

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
 Data File : VX032829.D
 Acq On : 15 Nov 2022 17:44
 Operator : JC/MD
 Sample : N5614-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-24

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: VX032829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.752	103	109	118	rVB	35164	47763	8.15%	0.878%
2	2.343	198	206	214	rBV	15692	30649	5.23%	0.563%
3	2.782	268	278	283	rBV	16761	36032	6.15%	0.662%
4	2.825	283	285	299	rVB2	5780	11036	1.88%	0.203%
5	3.105	322	331	341	rVB	24512	53490	9.13%	0.983%
6	4.209	499	512	521	rBV3	4182	11560	1.97%	0.212%
7	4.312	521	529	539	rVB5	2459	6708	1.14%	0.123%
8	5.385	694	705	719	rBV	67818	198456	33.86%	3.646%
9	5.556	722	733	743	rBV	106081	311640	53.16%	5.726%
10	5.849	769	781	789	rBV4	2319	7546	1.29%	0.139%
11	5.958	789	799	811	rBV2	70766	192928	32.91%	3.545%
12	6.159	824	832	840	rBV3	9181	25754	4.39%	0.473%
13	6.257	840	848	857	rVV2	20948	61877	10.56%	1.137%
14	6.355	857	864	874	rVB4	6221	18671	3.19%	0.343%
15	6.763	921	931	942	rBV	166719	396890	67.71%	7.292%
16	7.360	1021	1029	1038	rBV5	8386	19855	3.39%	0.365%
17	7.501	1044	1052	1056	rBV3	3555	7530	1.28%	0.138%
18	7.562	1056	1062	1066	rVV3	5531	11992	2.05%	0.220%
19	7.775	1091	1097	1106	rVB2	6493	12643	2.16%	0.232%
20	7.982	1121	1131	1141	rVB	23407	54861	9.36%	1.008%
21	8.104	1141	1151	1160	rBV	43505	87824	14.98%	1.614%
22	8.190	1160	1165	1179	rVB7	4691	13900	2.37%	0.255%
23	8.312	1179	1185	1193	rBV5	7546	14187	2.42%	0.261%
24	8.513	1208	1218	1225	rVB5	6318	16484	2.81%	0.303%
25	8.610	1226	1234	1235	rBV3	12507	22005	3.75%	0.404%
26	8.647	1235	1240	1252	rVB	361302	586188	100.00%	10.770%
27	8.775	1252	1261	1265	rBV4	6079	11742	2.00%	0.216%
28	8.976	1289	1294	1299	rVB3	7676	14055	2.40%	0.258%
29	9.104	1307	1315	1320	rVB3	15389	28178	4.81%	0.518%
30	9.159	1320	1324	1337	rVB	37274	64393	10.99%	1.183%
31	9.427	1364	1368	1371	rBV2	11747	17419	2.97%	0.320%
32	9.500	1376	1380	1389	rVB3	13936	27833	4.75%	0.511%
33	9.659	1403	1406	1415	rVB2	6965	12415	2.12%	0.228%
34	9.762	1417	1423	1429	rBV2	16109	26142	4.46%	0.480%
35	9.921	1444	1449	1455	rVB3	3916	8143	1.39%	0.150%
36	10.055	1466	1471	1477	rVV	357225	472838	80.66%	8.687%

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Integrator: RTE

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37	10.128	1480	1483	1486	rVB	5342	6626	1.13%	0.122%
38	10.275	1503	1507	1510	rBV3	6889	11432	1.95%	0.210%
39	10.305	1510	1512	1518	rVB5	6787	9400	1.60%	0.173%
40	10.585	1549	1558	1566	rBV4	9168	18801	3.21%	0.345%
41	10.774	1583	1589	1592	rBV2	5944	9382	1.60%	0.172%
42	10.866	1598	1604	1610	rVB7	3835	8087	1.38%	0.149%
43	11.079	1634	1639	1644	rBV	332737	421931	71.98%	7.752%
44	11.122	1644	1646	1654	rVB3	9277	13284	2.27%	0.244%
45	11.616	1719	1727	1733	rBV	19085	26483	4.52%	0.487%
46	12.024	1788	1794	1803	rBV	357065	466913	79.65%	8.578%
47	12.177	1815	1819	1824	rVB	12355	15224	2.60%	0.280%
48	12.250	1824	1831	1837	rBV	264403	328313	56.01%	6.032%
49	12.311	1837	1841	1848	rVB	72320	89432	15.26%	1.643%
50	12.402	1852	1856	1862	rVB2	25547	34509	5.89%	0.634%
51	12.469	1862	1867	1872	rBV2	16468	21962	3.75%	0.404%
52	12.646	1891	1896	1900	rBV	68198	83593	14.26%	1.536%
53	12.701	1900	1905	1912	rVV	333845	439872	75.04%	8.082%
54	12.762	1912	1915	1921	rVB	7862	8687	1.48%	0.160%
55	12.841	1921	1928	1934	rVB	17447	24335	4.15%	0.447%
56	12.902	1934	1938	1940	rBV3	3881	5886	1.00%	0.108%
57	13.024	1953	1958	1968	rBV2	32822	49286	8.41%	0.906%
58	13.134	1968	1976	1980	rBV2	26516	46524	7.94%	0.855%
59	13.195	1980	1986	1989	rVV2	14876	20049	3.42%	0.368%
60	13.237	1989	1993	1998	rVB2	7120	9830	1.68%	0.181%
61	13.298	1998	2003	2006	rBV3	12013	15175	2.59%	0.279%
62	13.347	2006	2011	2015	rVV3	19770	29206	4.98%	0.537%
63	13.390	2015	2018	2020	rVV3	6302	8268	1.41%	0.152%
64	13.426	2020	2024	2029	rVB	16135	21973	3.75%	0.404%
65	13.542	2032	2043	2047	rBV2	14849	28029	4.78%	0.515%
66	13.640	2052	2059	2067	rVB2	24917	50648	8.64%	0.931%
67	13.798	2080	2085	2091	rBV6	2868	7498	1.28%	0.138%
68	13.853	2091	2094	2098	rVB2	7925	9614	1.64%	0.177%
69	13.926	2098	2106	2110	rBV	25632	36065	6.15%	0.663%
70	14.073	2126	2130	2137	rBV	22965	29976	5.11%	0.551%
71	14.219	2148	2154	2166	rVB3	8812	19011	3.24%	0.349%
72	14.323	2166	2171	2176	rBV	16098	25907	4.42%	0.476%
73	14.371	2176	2179	2185	rVB	20829	26220	4.47%	0.482%
74	14.603	2209	2217	2221	rBV5	8415	15872	2.71%	0.292%
75	14.792	2243	2248	2251	rBV2	5708	7907	1.35%	0.145%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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

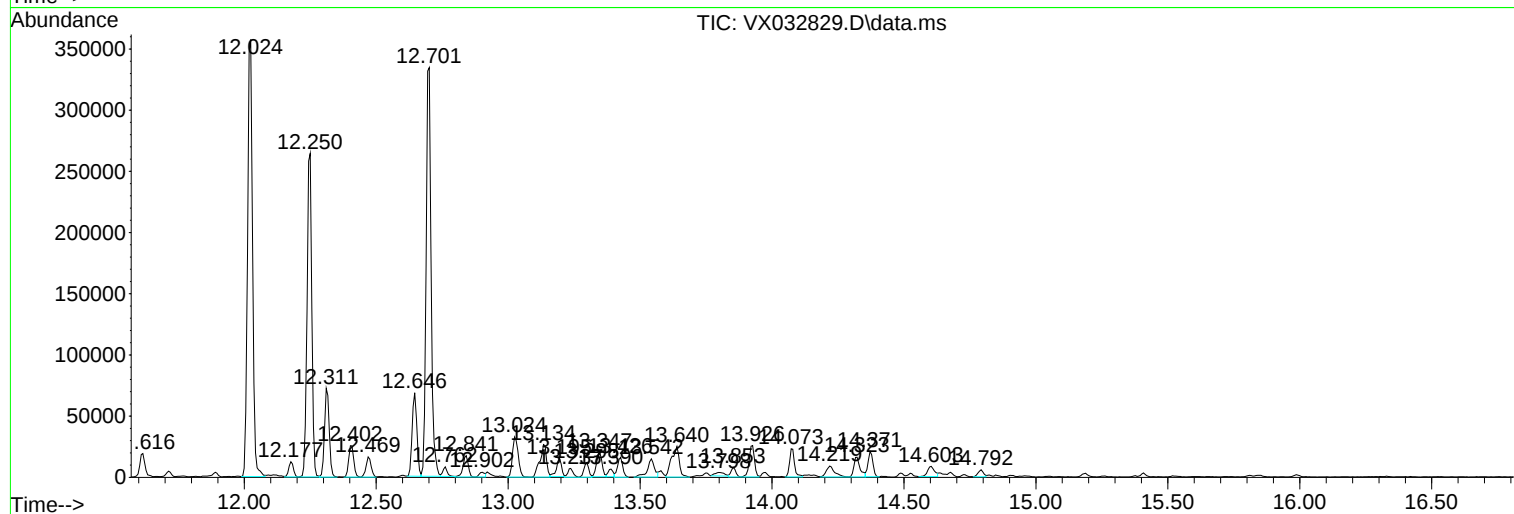
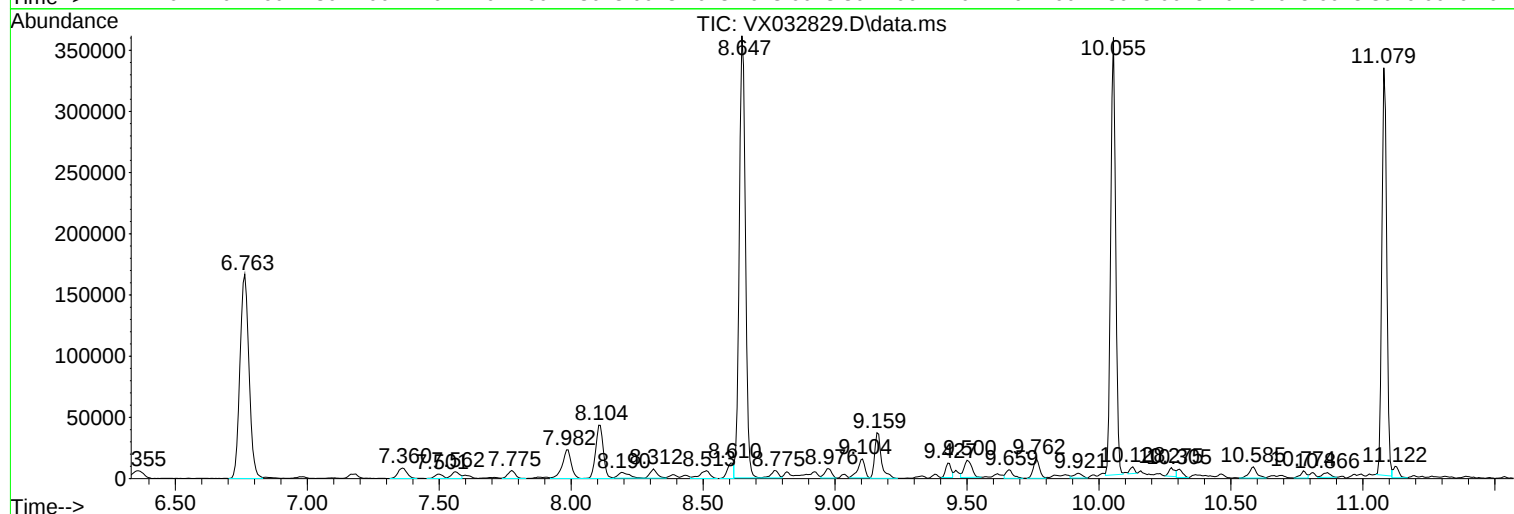
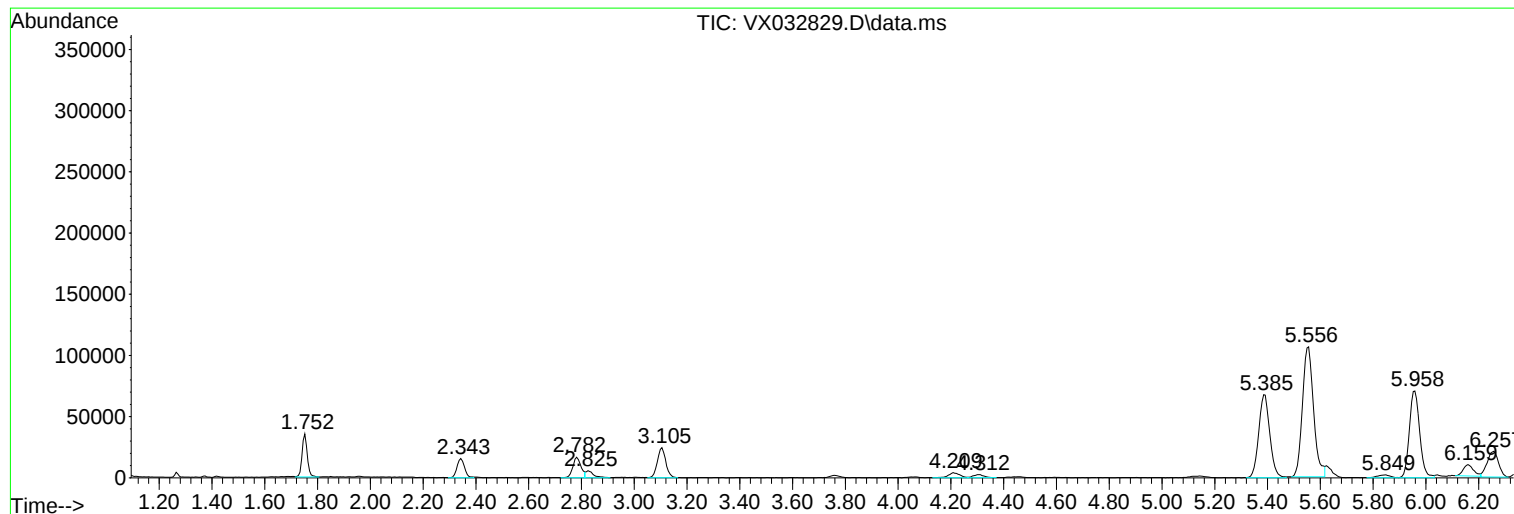
Sum of corrected areas: 5442837

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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 : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
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MW-24

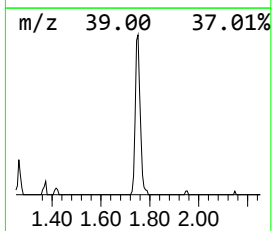
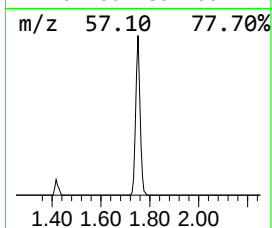
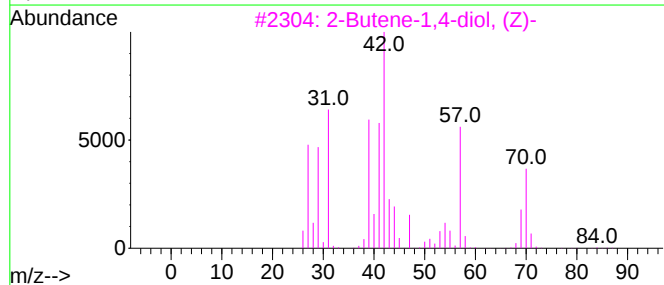
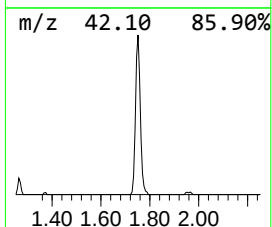
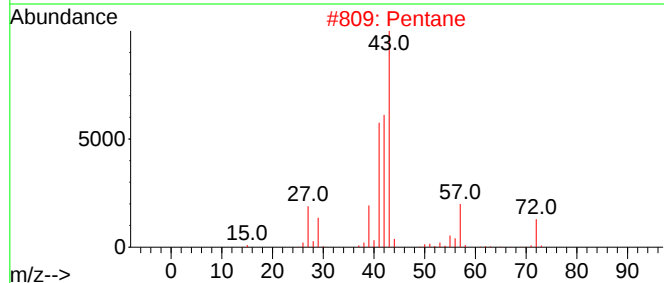
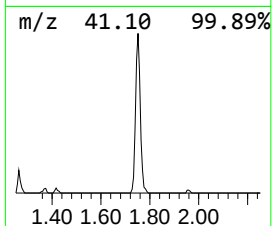
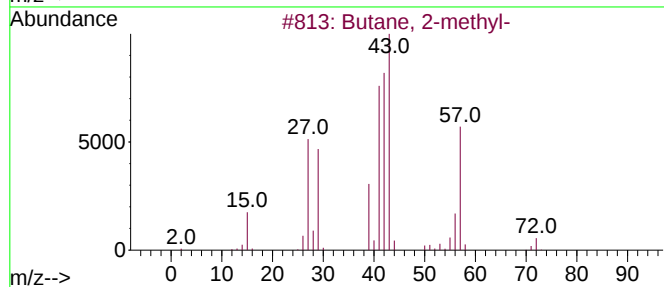
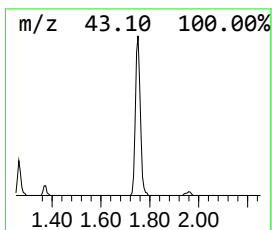
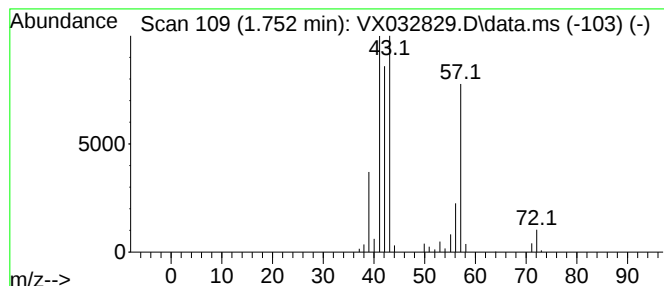
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	7.66 ug/l	47763	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	32
3			2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	25
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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Instrument :
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ClientSampleId :
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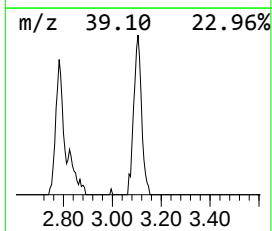
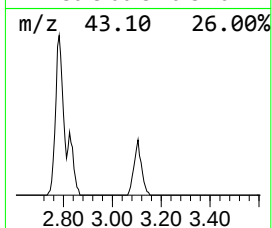
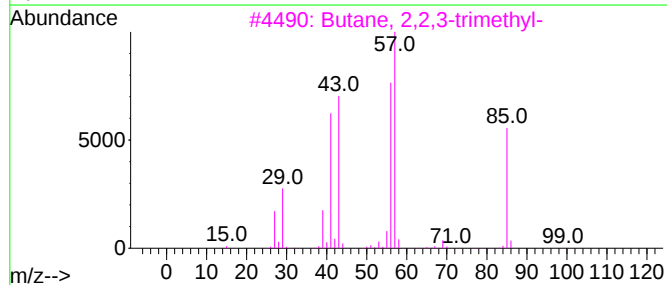
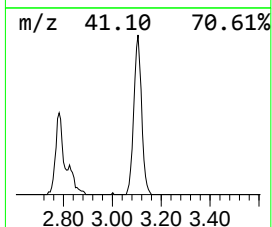
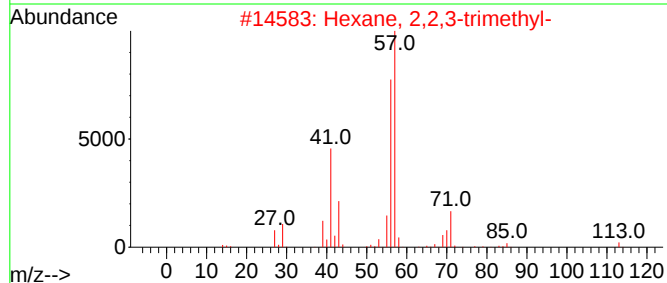
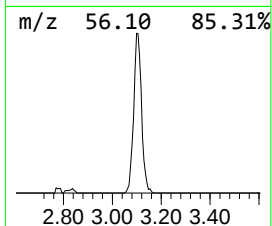
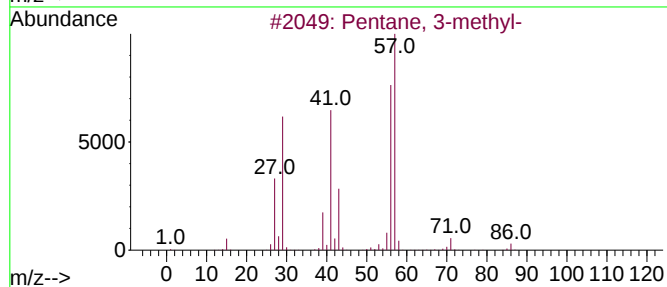
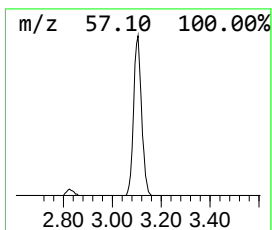
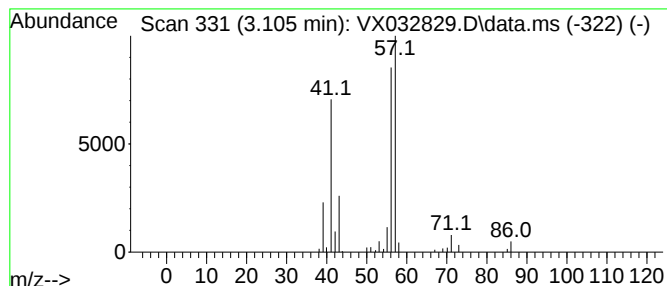
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	8.58 ug/l	53490	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45



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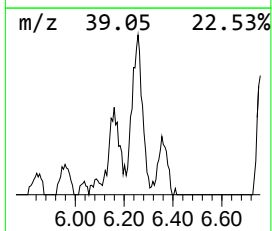
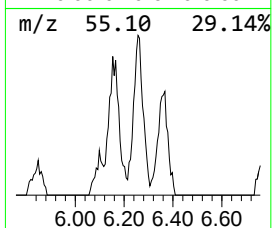
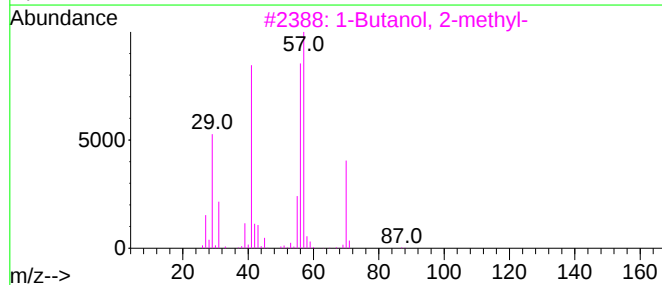
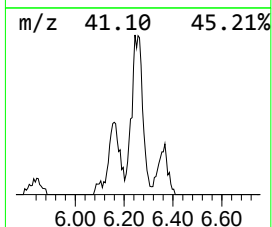
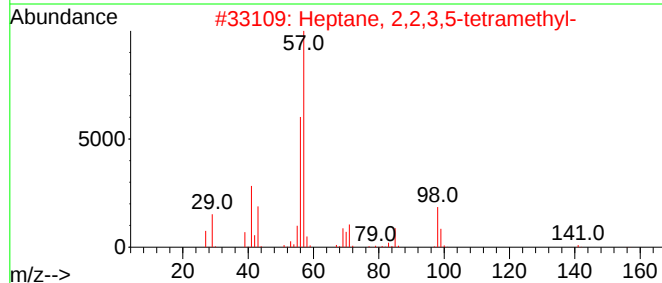
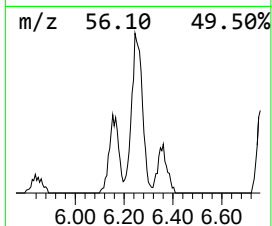
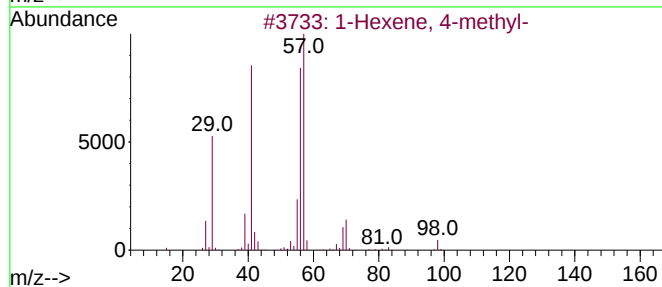
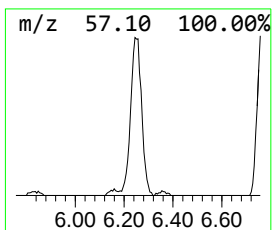
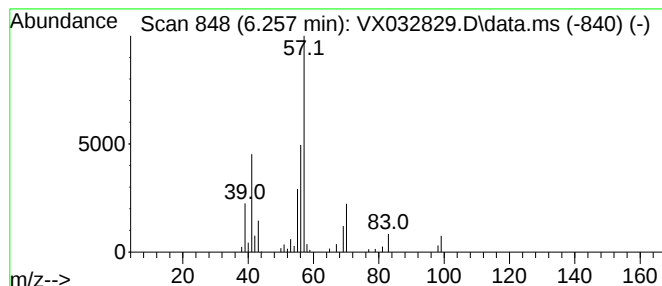
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Quant Title : SW846 8260

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

Peak Number 3 1-Hexene, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	7.80 ug/l	61877	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 4-methyl-			98	C7H14	003769-23-1	50
2	Heptane, 2,2,3,5-tetramethyl-			156	C11H24	061868-42-6	38
3	1-Butanol, 2-methyl-			88	C5H12O	000137-32-6	33
4	Octane, 2,3-dimethyl-			142	C10H22	007146-60-3	28
5	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	28



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MW-24

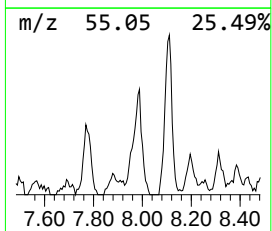
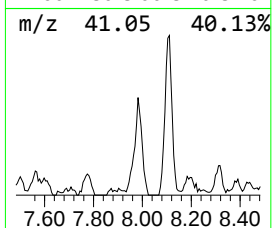
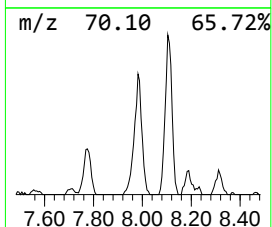
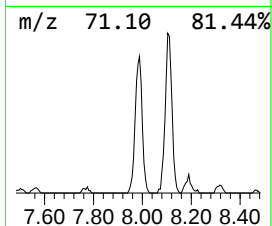
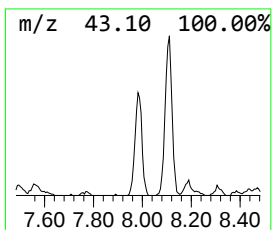
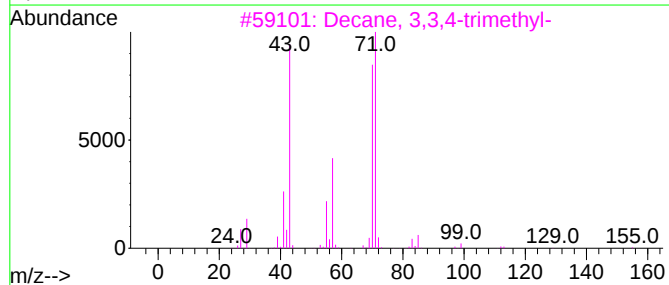
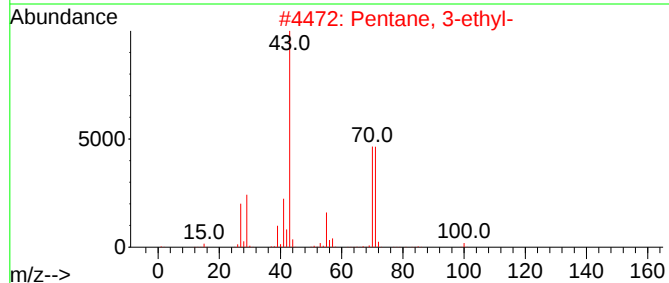
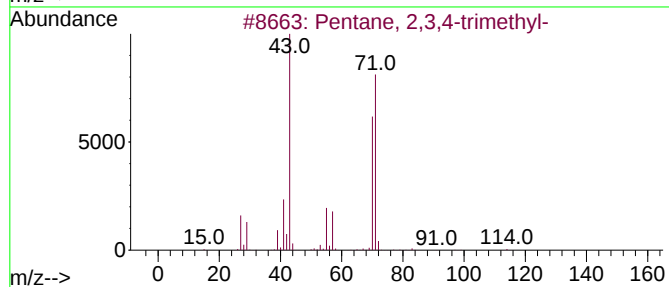
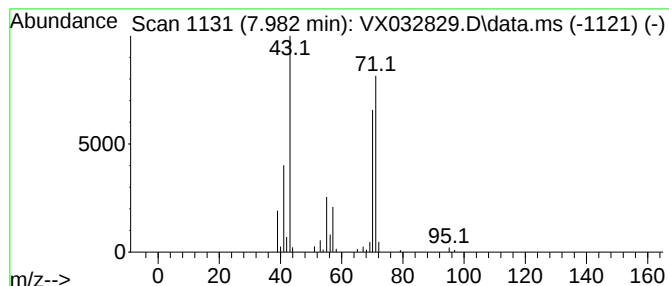
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	6.91 ug/l	54861	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	83
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

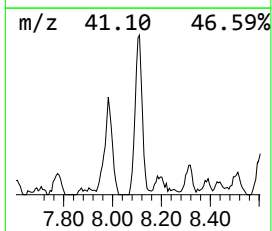
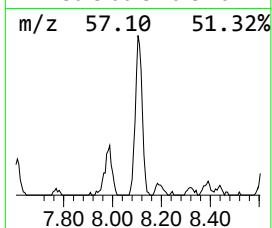
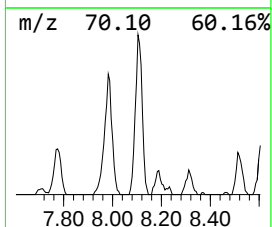
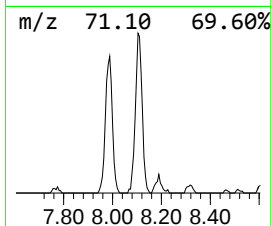
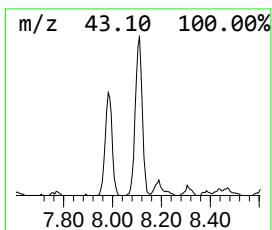
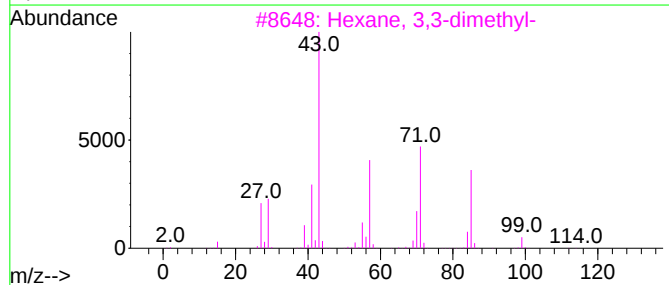
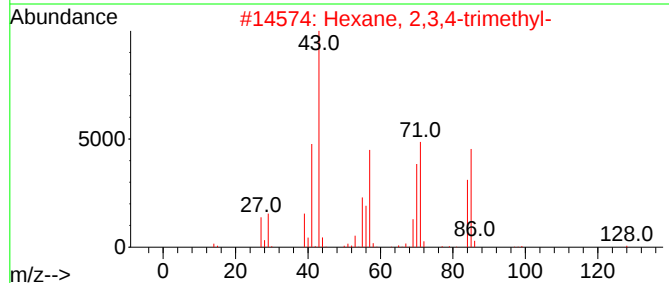
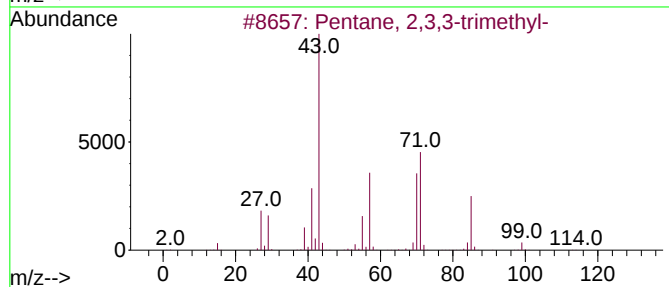
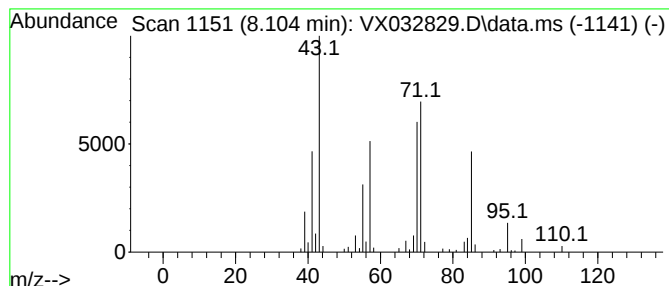
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	11.06 ug/l	87824	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	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

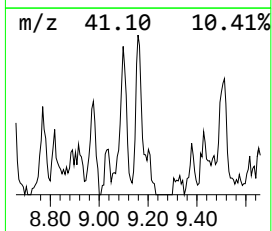
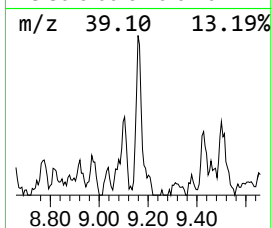
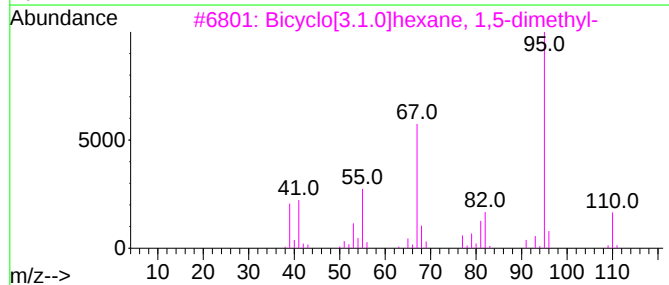
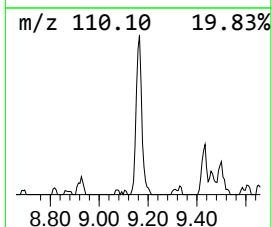
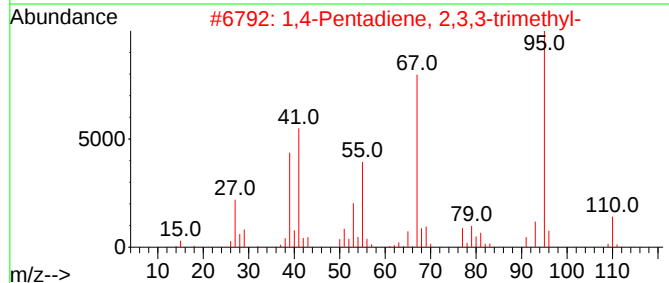
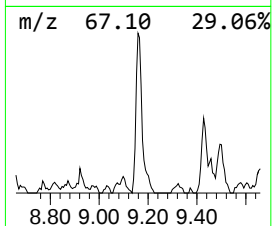
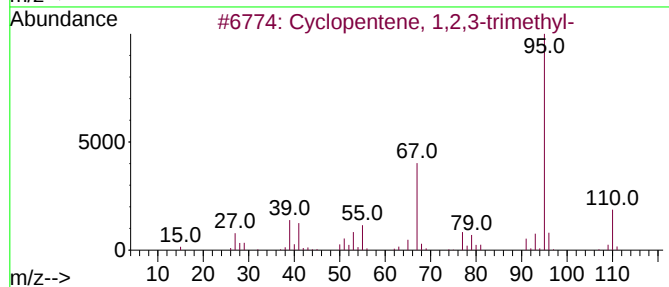
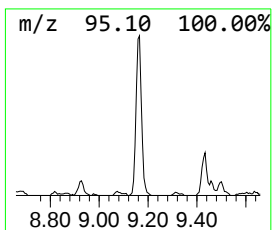
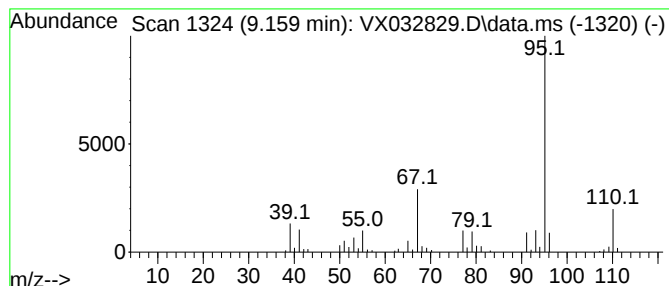
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	6.81 ug/l	64393	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	91
2			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	87
3			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	80
4			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	80
5			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

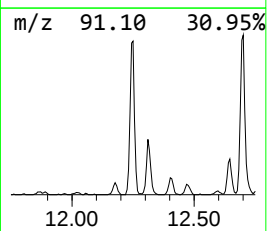
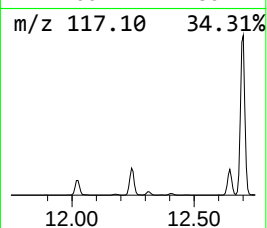
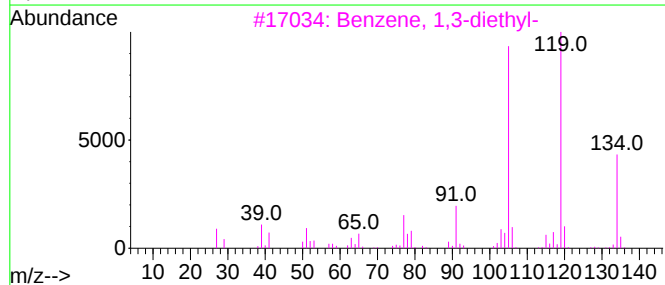
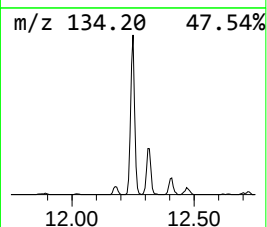
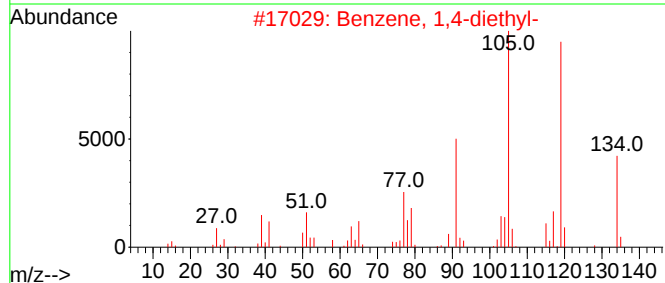
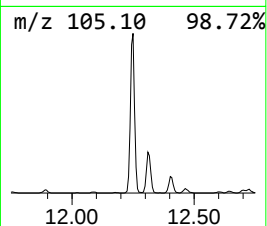
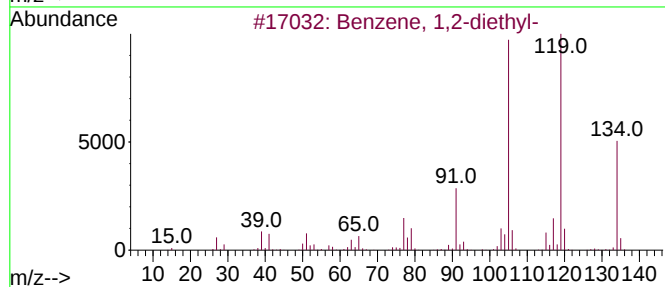
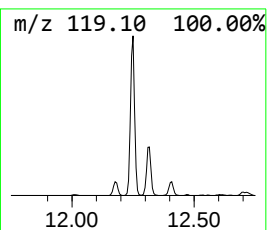
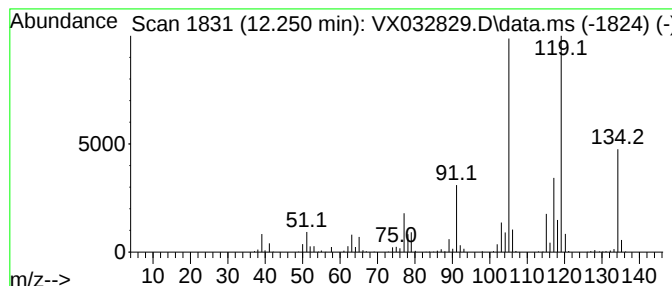
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2-diethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	35.16 ug/l	328313	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	93
3		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	90
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	83
5		Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

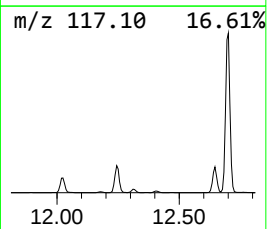
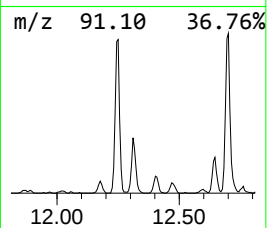
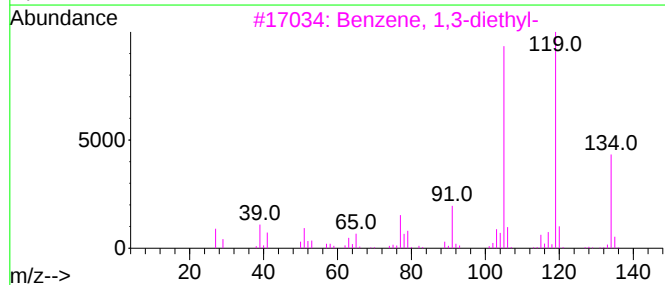
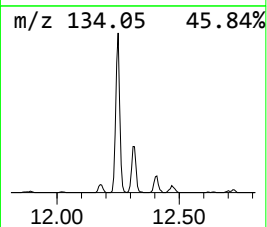
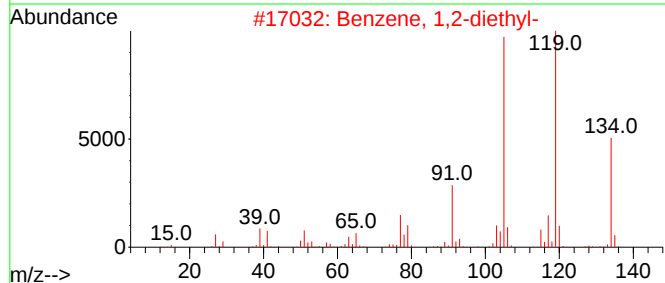
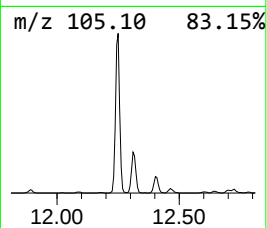
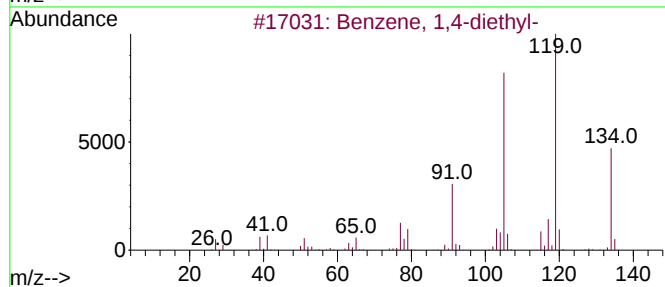
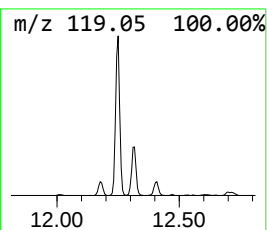
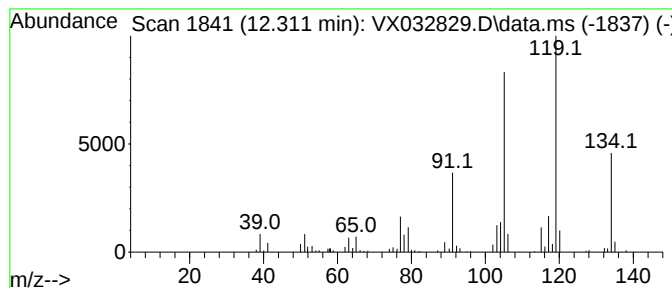
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,4-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.311	9.58 ug/l	89432	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

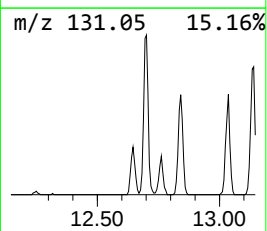
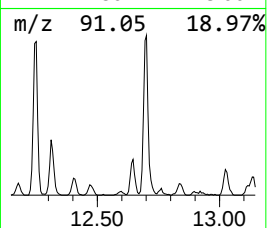
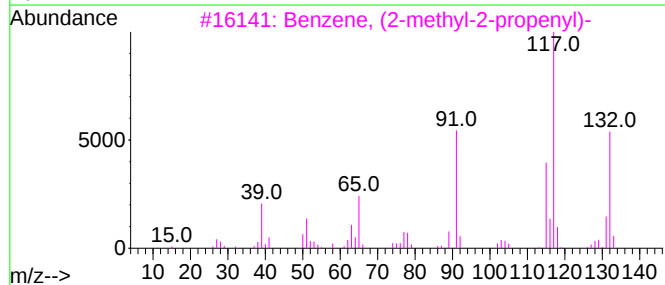
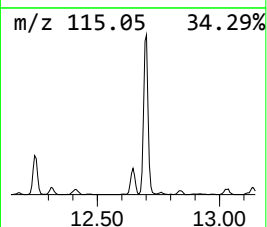
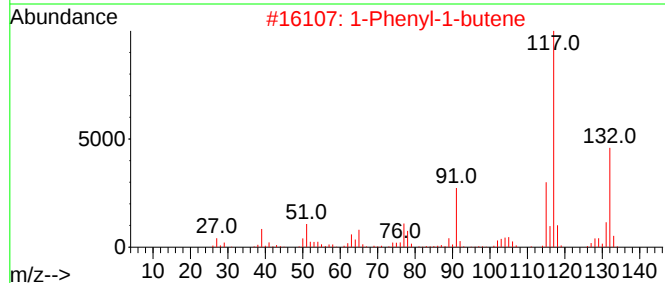
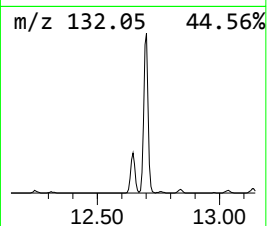
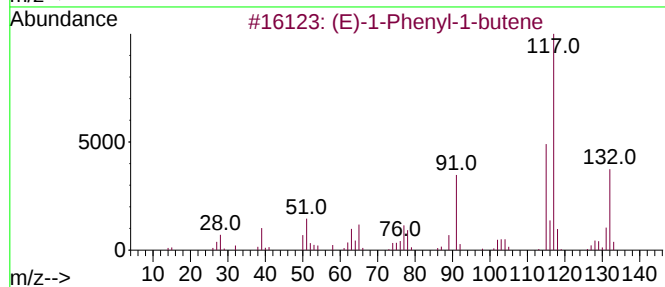
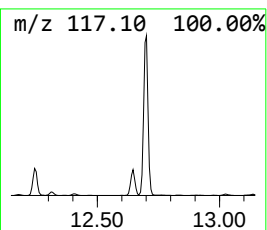
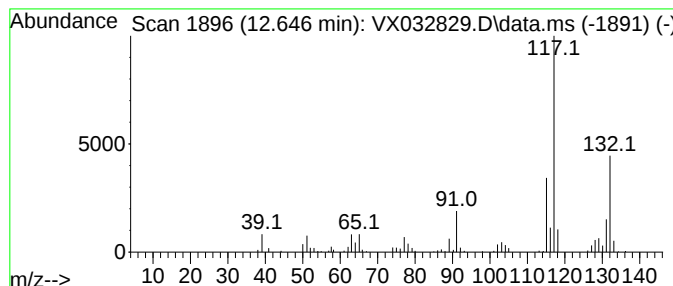
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Quant Title : SW846 8260

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

Peak Number 9 (E)-1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.646	8.95 ug/l	83593	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, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	94
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

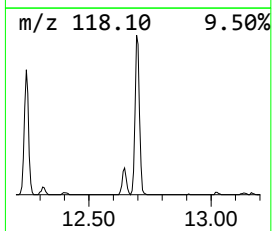
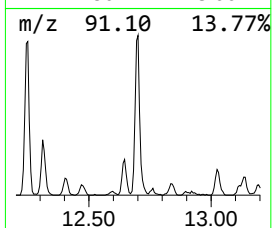
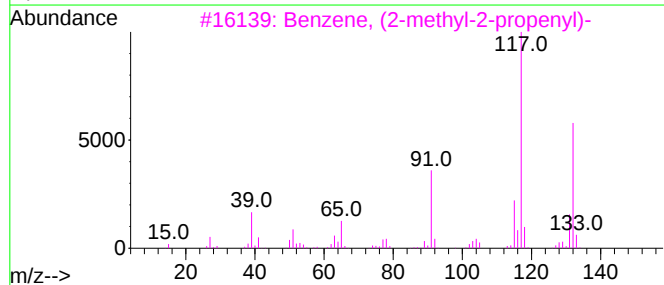
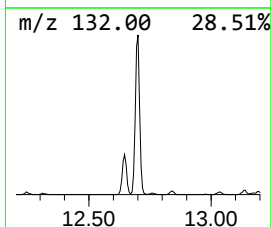
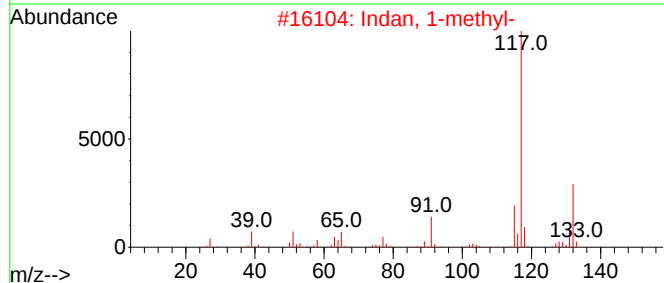
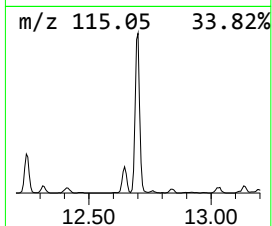
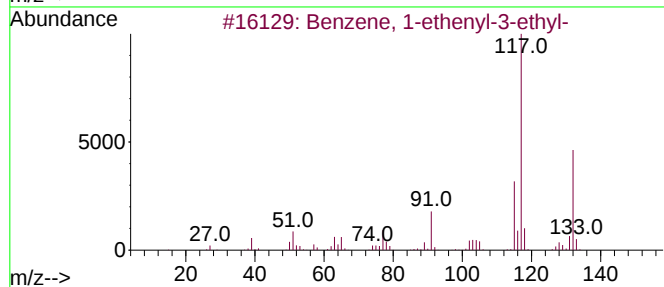
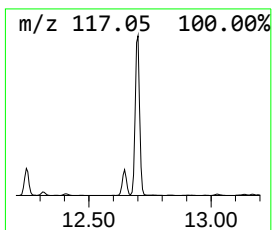
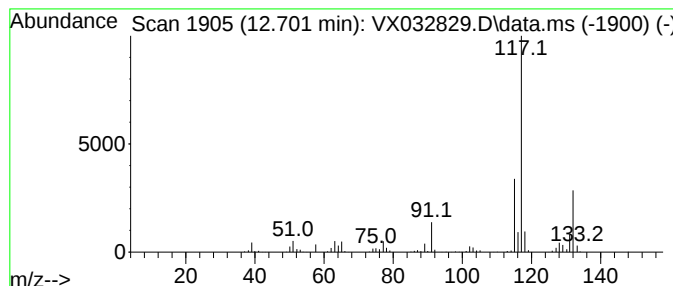
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	47.10 ug/l	439872	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, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111522\
Data File : VX032829.D
Acq On : 15 Nov 2022 17:44
Operator : JC/MD
Sample : N5614-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

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
Butane, 2-methyl-	1.752	7.7	ug/l	47763	1	5.556	311640	50.0
Pentane, 3-methyl-	3.105	8.6	ug/l	53490	1	5.556	311640	50.0
1-Hexene, 4-met...	6.257	7.8	ug/l	61877	2	6.763	396890	50.0
Pentane, 2,3,4-...	7.982	6.9	ug/l	54861	2	6.763	396890	50.0
Pentane, 2,3,3-...	8.104	11.1	ug/l	87824	2	6.763	396890	50.0
Cyclopentene, 1...	9.159	6.8	ug/l	64393	3	10.055	472838	50.0
Benzene, 1,2-di...	12.250	35.2	ug/l	328313	4	12.024	466913	50.0
Benzene, 1,4-di...	12.311	9.6	ug/l	89432	4	12.024	466913	50.0
(E)-1-Phenyl-1-...	12.646	8.9	ug/l	83593	4	12.024	466913	50.0
Benzene, 1-ethe...	12.701	47.1	ug/l	439872	4	12.024	466913	50.0