

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
 Data File : VN071761.D
 Acq On : 01 Apr 2022 18:32
 Operator : JC\MD
 Sample : N2090-11
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-55

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_N\methods\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	37	43	45	rBV2	50810	96754	2.78%	0.354%
2	4.263	374	387	401	rBV6	33892	135457	3.89%	0.496%
3	4.581	428	441	448	rBV2	13838	42809	1.23%	0.157%
4	5.075	513	525	557	rVB3	80916	371507	10.67%	1.359%
5	5.369	564	575	585	rBV3	22683	85019	2.44%	0.311%
6	5.622	603	618	631	rBV3	64829	230207	6.61%	0.842%
7	7.045	852	860	870	rBV5	17938	56035	1.61%	0.205%
8	7.334	898	909	921	rVB5	12121	40755	1.17%	0.149%
9	7.845	977	996	1005	rBV5	23683	84186	2.42%	0.308%
10	8.022	1013	1026	1031	rBV	398306	993366	28.54%	3.635%
11	8.081	1031	1036	1045	rVV	767186	1780413	51.14%	6.515%
12	8.169	1045	1051	1063	rVV3	71577	192619	5.53%	0.705%
13	8.298	1065	1073	1077	rVV3	27825	62058	1.78%	0.227%
14	8.357	1078	1083	1088	rVV5	16173	38464	1.10%	0.141%
15	8.439	1088	1097	1109	rVV	417765	993591	28.54%	3.636%
16	8.616	1109	1127	1136	rVV	400902	1124745	32.31%	4.116%
17	8.704	1137	1142	1154	rVB4	49391	127600	3.67%	0.467%
18	8.963	1176	1186	1199	rBV	1123407	2393741	68.76%	8.759%
19	9.198	1219	1226	1232	rBV4	17523	35029	1.01%	0.128%
20	9.422	1253	1264	1275	rBV4	92190	253318	7.28%	0.927%
21	9.592	1287	1293	1300	rBV2	45070	92008	2.64%	0.337%
22	9.728	1308	1316	1323	rBV2	45107	94364	2.71%	0.345%
23	9.881	1334	1342	1351	rVB	372019	736160	21.15%	2.694%
24	10.010	1351	1364	1377	rBV	680801	1457258	41.86%	5.332%
25	10.198	1388	1396	1402	rBV4	38417	86398	2.48%	0.316%
26	10.363	1419	1424	1429	rVB2	44368	77301	2.22%	0.283%
27	10.439	1429	1437	1456	rVV	1879362	3481186	100.00%	12.738%
28	10.633	1459	1470	1477	rVV5	55458	172546	4.96%	0.631%
29	10.781	1490	1495	1500	rVV5	24849	44805	1.29%	0.164%
30	10.857	1500	1508	1517	rVV2	101816	244756	7.03%	0.896%
31	10.945	1517	1523	1532	rVB8	23230	63059	1.81%	0.231%
32	11.251	1566	1575	1581	rBV6	43960	92011	2.64%	0.337%
33	11.398	1595	1600	1605	rBV3	20706	36549	1.05%	0.134%
34	11.551	1622	1626	1635	rVB9	15347	42064	1.21%	0.154%
35	11.739	1651	1658	1671	rBV	1715779	3133064	90.00%	11.464%
36	12.580	1794	1801	1807	rBV	41618	77804	2.23%	0.285%

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37	12.727	1819	1826	1835	rBV	1231313	2121339	60.94%	7.762%
38	12.916	1851	1858	1867	rVB	38420	78243	2.25%	0.286%
39	13.480	1946	1954	1963	rBV2	119834	260688	7.49%	0.954%
40	13.674	1979	1987	1998	rBV	1296438	2299047	66.04%	8.413%
41	13.769	1999	2003	2007	rVV	22283	35396	1.02%	0.130%
42	13.833	2008	2014	2020	rVV	257337	426003	12.24%	1.559%
43	13.916	2024	2028	2037	rVV2	45247	114036	3.28%	0.417%
44	13.998	2037	2042	2048	rVB	73797	118483	3.40%	0.434%
45	14.145	2058	2067	2073	rBV3	81104	161887	4.65%	0.592%
46	14.216	2073	2079	2085	rVV	348286	542583	15.59%	1.985%
47	14.274	2085	2089	2092	rVV	24279	39844	1.14%	0.146%
48	14.327	2092	2098	2104	rVV2	188160	329087	9.45%	1.204%
49	14.404	2104	2111	2116	rVB5	70214	150004	4.31%	0.549%
50	14.463	2116	2121	2125	rBV	39538	58575	1.68%	0.214%
51	14.539	2125	2134	2141	rVB	434717	719510	20.67%	2.633%
52	14.810	2175	2180	2185	rVV3	58274	108975	3.13%	0.399%
53	14.921	2192	2199	2206	rVV4	91098	213604	6.14%	0.782%
54	14.992	2206	2211	2216	rVB3	21623	48663	1.40%	0.178%
55	15.192	2238	2245	2251	rBV2	76851	162810	4.68%	0.596%
56	15.304	2256	2264	2277	rVB4	80875	207171	5.95%	0.758%
57	16.110	2390	2401	2406	rBV2	30773	63588	1.83%	0.233%

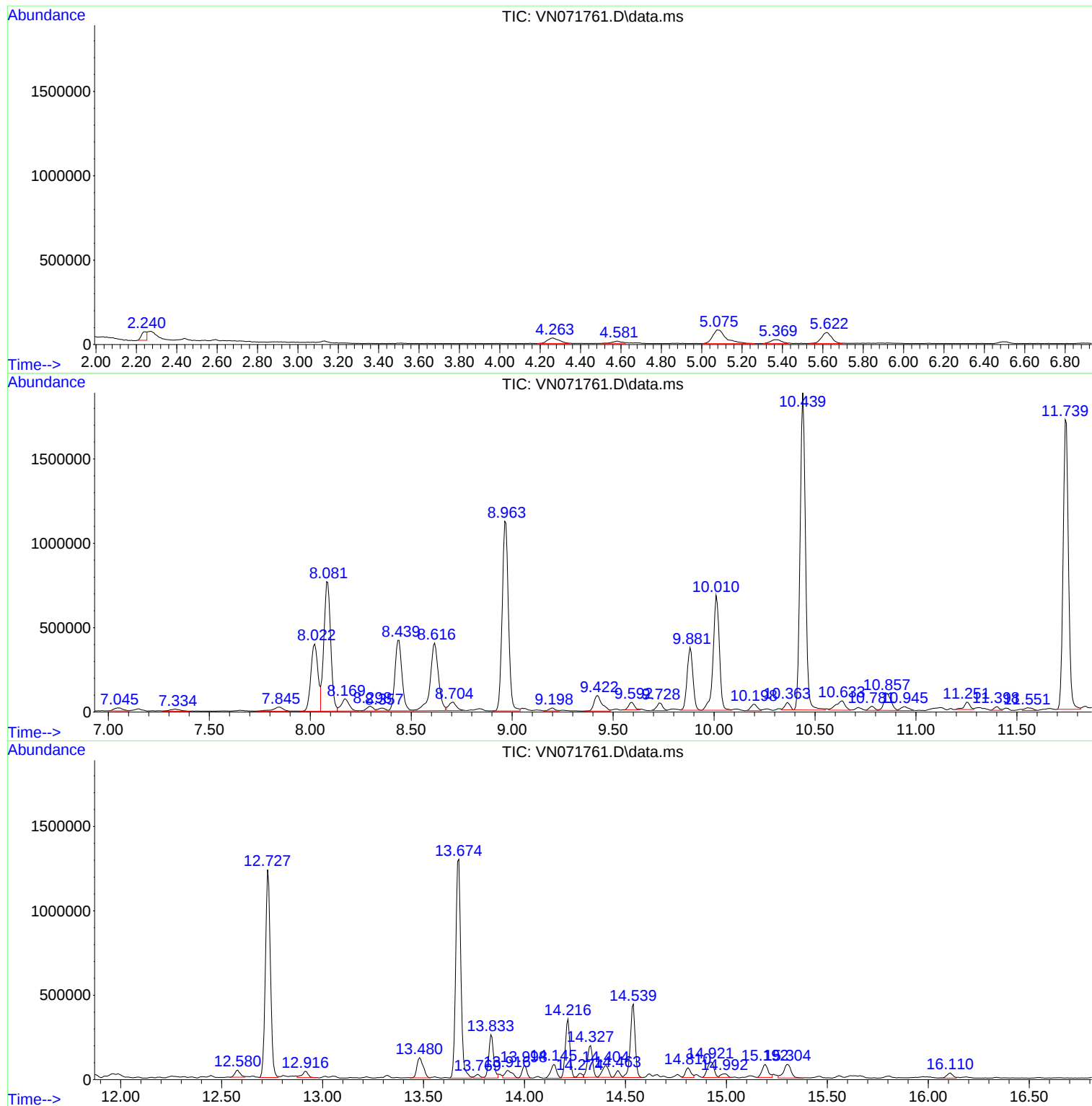
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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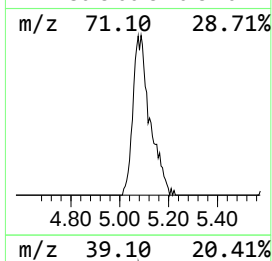
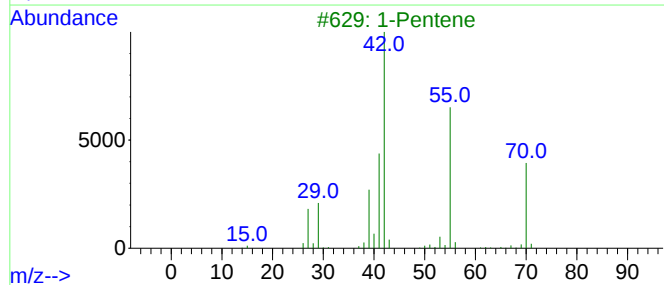
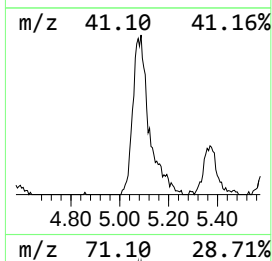
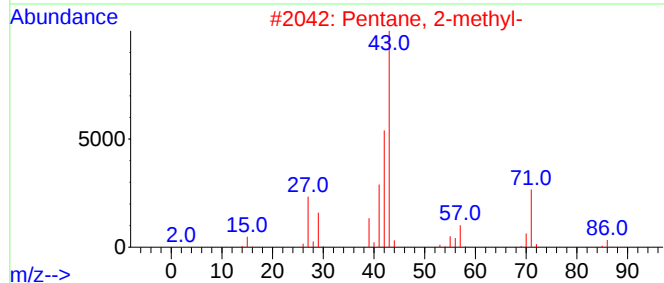
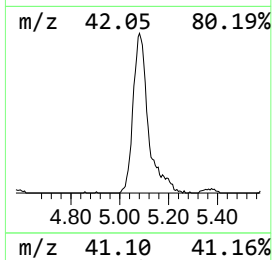
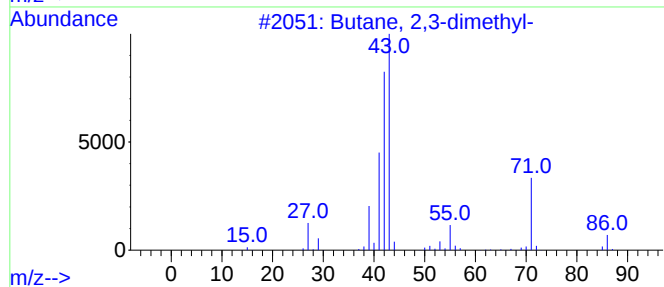
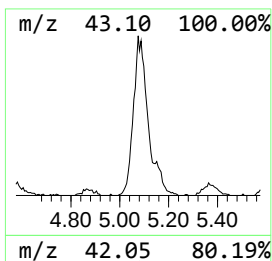
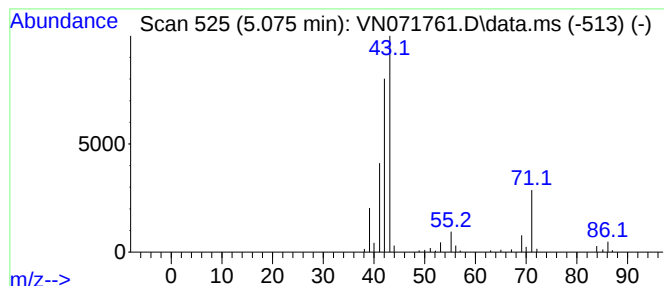
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	10.43 ug/l	371507	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			1-Pentene	70	C5H10	000109-67-1	28
4			1,2,4,5-Tetrazine, 1,4-dihydro-3...	112	C4H8N4	037454-64-1	28
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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Instrument :
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ClientSampleId :
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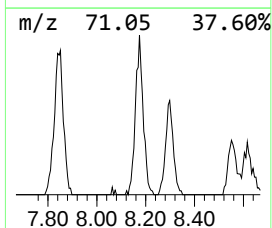
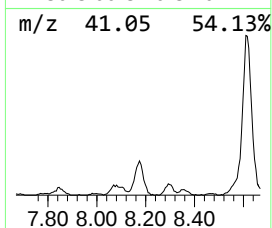
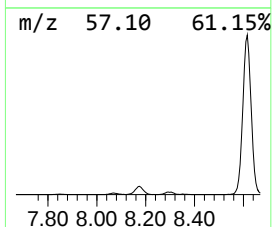
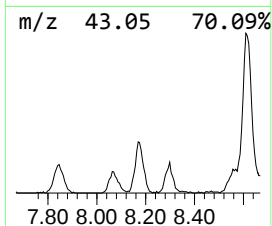
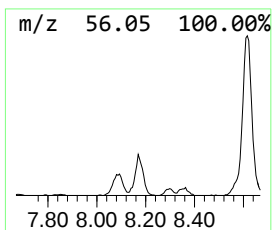
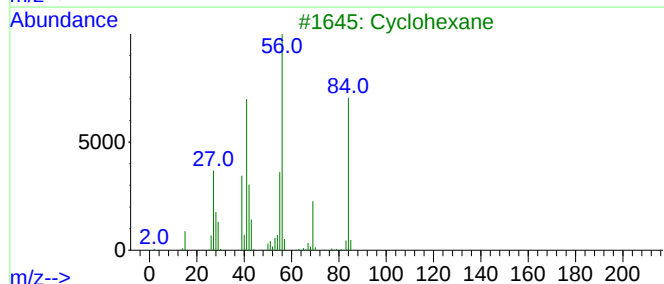
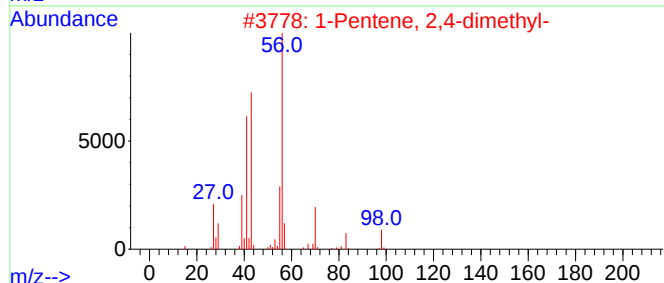
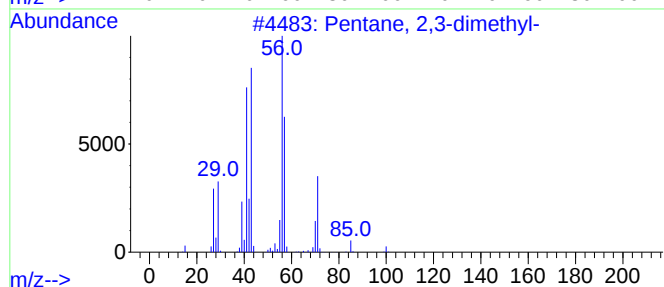
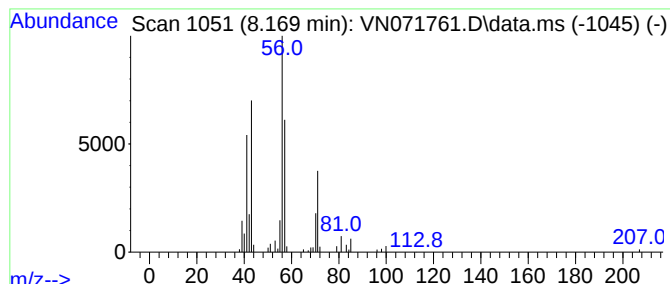
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.169	5.41 ug/l	192619	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	53
3			Cyclohexane	84	C6H12	000110-82-7	50
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	47
5			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	45



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Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

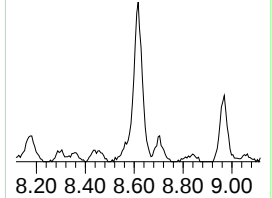
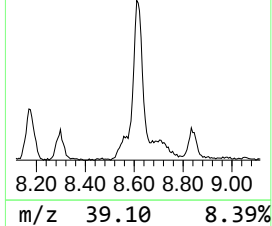
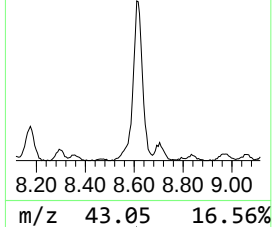
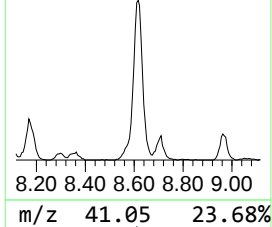
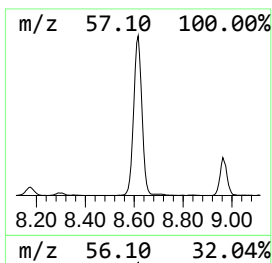
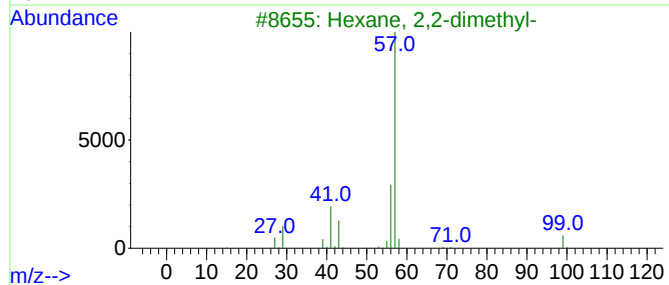
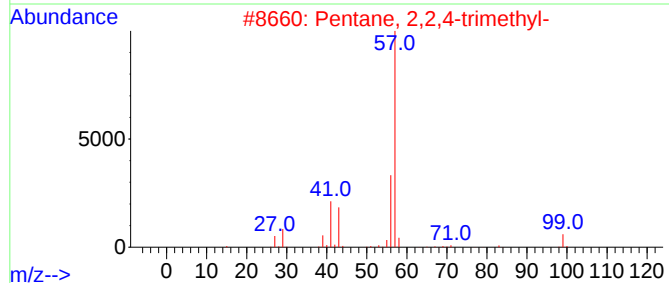
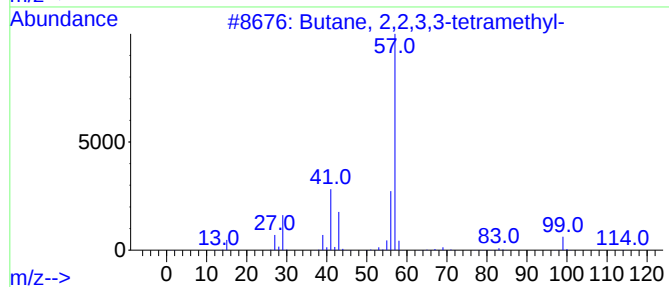
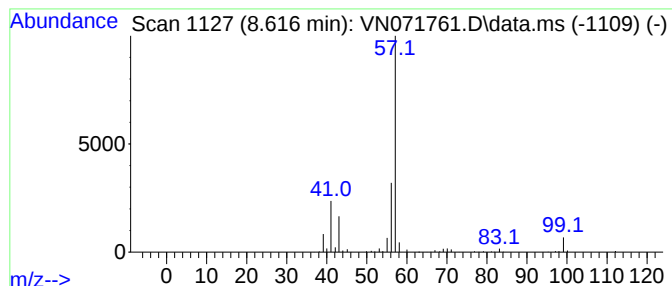
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	23.49 ug/l	1124750	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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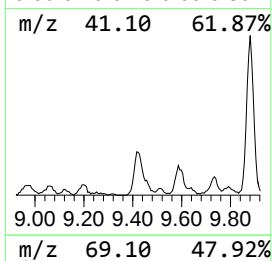
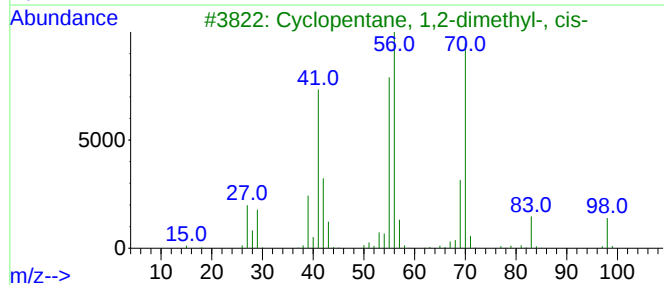
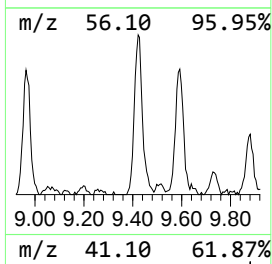
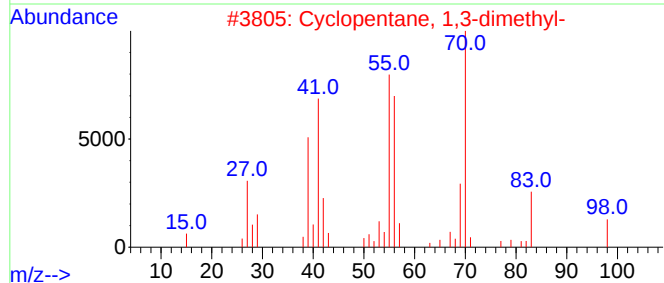
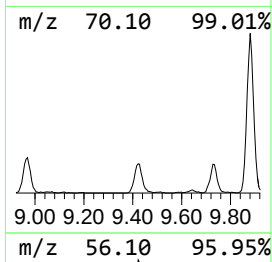
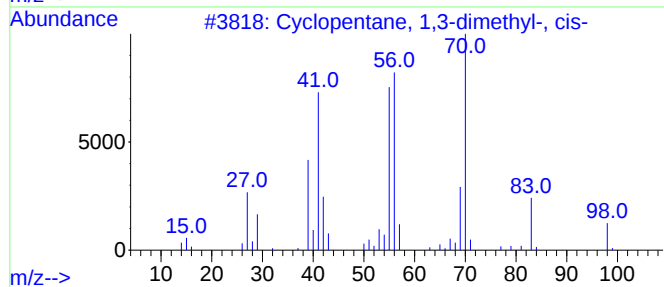
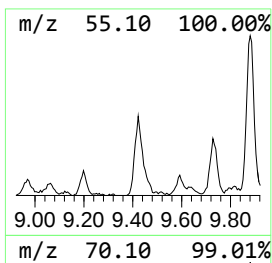
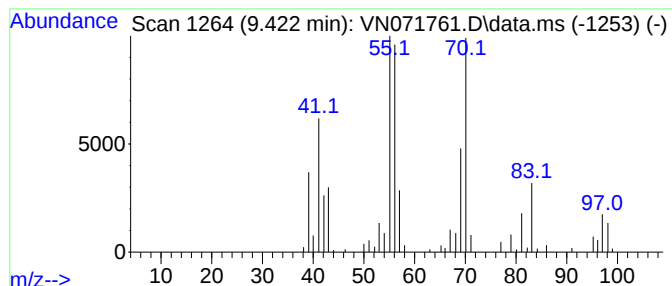
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, 1,3-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.422	5.29 ug/l	253318	1,4-Difluorobenzene	8.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	87
2		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	87
3		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	87
4		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	83
5		Cycloheptane	98	C7H14	000291-64-5	72



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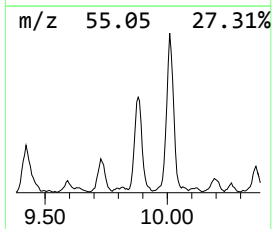
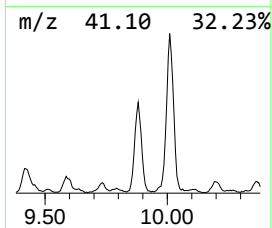
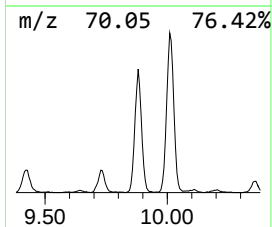
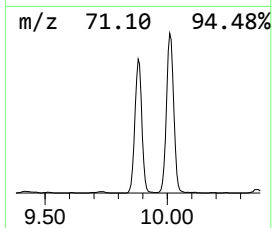
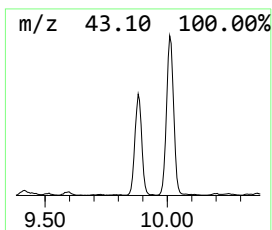
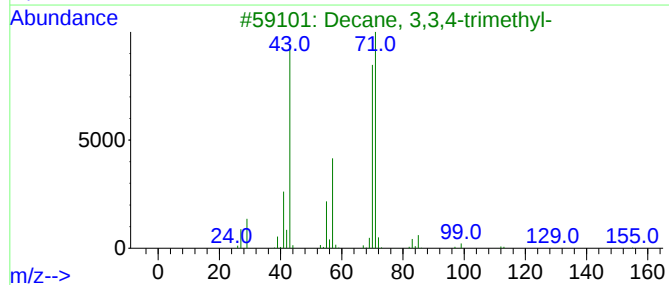
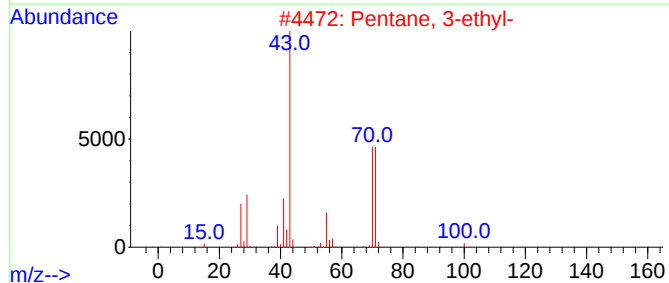
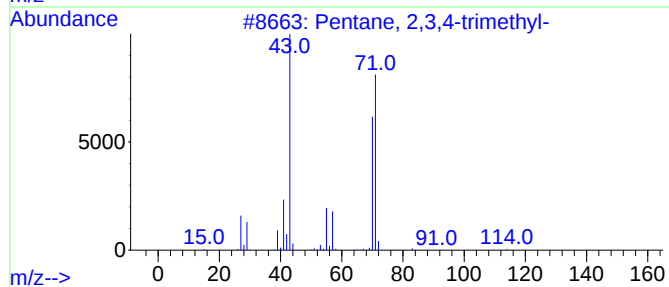
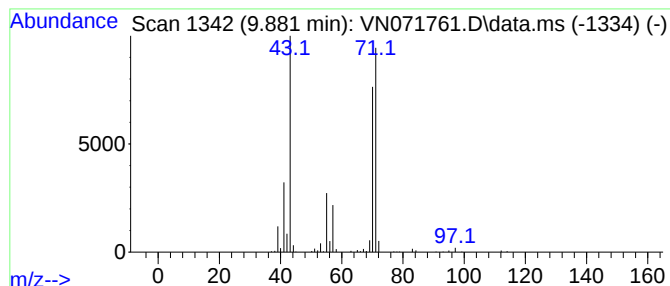
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.881	15.38 ug/l	736160	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	74
5			3,4-Diethyl hexane	142	C10H22	019398-77-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

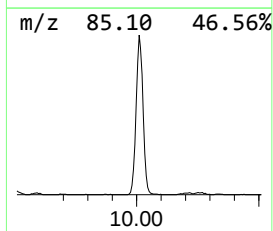
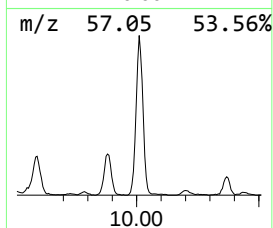
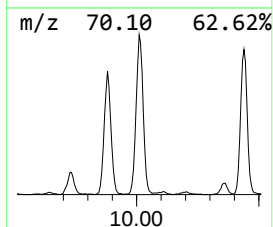
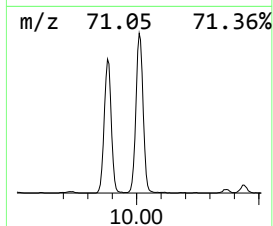
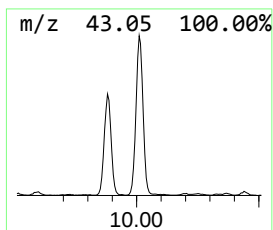
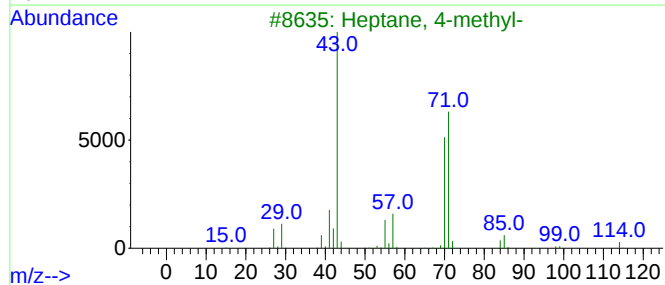
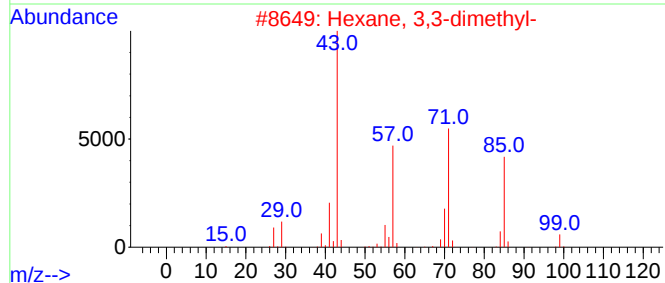
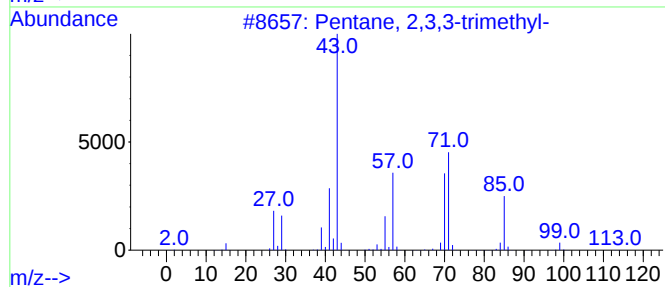
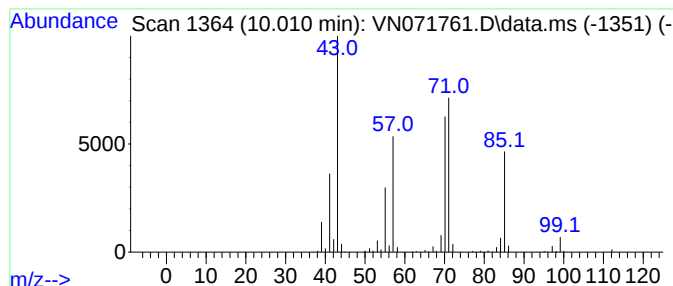
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	30.44 ug/l	1457260	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

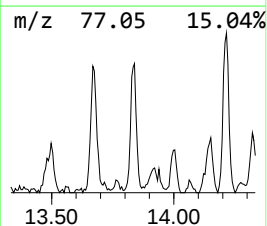
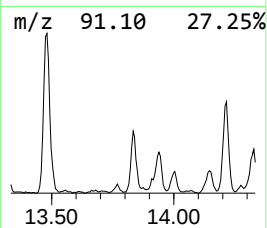
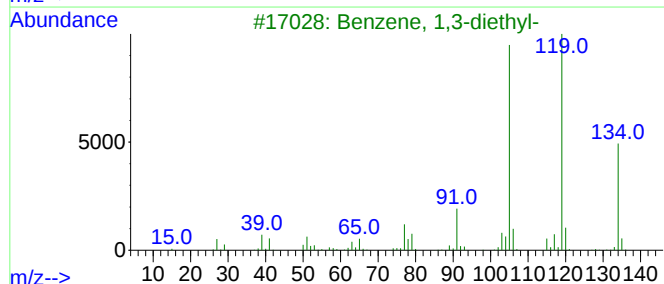
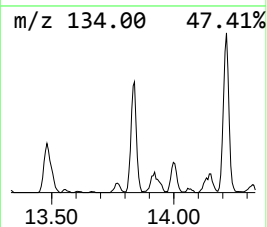
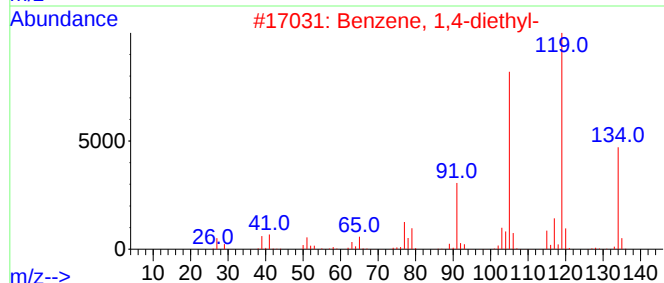
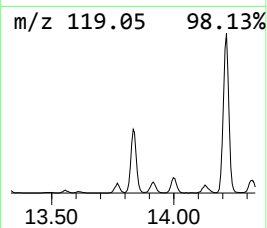
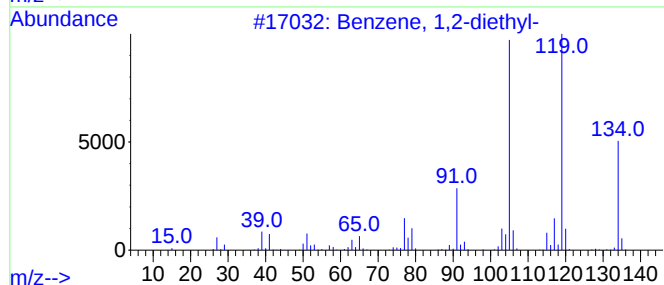
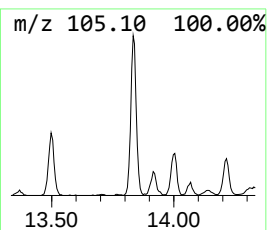
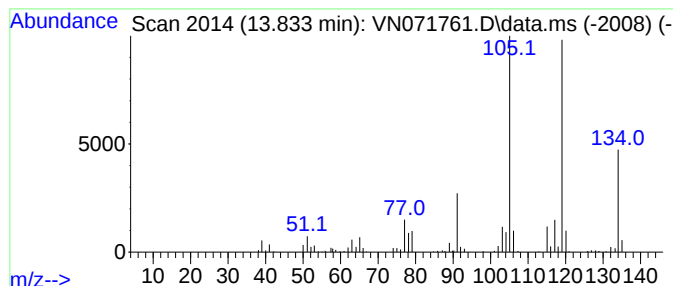
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	9.26 ug/l	426003	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

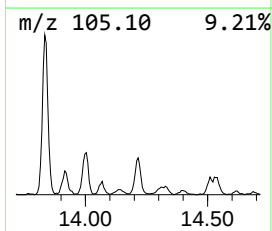
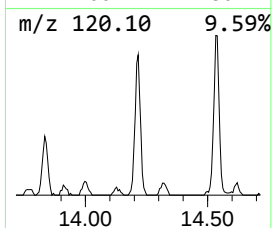
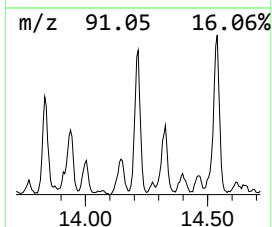
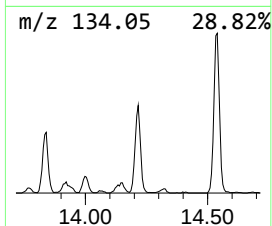
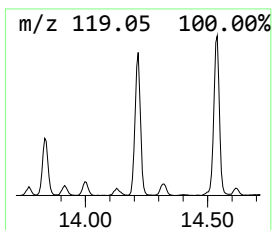
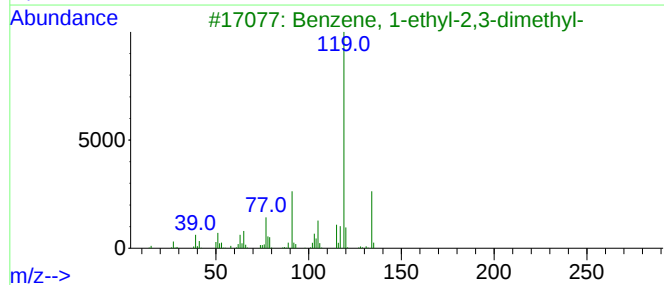
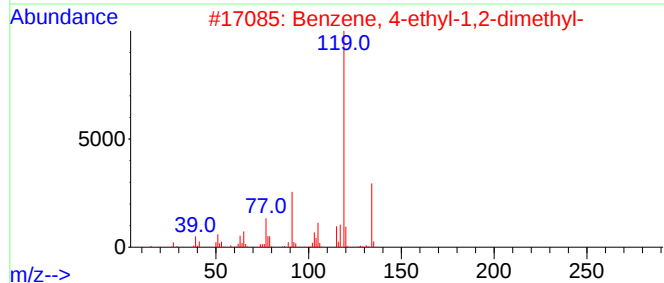
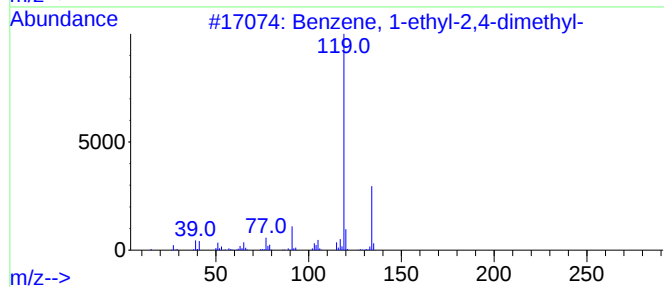
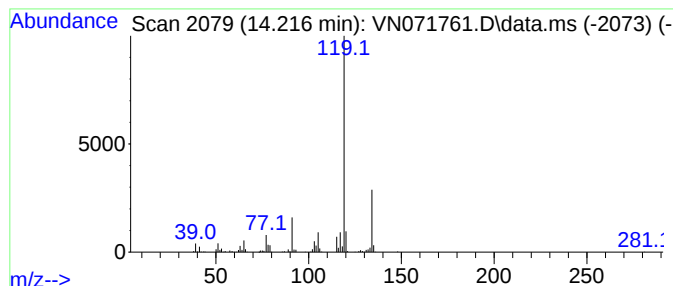
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	11.80 ug/l	542583	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

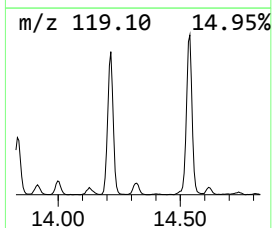
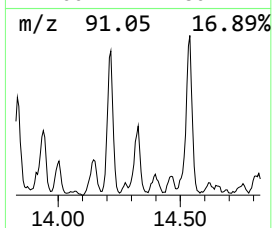
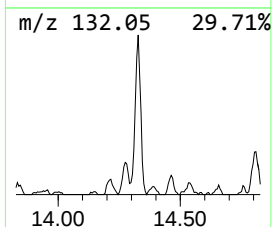
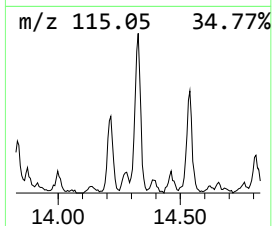
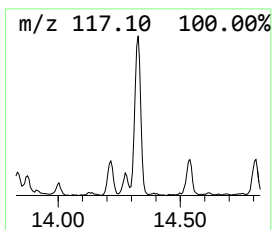
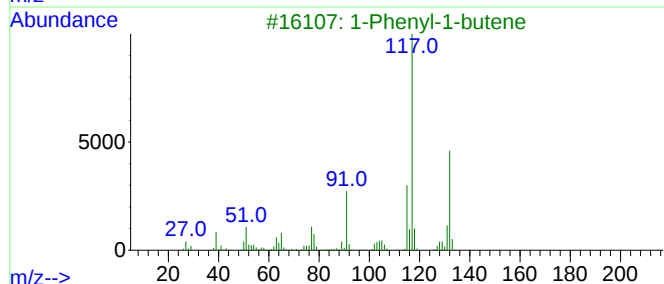
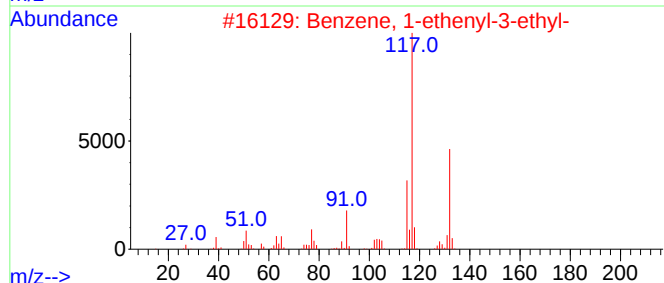
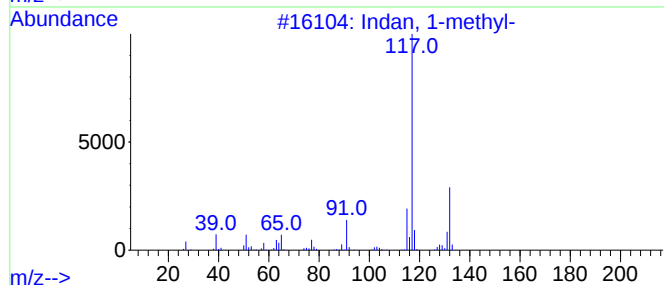
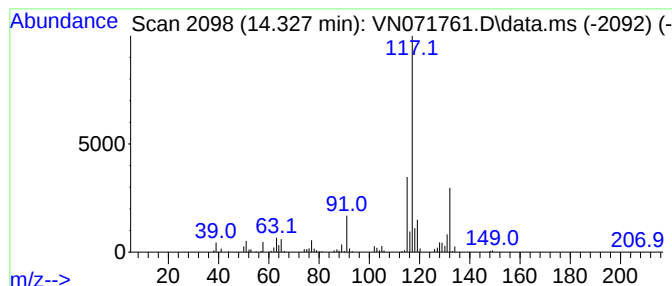
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Quant Title : SW846 8260

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

Peak Number 9 Indan, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	7.16 ug/l	329087	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	80
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	72
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

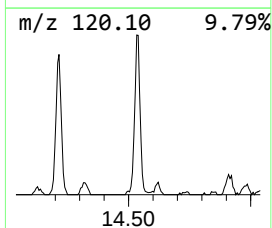
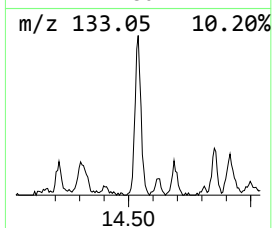
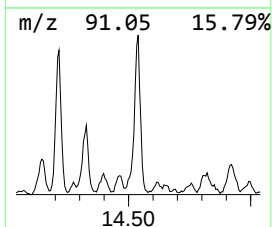
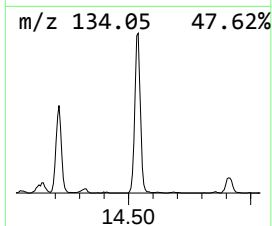
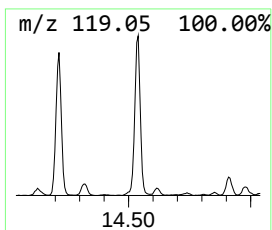
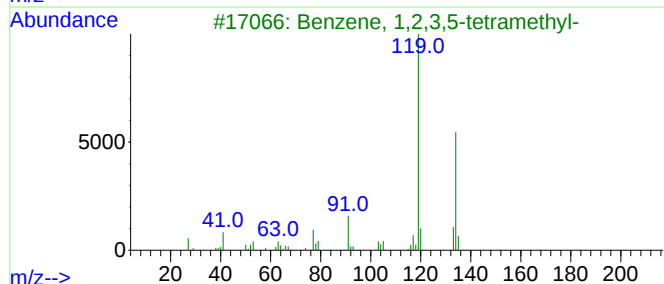
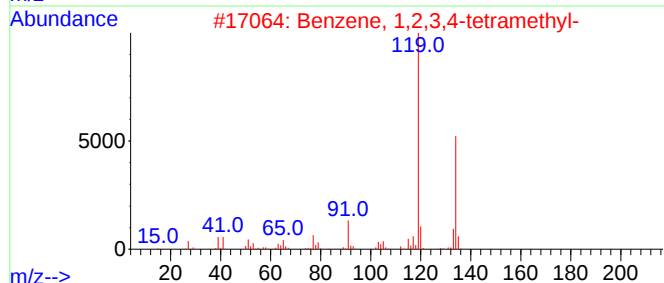
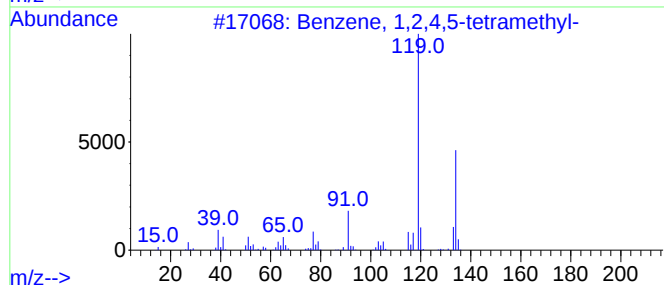
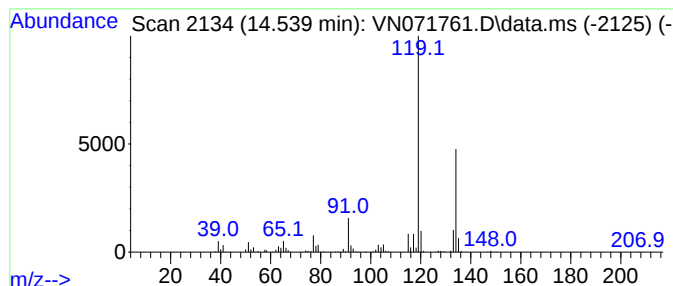
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	15.65 ug/l	719510	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071761.D
Acq On : 01 Apr 2022 18:32
Operator : JC\MD
Sample : N2090-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-55

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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, 2,3-dim...	5.075	10.4	ug/l	371507	1	8.081	1780410	50.0
Pentane, 2,3-di...	8.169	5.4	ug/l	192619	1	8.081	1780410	50.0
Butane, 2,2,3,3...	8.616	23.5	ug/l	1124750	2	8.969	2393740	50.0
Cyclopentane, 1...	9.422	5.3	ug/l	253318	2	8.969	2393740	50.0
Pentane, 2,3,4-...	9.881	15.4	ug/l	736160	2	8.969	2393740	50.0
Pentane, 2,3,3-...	10.010	30.4	ug/l	1457260	2	8.969	2393740	50.0
Benzene, 1,2-di...	13.833	9.3	ug/l	426003	4	13.674	2299050	50.0
Benzene, 1-ethy...	14.216	11.8	ug/l	542583	4	13.674	2299050	50.0
Indan, 1-methyl-	14.327	7.2	ug/l	329087	4	13.674	2299050	50.0
Benzene, 1,2,4,...	14.539	15.7	ug/l	719510	4	13.674	2299050	50.0