

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
 Data File : VX032867.D
 Acq On : 16 Nov 2022 14:51
 Operator : JC/MD
 Sample : N5614-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-16S

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	199	206	216	rBV2	12183	23464	4.04%	0.424%
2	2.782	270	278	288	rBV2	10455	22973	3.95%	0.416%
3	2.977	299	310	325	rBV	86287	276348	47.55%	4.999%
4	3.111	325	332	346	rVB	42547	100375	17.27%	1.816%
5	3.757	429	438	456	rVB	38741	102579	17.65%	1.856%
6	4.202	495	511	512	rBV3	2146	5843	1.01%	0.106%
7	5.153	651	667	668	rBV7	3666	10362	1.78%	0.187%
8	5.385	694	705	719	rBV	65377	191906	33.02%	3.472%
9	5.550	721	732	743	rBV	104508	300596	51.72%	5.438%
10	5.958	788	799	808	rBV	71892	186833	32.15%	3.380%
11	6.044	808	813	818	rVB4	7400	16926	2.91%	0.306%
12	6.245	836	846	860	rBV2	77697	247727	42.62%	4.481%
13	6.361	860	865	875	rVB5	7698	21660	3.73%	0.392%
14	6.763	920	931	941	rBV	164778	394298	67.84%	7.133%
15	6.854	943	946	956	rVV5	4950	10622	1.83%	0.192%
16	7.177	991	999	1005	rBV5	7909	16479	2.84%	0.298%
17	7.366	1022	1030	1037	rVB6	2741	6182	1.06%	0.112%
18	7.562	1057	1062	1065	rVV3	3445	6340	1.09%	0.115%
19	7.775	1090	1097	1105	rVB3	6277	11950	2.06%	0.216%
20	7.885	1105	1115	1122	rBV6	5108	17023	2.93%	0.308%
21	7.982	1122	1131	1140	rVB4	18622	46300	7.97%	0.838%
22	8.104	1144	1151	1162	rBV2	32724	73077	12.57%	1.322%
23	8.214	1162	1169	1173	rBV7	3589	9202	1.58%	0.166%
24	8.305	1179	1184	1192	rBV5	6830	13194	2.27%	0.239%
25	8.427	1200	1204	1210	rVB2	7047	11968	2.06%	0.217%
26	8.506	1210	1217	1224	rVB4	10300	20533	3.53%	0.371%
27	8.647	1228	1240	1251	rBV	359480	581194	100.00%	10.514%
28	8.921	1281	1285	1289	rVB2	4804	6384	1.10%	0.115%
29	8.976	1289	1294	1299	rVB4	5959	11384	1.96%	0.206%
30	9.104	1312	1315	1319	rVB	4926	6817	1.17%	0.123%
31	9.165	1319	1325	1335	rVB	36904	64486	11.10%	1.167%
32	9.427	1363	1368	1376	rBV4	16165	37691	6.49%	0.682%
33	9.500	1376	1380	1388	rVB4	10720	20395	3.51%	0.369%
34	9.659	1402	1406	1416	rVB2	5325	9443	1.62%	0.171%
35	9.762	1416	1423	1432	rBV4	15255	24501	4.22%	0.443%
36	10.012	1460	1464	1466	rVV	17729	25455	4.38%	0.460%

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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\82X102622W.M
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37	10.055	1466	1471	1476	rVV	333501	443777	76.36%	8.028%
38	10.104	1476	1479	1484	rVV5	6368	12318	2.12%	0.223%
39	10.153	1484	1487	1491	rVV4	4717	7427	1.28%	0.134%
40	10.195	1491	1494	1498	rVB	13922	16971	2.92%	0.307%
41	10.305	1509	1512	1518	rVB2	4636	7081	1.22%	0.128%
42	10.372	1518	1523	1528	rBV2	10814	17319	2.98%	0.313%
43	10.585	1551	1558	1564	rBV4	3602	6706	1.15%	0.121%
44	10.787	1581	1591	1593	rBV7	4511	8180	1.41%	0.148%
45	10.963	1615	1620	1625	rBV	87000	111335	19.16%	2.014%
46	11.018	1625	1629	1632	rVV2	8294	12633	2.17%	0.229%
47	11.079	1634	1639	1645	rVV	292902	397922	68.47%	7.198%
48	11.158	1649	1652	1660	rVB7	4162	7624	1.31%	0.138%
49	11.305	1673	1676	1679	rBV	8687	10263	1.77%	0.186%
50	11.335	1679	1681	1686	rVB2	5182	6283	1.08%	0.114%
51	11.616	1723	1727	1731	rBV	19570	25175	4.33%	0.455%
52	11.713	1736	1743	1746	rBV2	9991	14312	2.46%	0.259%
53	11.750	1746	1749	1754	rVB	9719	12780	2.20%	0.231%
54	11.890	1765	1772	1779	rBV4	8696	15448	2.66%	0.279%
55	12.024	1788	1794	1802	rBV	317472	403692	69.46%	7.303%
56	12.091	1802	1805	1812	rVB3	4799	8648	1.49%	0.156%
57	12.177	1816	1819	1824	rVB	10739	12853	2.21%	0.233%
58	12.250	1824	1831	1836	rBV	67516	88071	15.15%	1.593%
59	12.317	1836	1842	1845	rBV	11827	15777	2.71%	0.285%
60	12.414	1853	1858	1863	rVB2	6897	9081	1.56%	0.164%
61	12.646	1892	1896	1900	rBV	34603	41247	7.10%	0.746%
62	12.701	1900	1905	1912	rVV	334994	422203	72.64%	7.638%
63	12.762	1912	1915	1921	rVB4	5264	6942	1.19%	0.126%
64	12.841	1921	1928	1933	rBV	11333	15879	2.73%	0.287%
65	13.036	1955	1960	1965	rVB	9223	11884	2.04%	0.215%
66	13.134	1965	1976	1978	rBV2	11282	16965	2.92%	0.307%
67	13.170	1978	1982	1989	rVB	62238	82905	14.26%	1.500%
68	13.237	1989	1993	1997	rVB2	4623	5940	1.02%	0.107%
69	13.292	1997	2002	2007	rBV	126101	156204	26.88%	2.826%
70	13.347	2007	2011	2015	rVB2	14908	18230	3.14%	0.330%
71	13.426	2020	2024	2031	rVB2	14477	19447	3.35%	0.352%
72	13.542	2039	2043	2047	rVV	26455	35517	6.11%	0.643%
73	13.585	2047	2050	2053	rVV	6958	8813	1.52%	0.159%
74	13.640	2053	2059	2060	rVV4	19900	28766	4.95%	0.520%
75	13.664	2060	2063	2068	rVB	29676	38057	6.55%	0.688%
76	13.780	2079	2082	2090	rVB4	2906	6045	1.04%	0.109%

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ClientSampleId :
MW-16S

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\82X102622W.M
Title : SW846 8260

77	13.926	2102	2106	2110	rBV2	6822	8657	1.49%	0.157%
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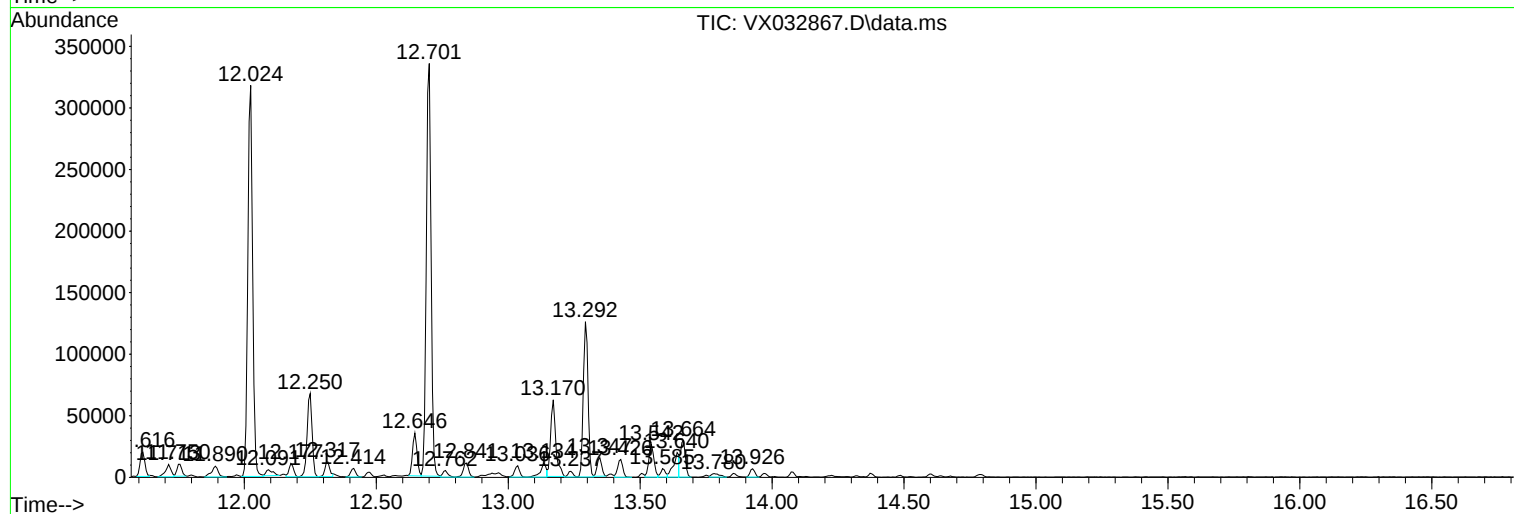
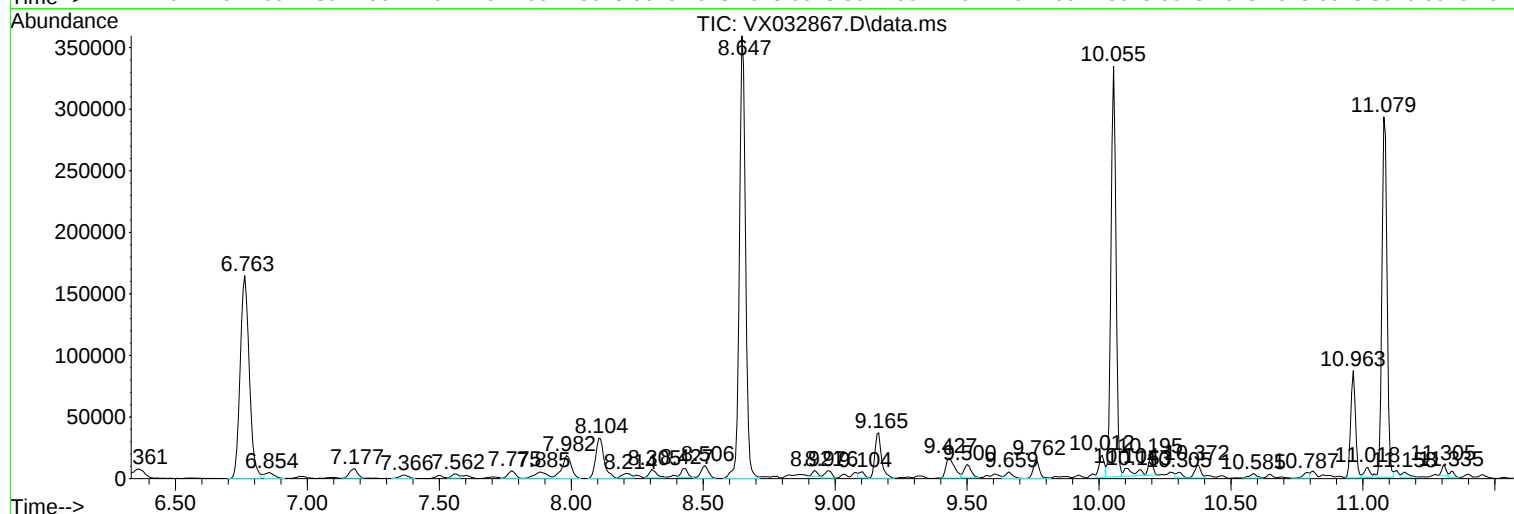
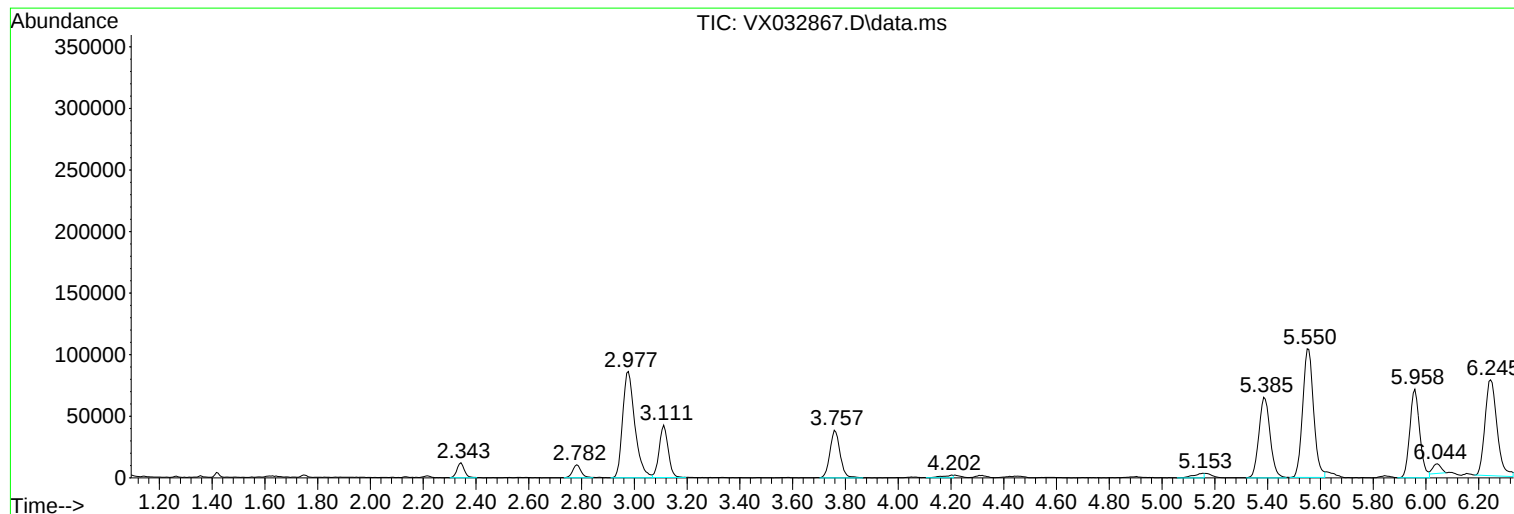
Sum of corrected areas: 5527887

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

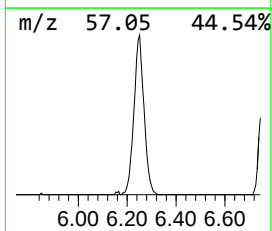
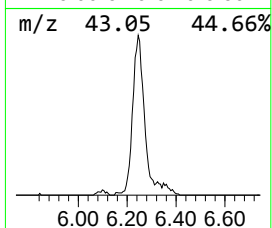
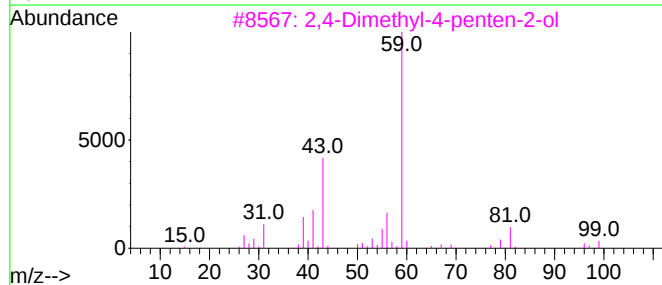
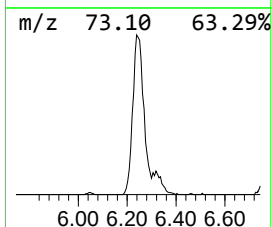
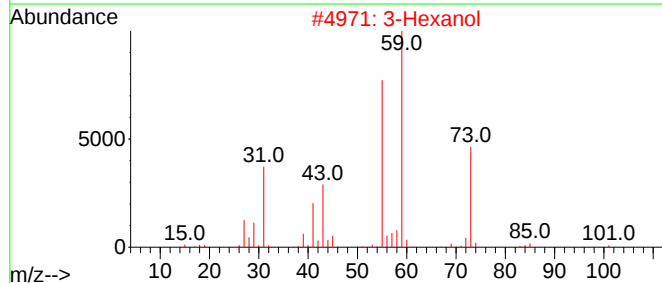
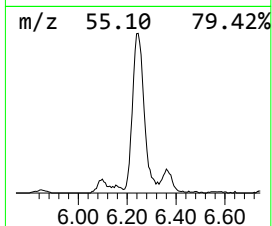
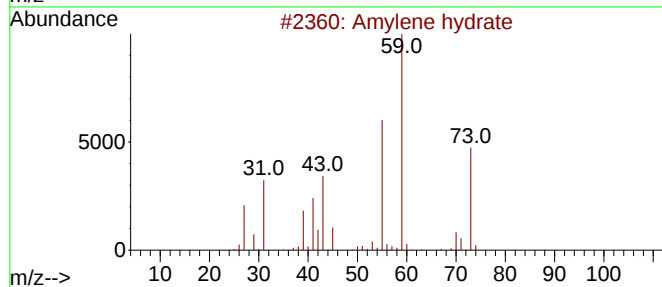
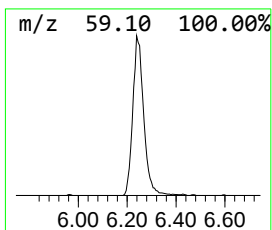
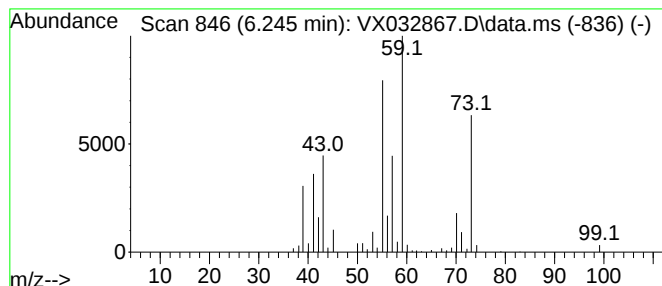
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	31.41 ug/l	247727	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	56
2			3-Hexanol	102	C6H14O	000623-37-0	53
3			2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	43
4			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	38
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	38



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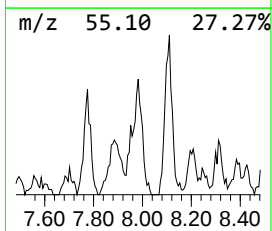
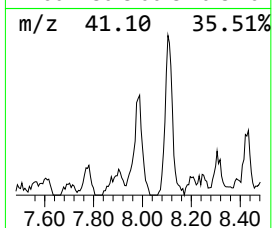
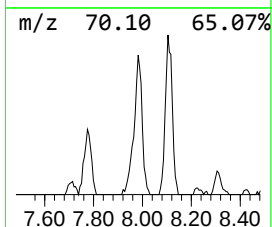
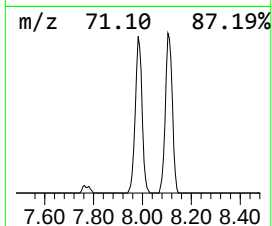
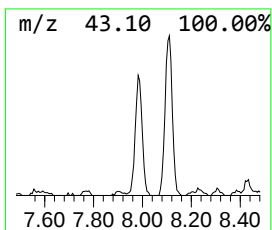
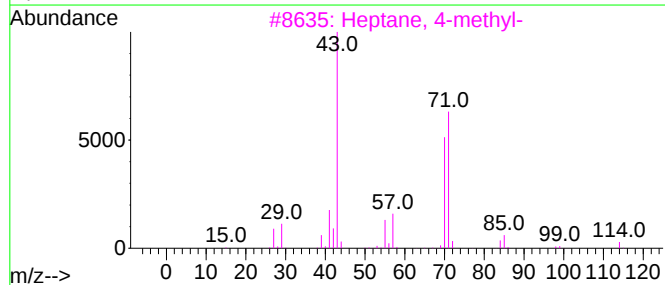
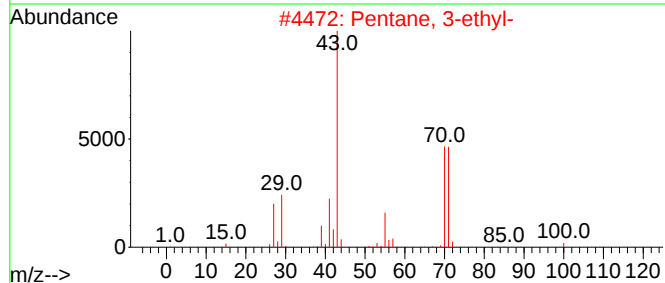
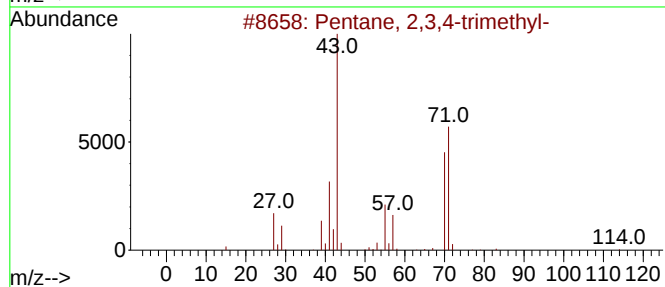
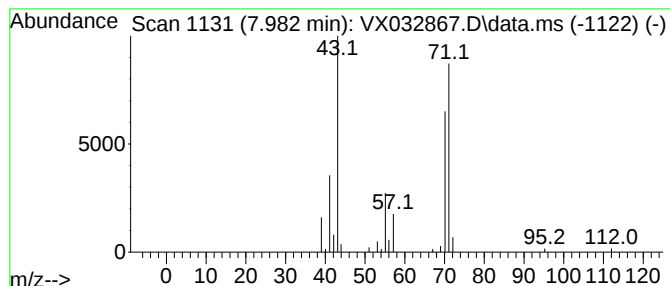
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	5.87 ug/l	46300	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	78
4		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	78
5		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
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MW-16S

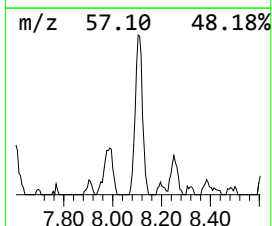
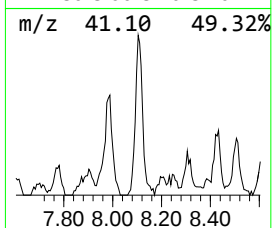
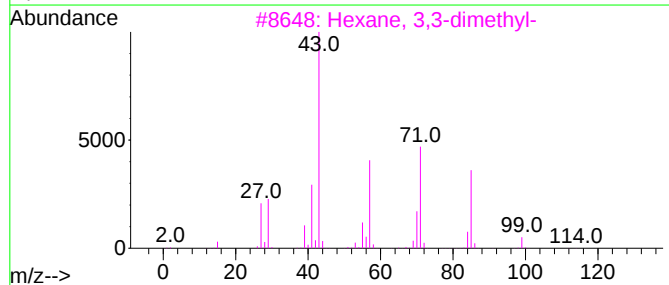
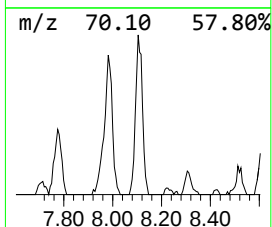
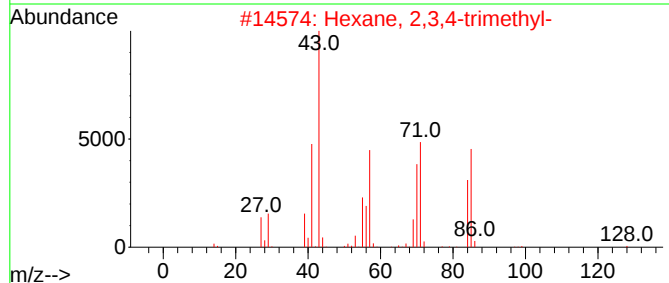
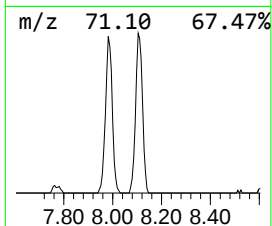
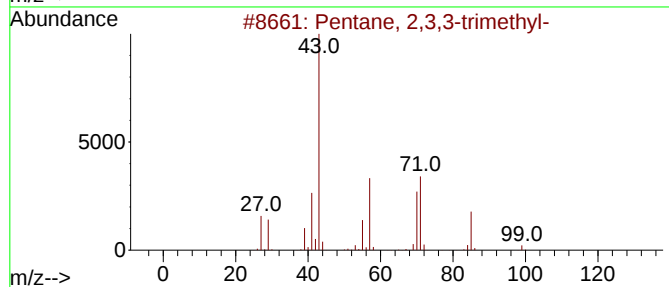
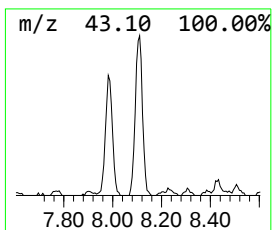
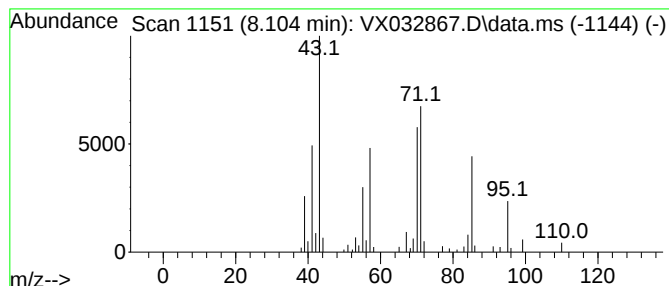
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	9.27 ug/l	73077	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
4			Butanal, 4-[(tetrahydro-2H-pyran...	172	C9H16O3	054911-85-2	43
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	43



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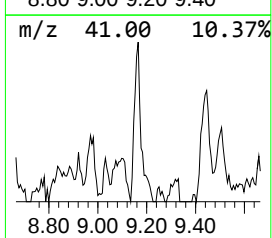
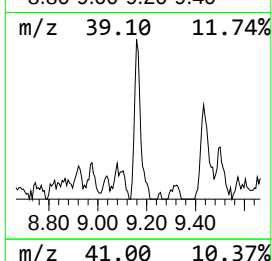
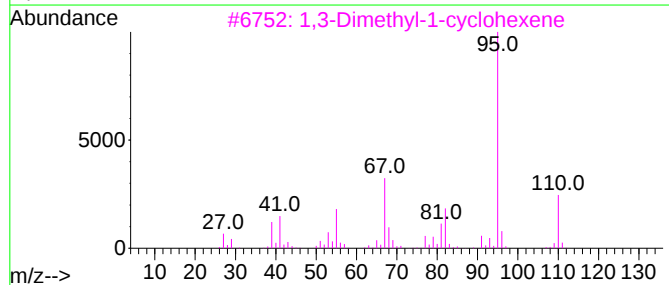
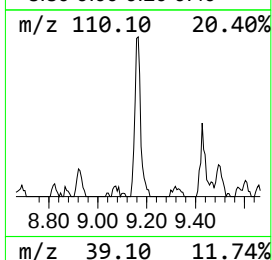
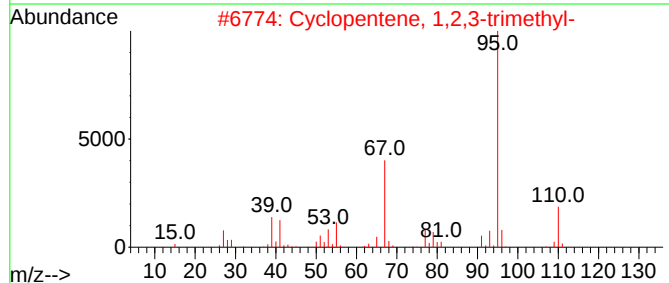
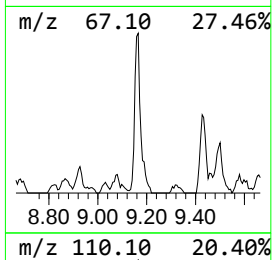
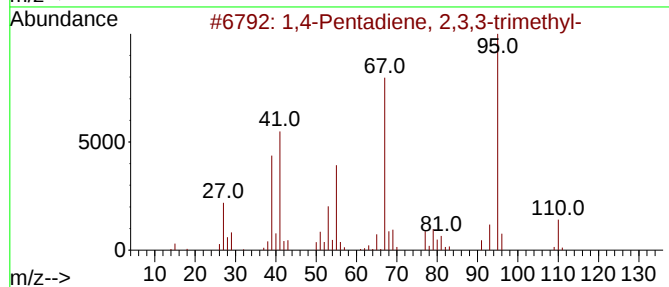
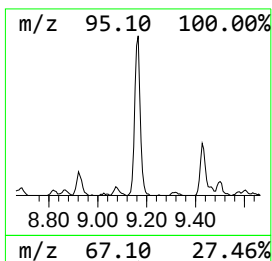
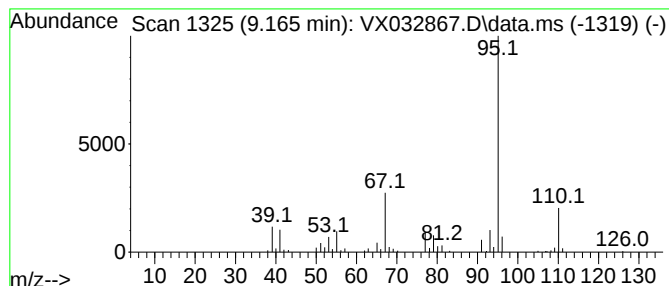
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Quant Title : SW846 8260

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

Peak Number 4 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	7.27 ug/l	64486	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	91
2		Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	91
3		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	86
4		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	80
5		1-(3H-Imidazol-4-yl)-ethanone	110	C5H6N2O	061985-25-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

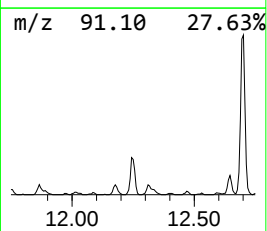
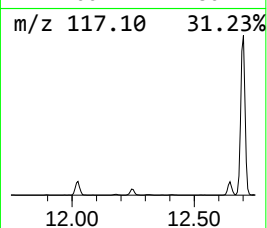
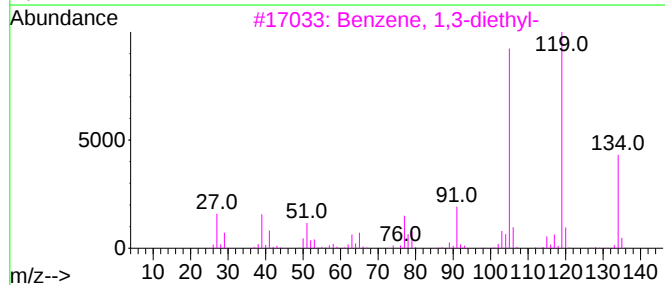
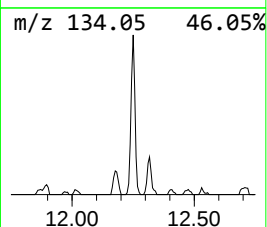
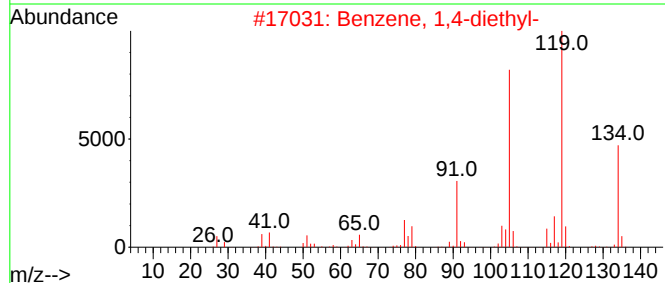
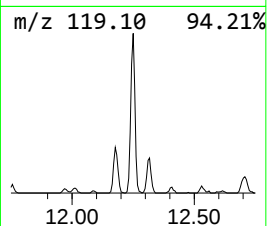
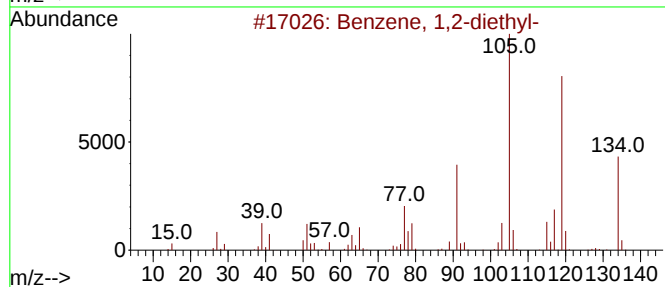
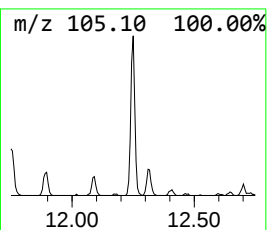
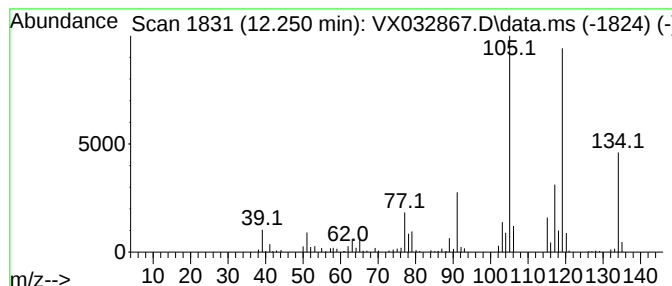
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	10.91 ug/l	88071	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	90
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	83
5			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

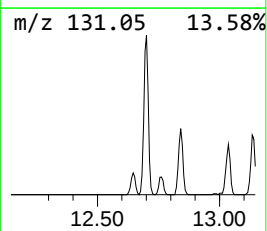
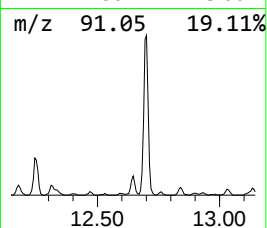
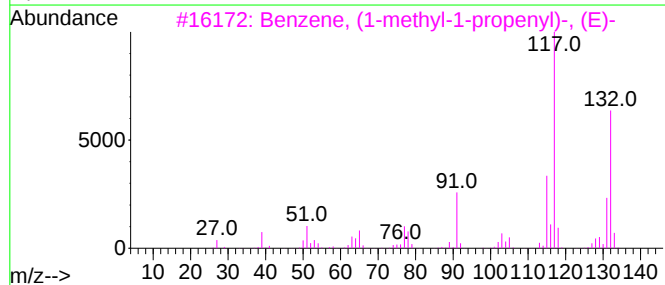
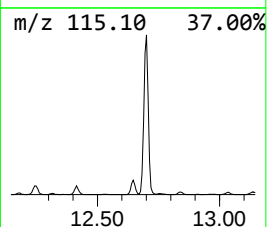
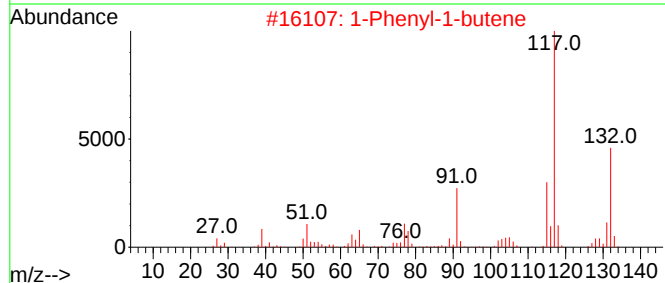
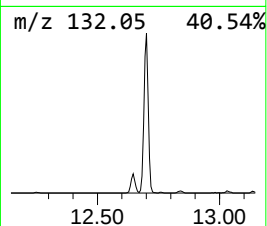
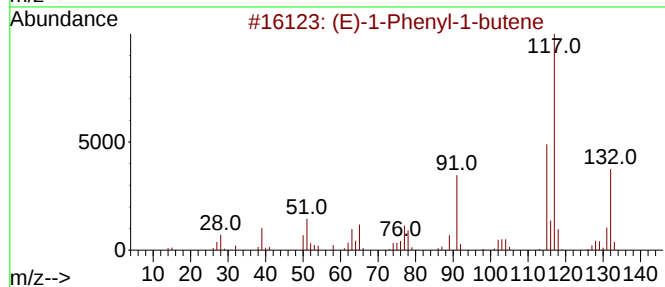
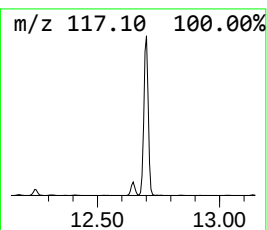
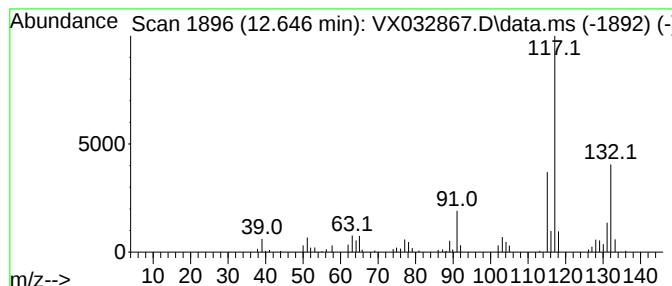
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Quant Title : SW846 8260

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

Peak Number 6 (E)-1-Phenyl-1-butene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.646	5.11 ug/l	41247	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	95
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	94
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	93
5			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

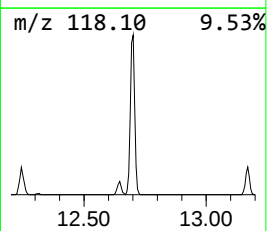
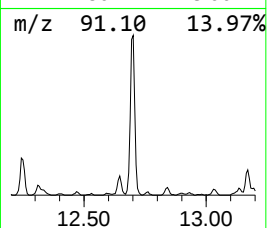
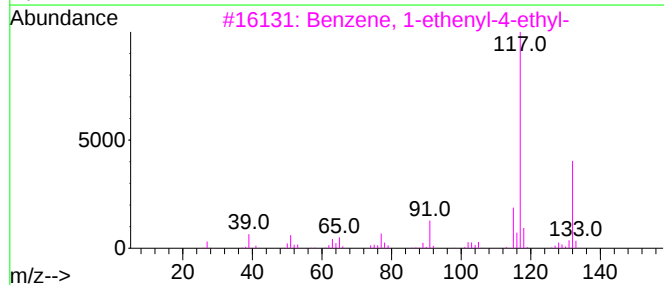
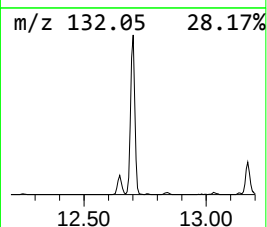
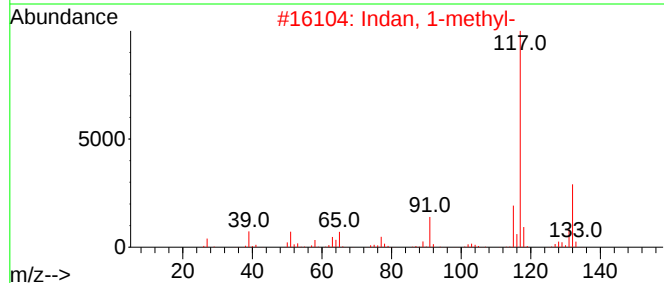
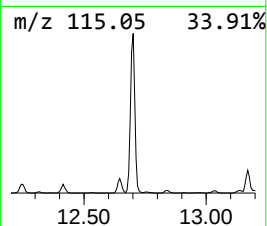
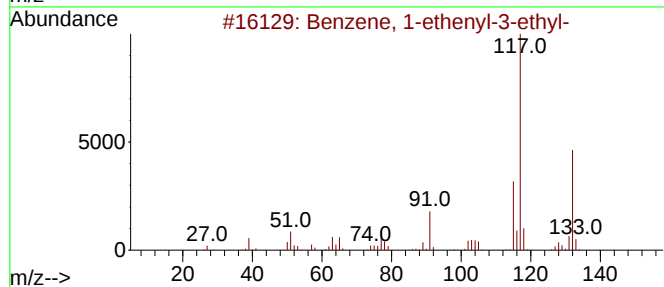
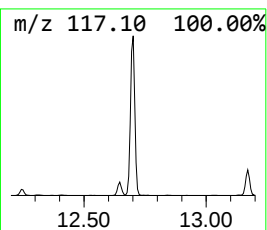
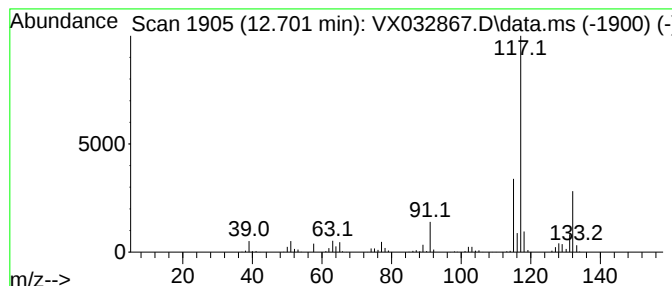
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	52.29 ug/l	422203	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

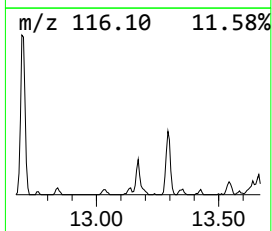
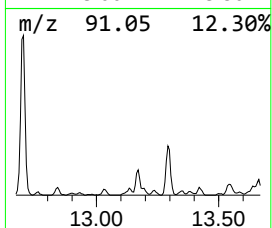
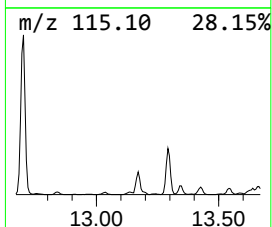
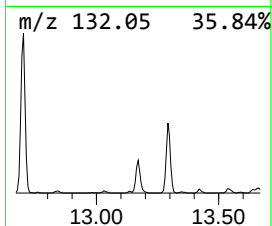
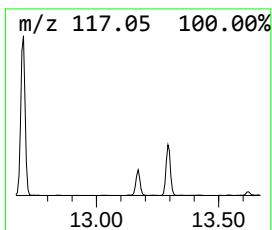
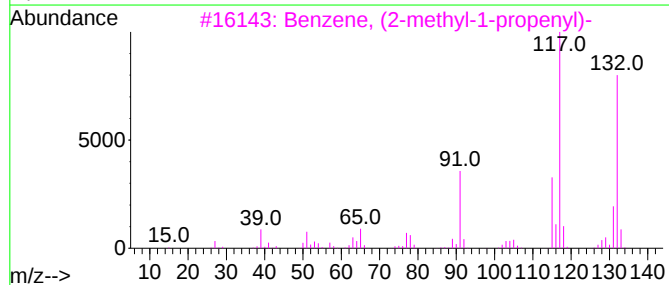
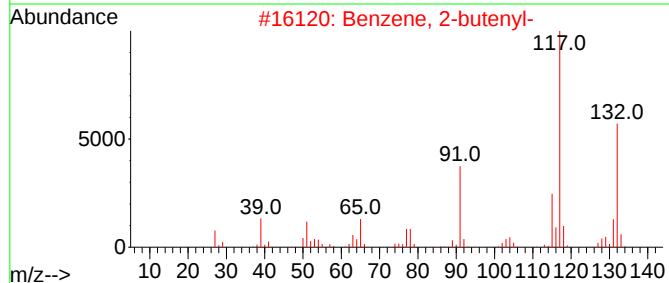
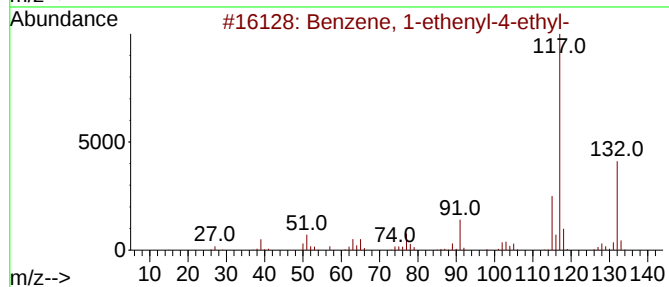
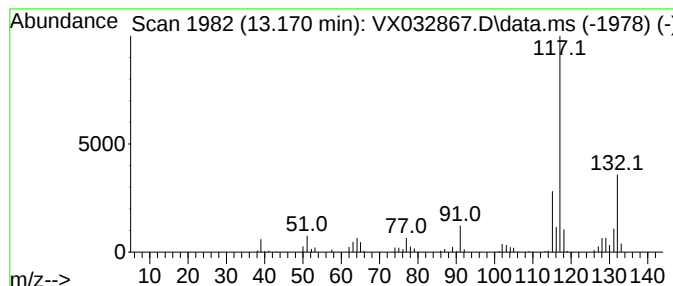
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	10.27 ug/l	82905	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	90
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

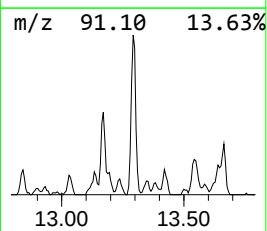
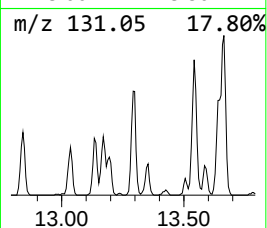
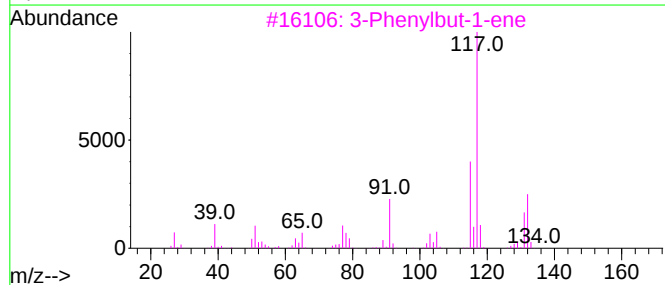
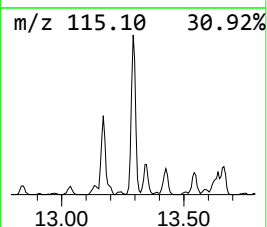
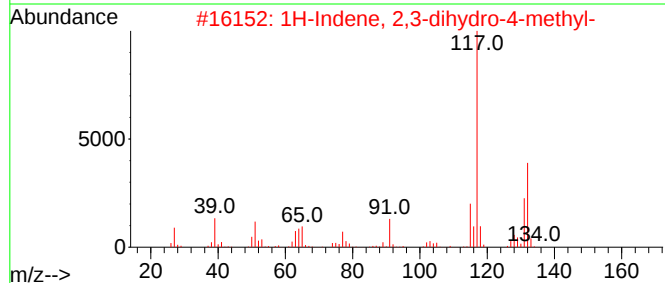
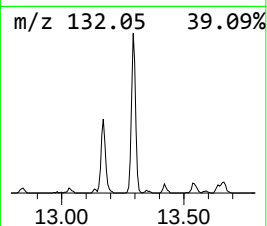
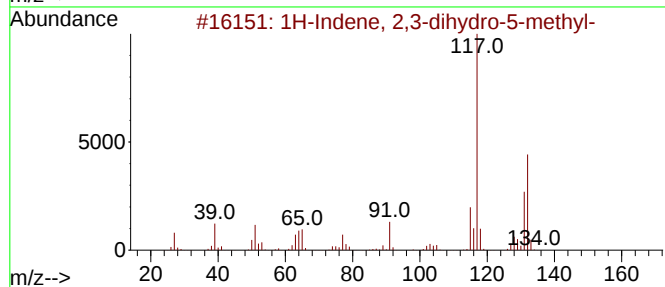
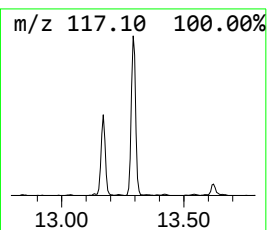
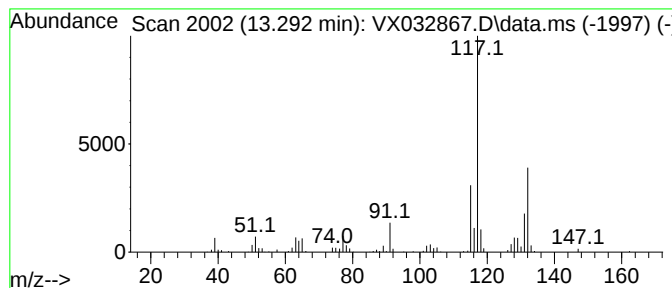
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	19.35 ug/l	156204	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
2		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111622\
Data File : VX032867.D
Acq On : 16 Nov 2022 14:51
Operator : JC/MD
Sample : N5614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane, 2,3,4-...	7.982	5.9	ug/l	46300	2	6.763	394298	50.0
Pentane, 2,3,3-...	8.104	9.3	ug/l	73077	2	6.763	394298	50.0
1,4-Pentadiene,...	9.165	7.3	ug/l	64486	3	10.055	443777	50.0
Benzene, 1,2-di...	12.250	10.9	ug/l	88071	4	12.024	403692	50.0
(E)-1-Phenyl-1-...	12.646	5.1	ug/l	41247	4	12.024	403692	50.0
Benzene, 1-ethe...	12.701	52.3	ug/l	422203	4	12.024	403692	50.0
Benzene, 1-ethe...	13.170	10.3	ug/l	82905	4	12.024	403692	50.0
1H-Indene, 2,3-...	13.292	19.4	ug/l	156204	4	12.024	403692	50.0