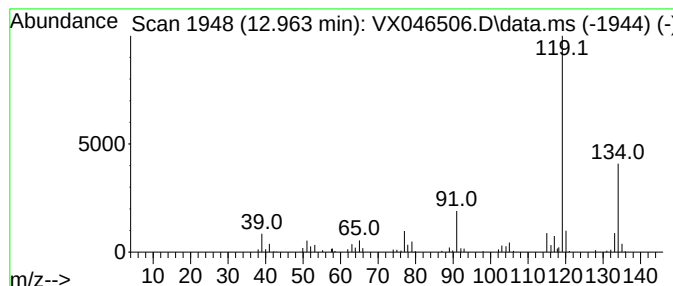
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	9.29 ug/l	61618	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			o-Cymene	134	C10H14	000527-84-4	94
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

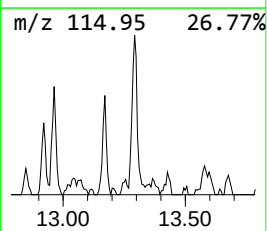
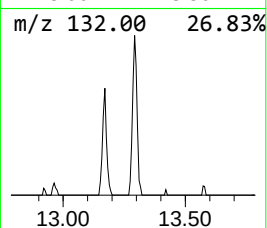
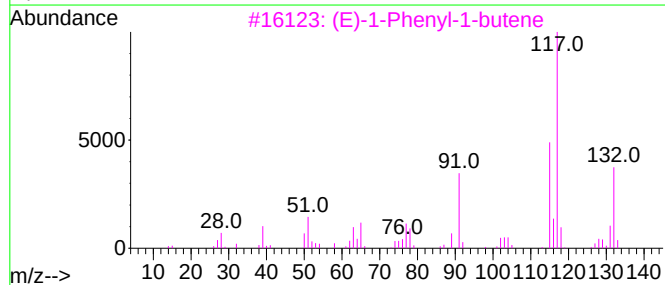
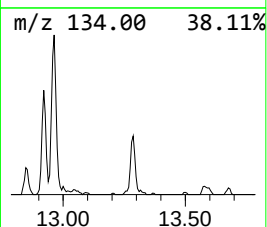
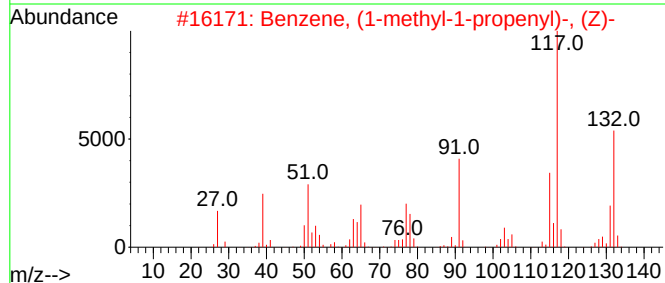
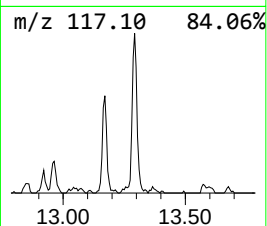
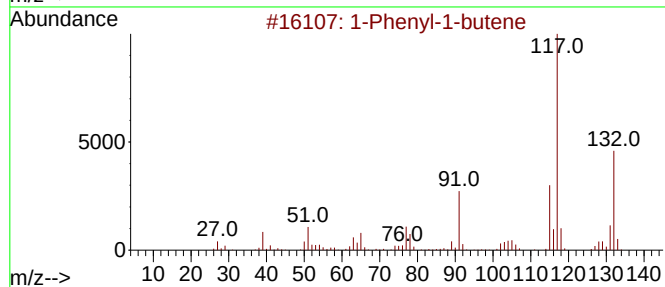
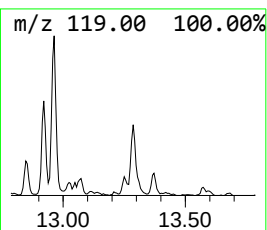
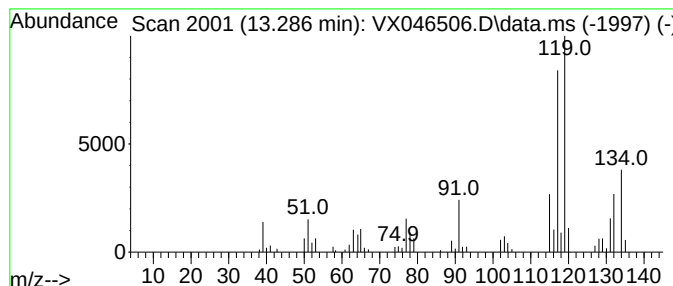
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	8.94 ug/l	59341	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	86
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	64
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	60
4			o-Cymene	134	C10H14	000527-84-4	55
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060425\
Data File : VX046506.D
Acq On : 04 Jun 2025 17:25
Operator : JC/MD
Sample : Q2198-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-202-GW01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
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
Sulfur dioxide	1.246	6.2	ug/l	24218	1	5.550	196943	50.0
o-Cymene	12.610	5.6	ug/l	36951	4	12.018	331799	50.0
Benzene, 1,2,3,...	12.921	5.5	ug/l	36764	4	12.018	331799	50.0
Benzene, 1,2,4,...	12.963	9.3	ug/l	61618	4	12.018	331799	50.0
1-Phenyl-1-butene	13.286	8.9	ug/l	59341	4	12.018	331799	50.0