

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
 Data File : VN075243.D
 Acq On : 11 Nov 2022 13:17
 Operator : JC\MD
 Sample : N5487-01
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FMC-0612

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\82N102622W.M
 Title : SW846 8260

Signal : TIC: VN075243.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.453	397	408	430	rBV	572190	1851533	27.26%	10.301%
2	8.171	1026	1040	1042	rBV	93728	194201	2.86%	1.080%
3	8.218	1042	1048	1058	rVV2	338020	819218	12.06%	4.558%
4	8.324	1058	1066	1076	rVB2	59457	143850	2.12%	0.800%
5	8.441	1076	1086	1095	rBV	250717	564660	8.31%	3.141%
6	8.582	1101	1110	1120	rVB	95058	214223	3.15%	1.192%
7	8.700	1120	1130	1138	rBV5	28486	81080	1.19%	0.451%
8	8.965	1167	1175	1184	rVB	138560	280332	4.13%	1.560%
9	9.100	1189	1198	1208	rBV	239664	475558	7.00%	2.646%
10	9.600	1271	1283	1295	rBV2	49191	120516	1.77%	0.670%
11	10.565	1439	1447	1452	rBV	339520	642560	9.46%	3.575%
12	10.629	1452	1458	1472	rVV	3798209	6793231	100.00%	37.794%
13	10.747	1472	1478	1487	rVB2	42591	83697	1.23%	0.466%
14	11.647	1623	1631	1634	rBV3	41894	85114	1.25%	0.474%
15	11.865	1661	1668	1679	rVB	296834	543074	7.99%	3.021%
16	11.965	1679	1685	1690	rBV	68219	119393	1.76%	0.664%
17	12.070	1694	1703	1708	rBV	310755	571502	8.41%	3.180%
18	12.400	1747	1759	1766	rBV2	119313	326703	4.81%	1.818%
19	12.482	1766	1773	1778	rVB2	43808	83487	1.23%	0.464%
20	12.600	1785	1793	1794	rBV5	37973	85560	1.26%	0.476%
21	12.853	1830	1836	1845	rVB2	236509	439613	6.47%	2.446%
22	13.035	1860	1867	1872	rVB	84287	154963	2.28%	0.862%
23	13.100	1872	1878	1881	rBV	169891	289707	4.26%	1.612%
24	13.159	1881	1888	1897	rVV3	238387	623657	9.18%	3.470%
25	13.335	1909	1918	1924	rBV	74535	162519	2.39%	0.904%
26	13.394	1924	1928	1937	rVV5	38145	85995	1.27%	0.478%
27	13.482	1937	1943	1953	rVB	187741	309292	4.55%	1.721%
28	13.676	1970	1976	1981	rBV5	65443	131217	1.93%	0.730%
29	13.794	1990	1996	2005	rBV2	313497	602986	8.88%	3.355%
30	13.988	2024	2029	2033	rBV2	78205	139897	2.06%	0.778%
31	14.111	2045	2050	2056	rBV5	132752	258419	3.80%	1.438%
32	14.447	2101	2107	2111	rVB2	55707	95380	1.40%	0.531%
33	14.629	2133	2138	2141	rBV2	74930	112469	1.66%	0.626%
34	14.788	2160	2165	2171	rVB5	34686	70561	1.04%	0.393%
35	14.958	2185	2194	2202	rBV9	60645	165369	2.43%	0.920%
36	15.053	2202	2210	2216	rBV7	58861	156875	2.31%	0.873%

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FMC-0612

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\82N102622W.M
Title : SW846 8260

37	15.211	2228	2237	2244	rBV2	38892	95890	1.41%	0.533%
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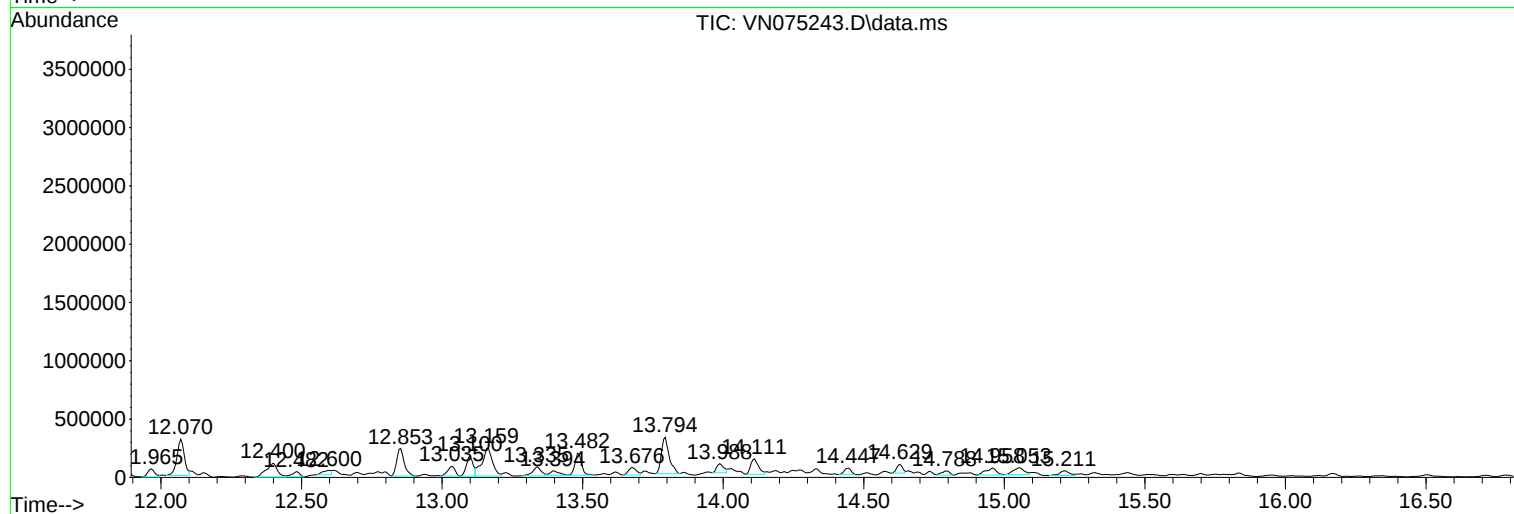
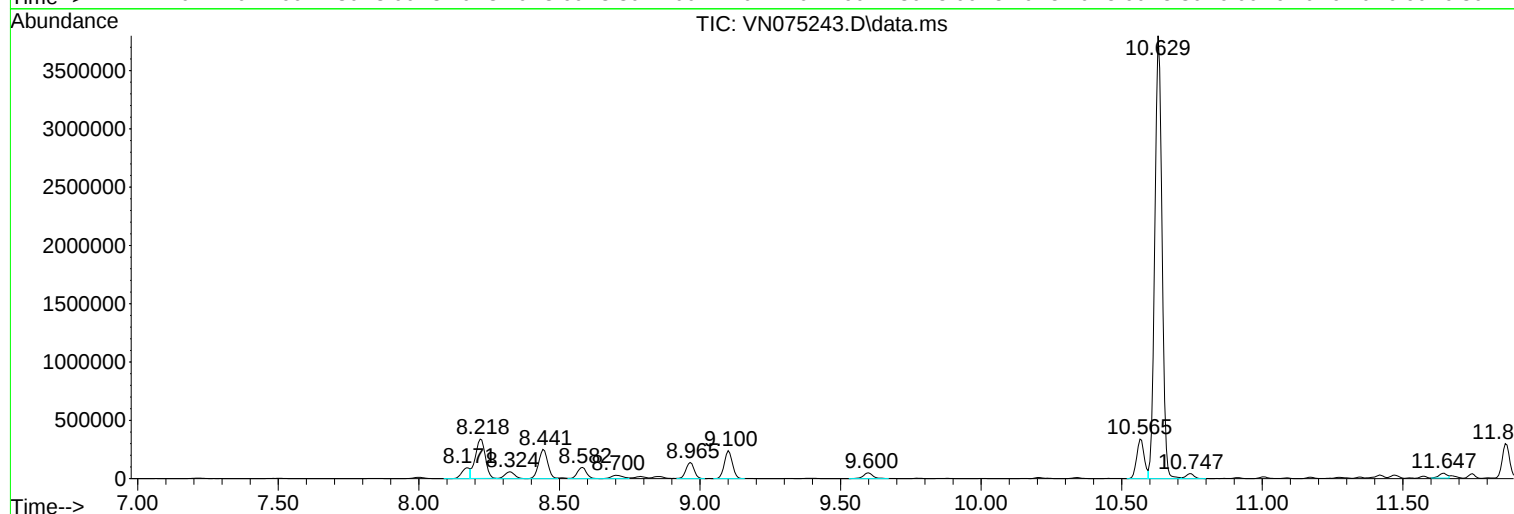
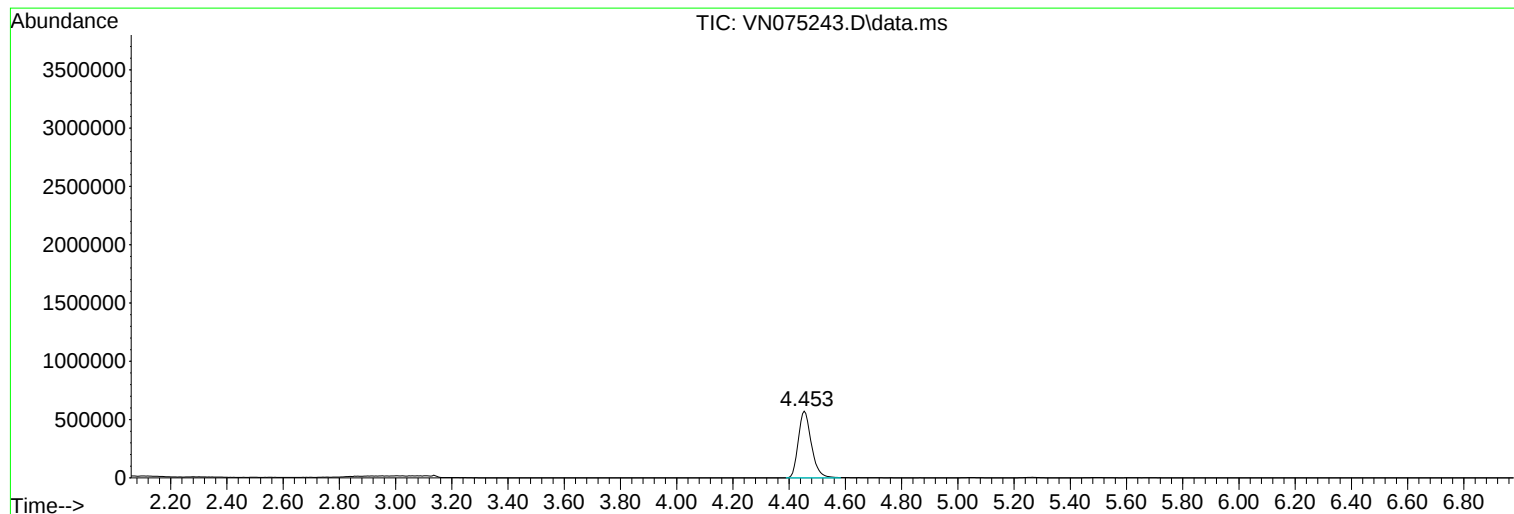
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

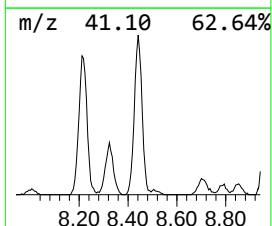
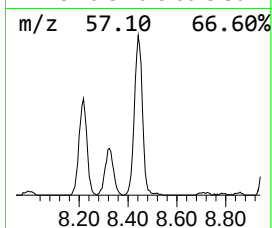
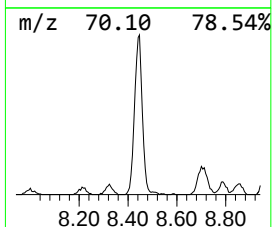
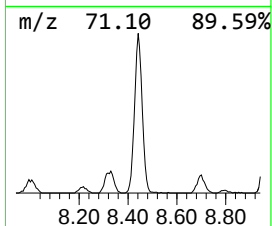
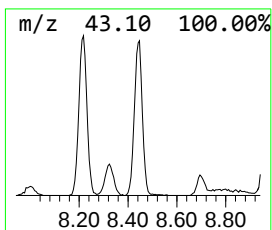
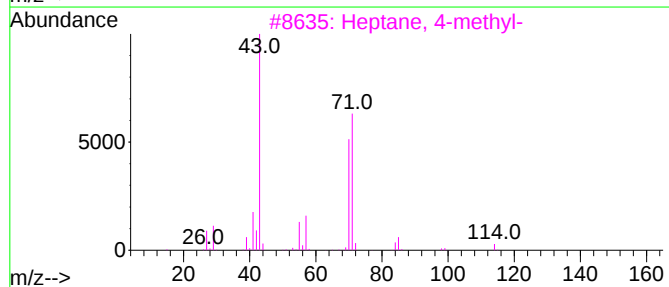
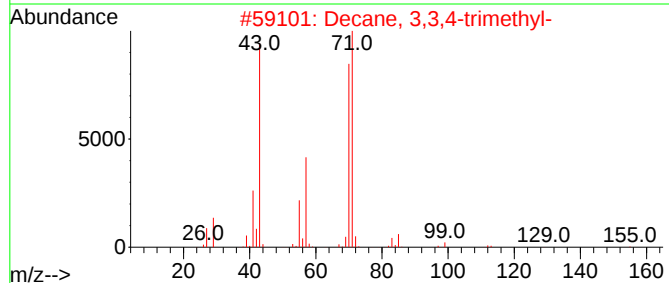
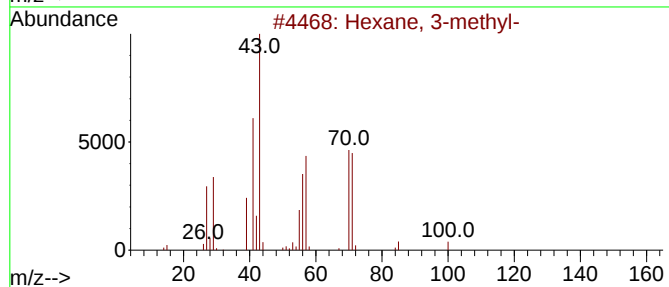
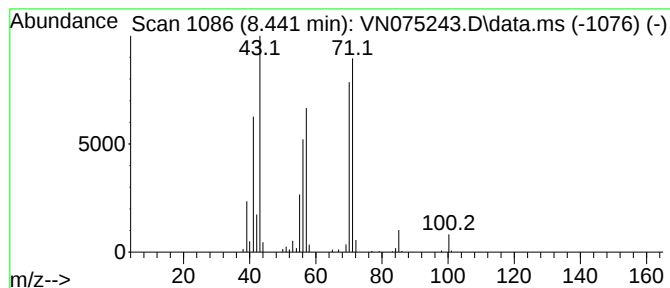
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	34.46 ug/l	564660	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59



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MSVOA_N
ClientSampleId :
FMC-0612

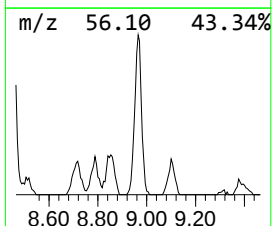
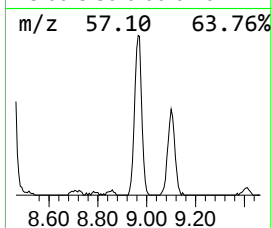
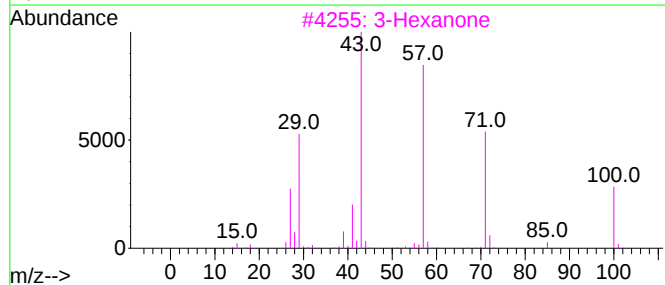
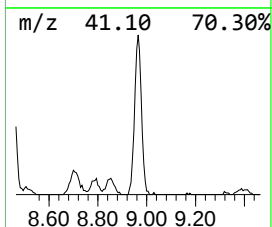
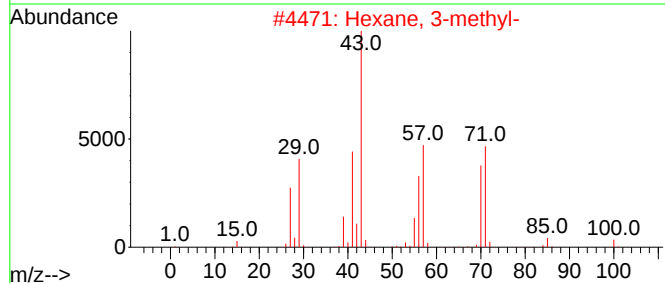
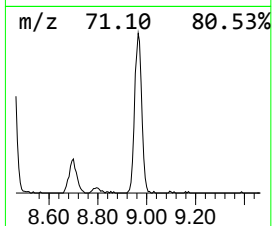
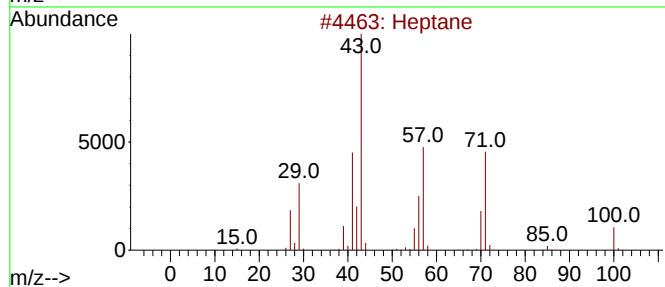
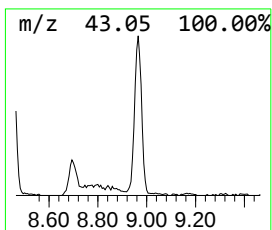
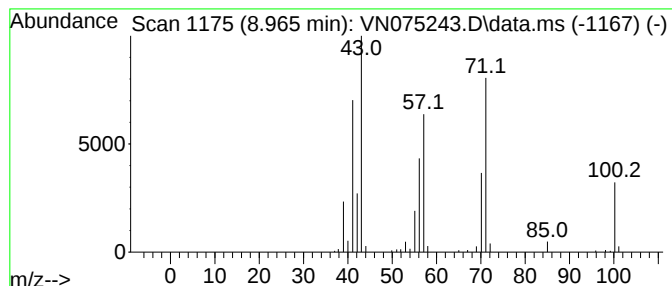
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	29.47 ug/l	280332	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	83
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3			3-Hexanone	100	C6H12O	000589-38-8	49
4			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	43
5			Oxirane, butyl-	100	C6H12O	001436-34-6	32



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

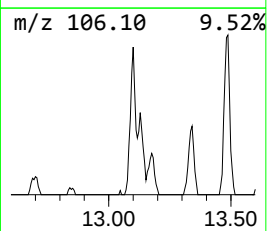
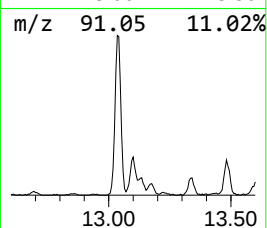
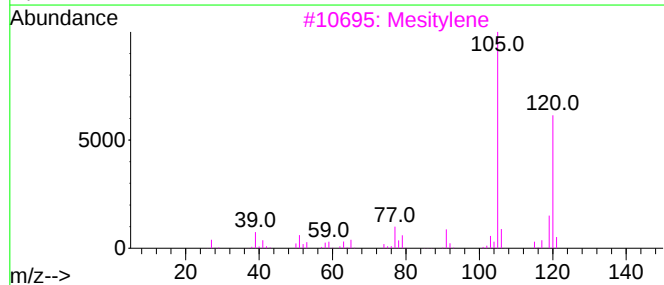
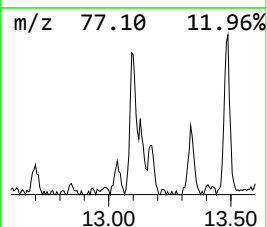
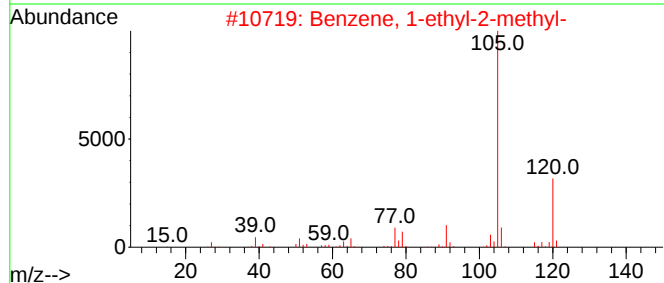
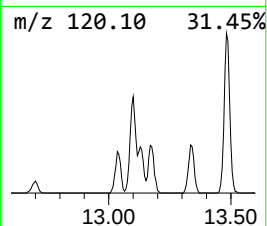
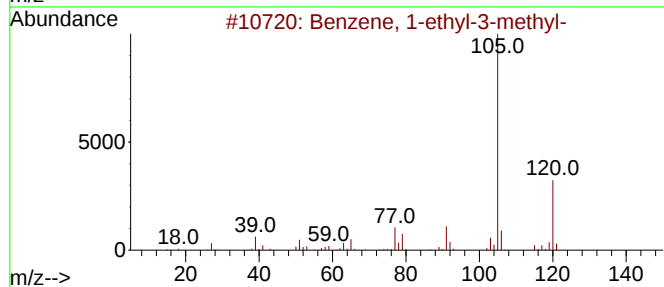
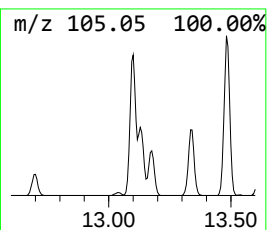
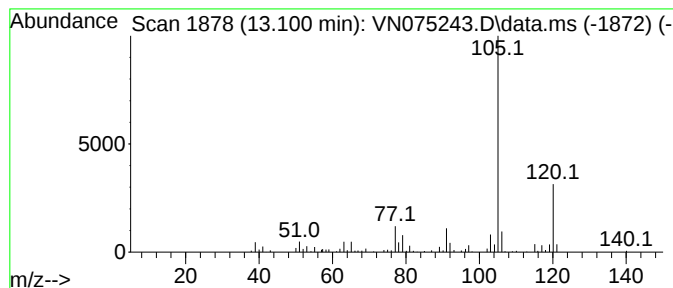
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	24.02 ug/l	289707	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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Instrument :
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ClientSampleId :
FMC-0612

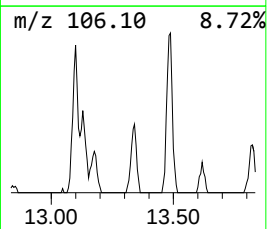
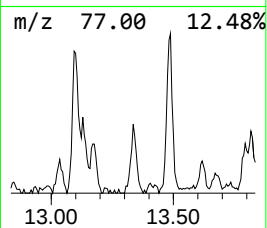
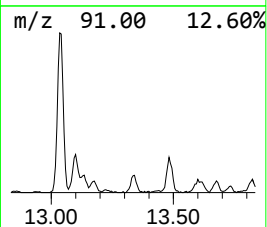
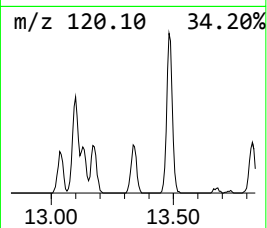
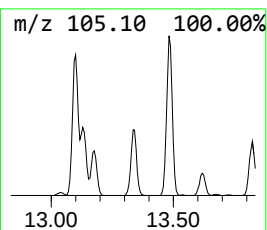
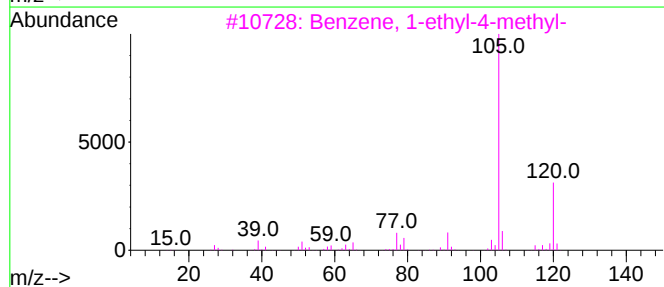
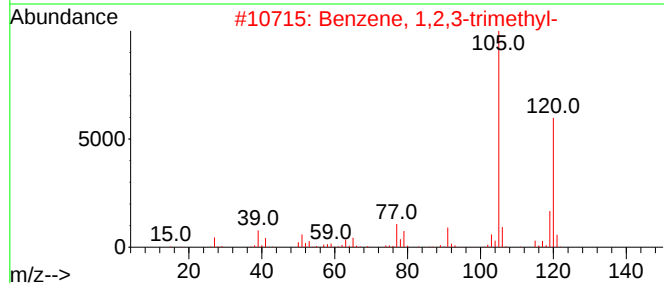
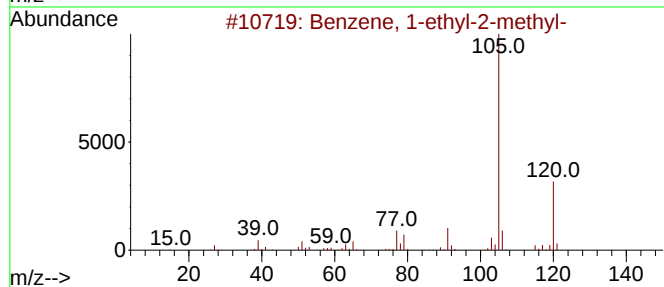
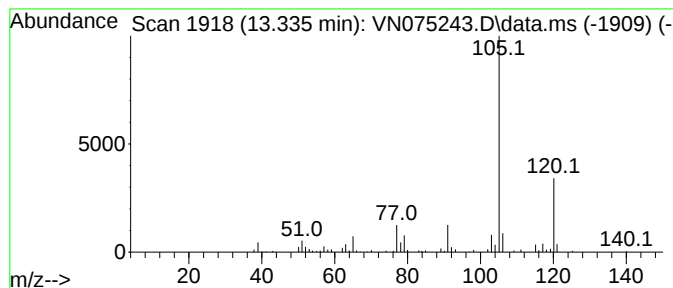
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	13.48 ug/l	162519	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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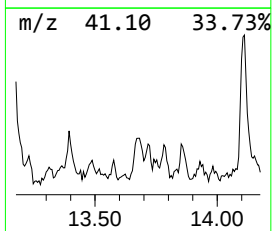
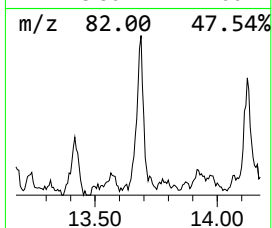
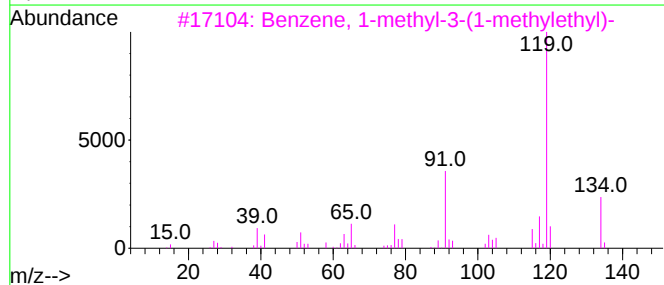
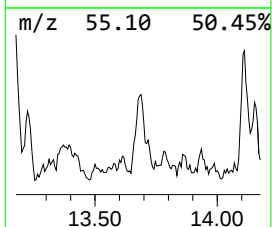
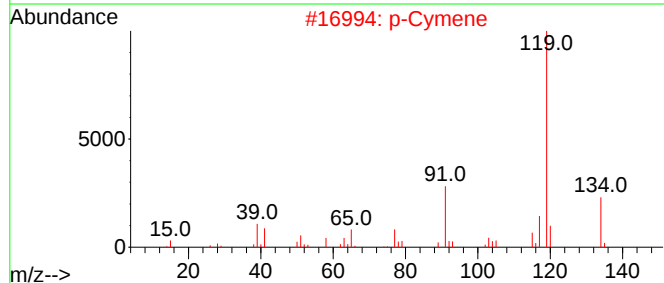
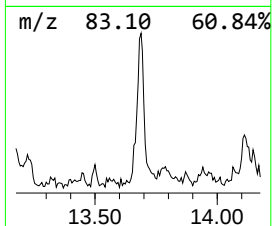
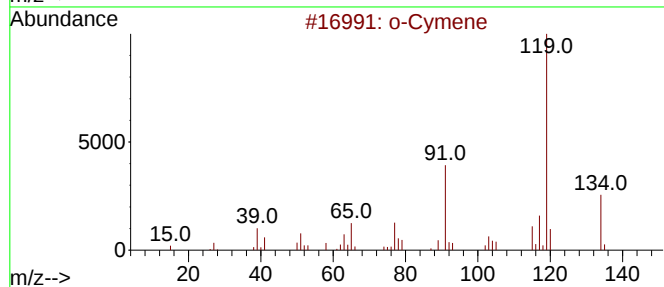
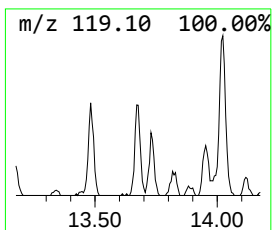
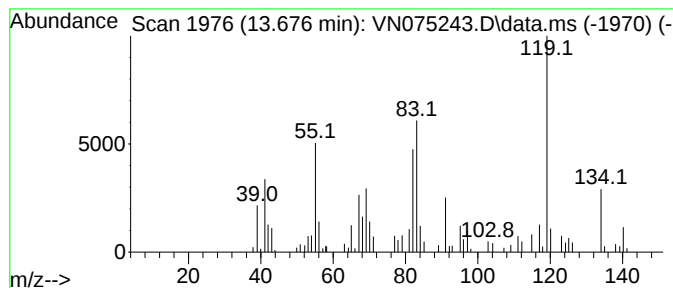
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	10.88 ug/l	131217	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	89
2			p-Cymene	134	C10H14	000099-87-6	86
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	50
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	50
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

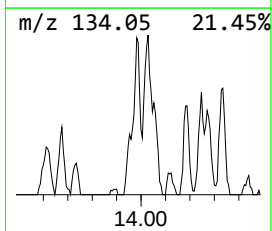
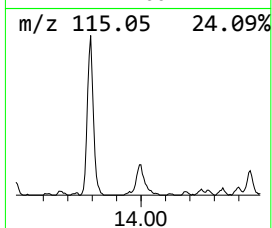
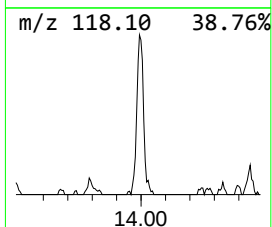
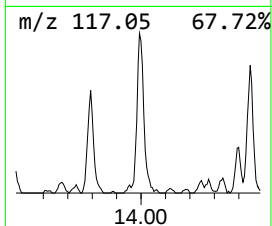
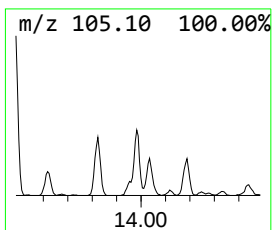
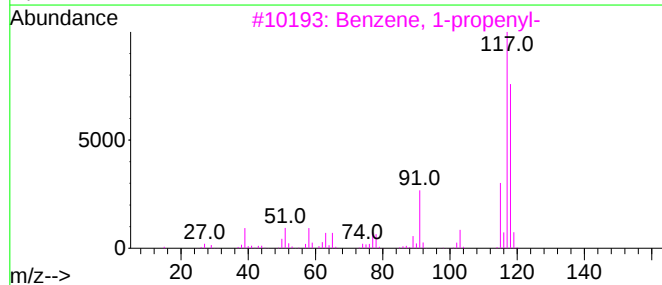
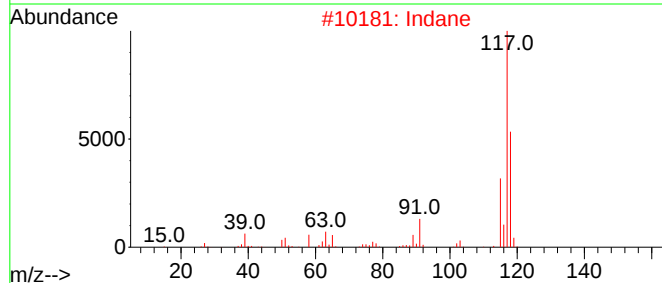
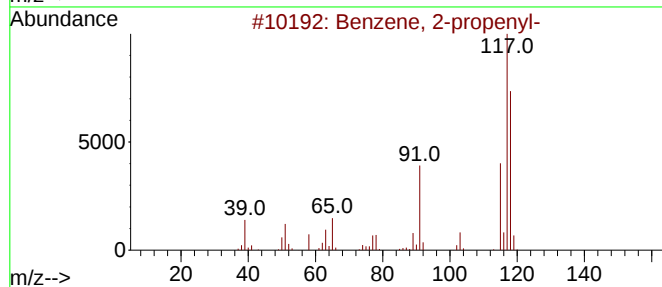
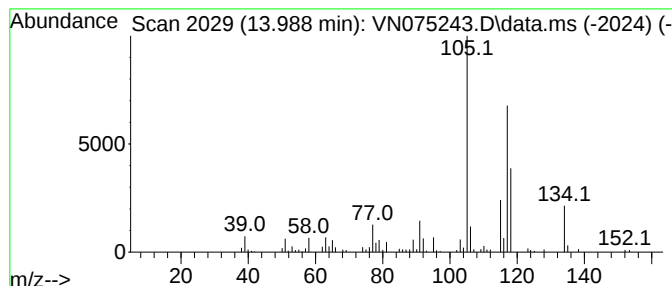
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	11.60 ug/l	139897	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
2			Indane	118	C9H10	000496-11-7	50
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	49
4			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	46
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

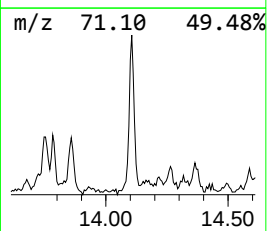
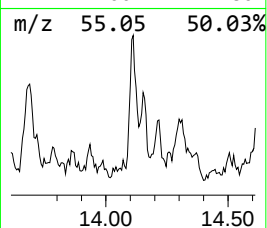
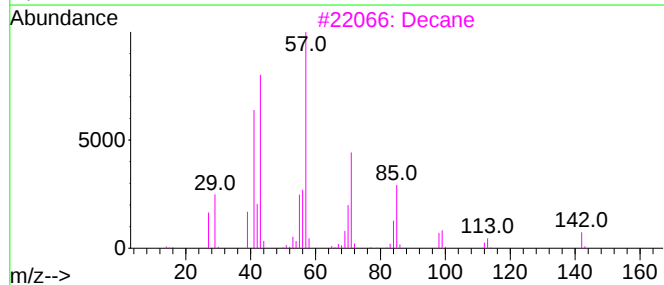
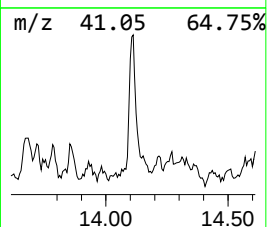
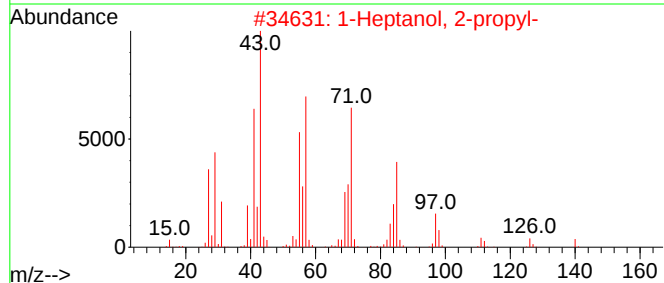
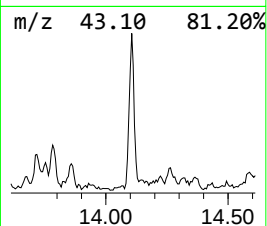
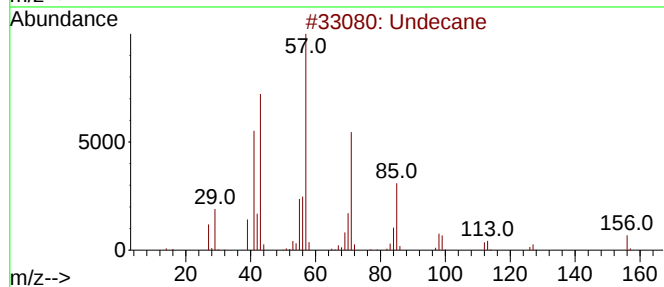
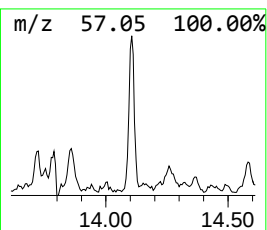
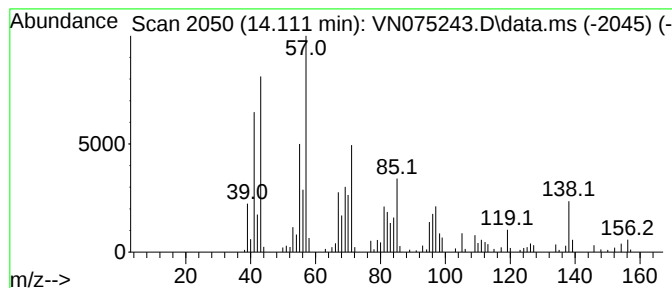
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Quant Title : SW846 8260

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

Peak Number 7 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	21.43 ug/l	258419	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	86
2	1-Heptanol, 2-propyl-			158	C10H22O	010042-59-8	47
3	Decane			142	C10H22	000124-18-5	43
4	Carbonic acid, decyl vinyl ester			228	C13H24O3	1000383-25-7	38
5	Decane, 2,3,8-trimethyl-			184	C13H28	062238-14-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

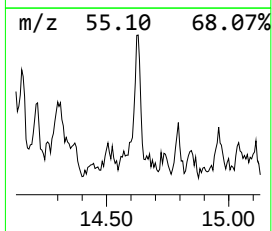
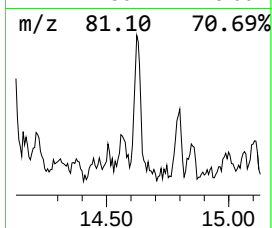
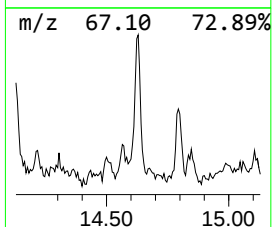
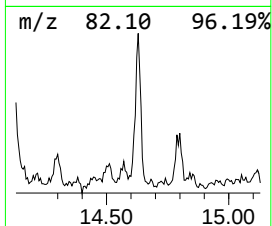
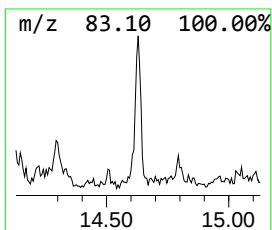
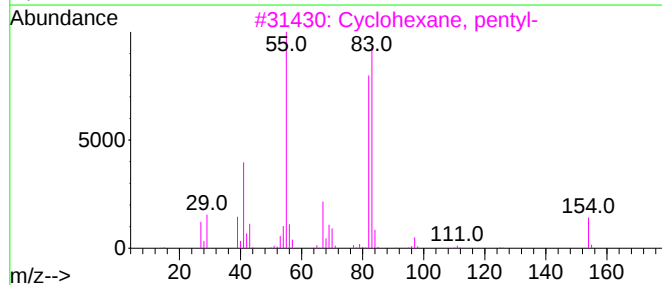
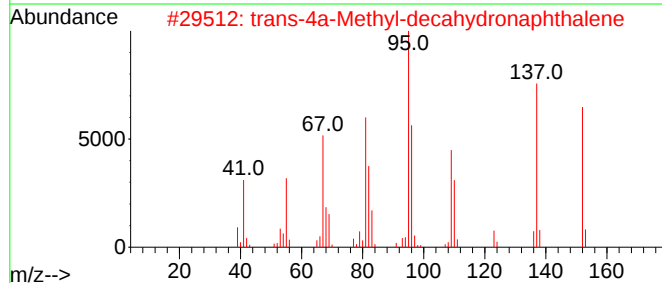
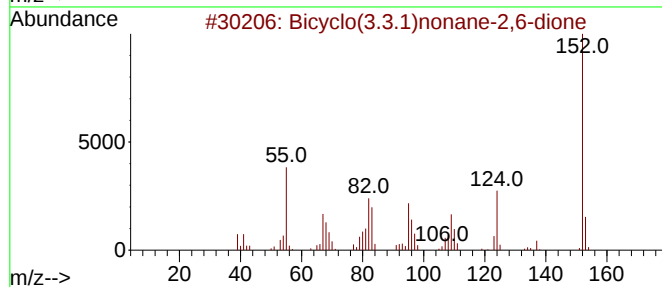
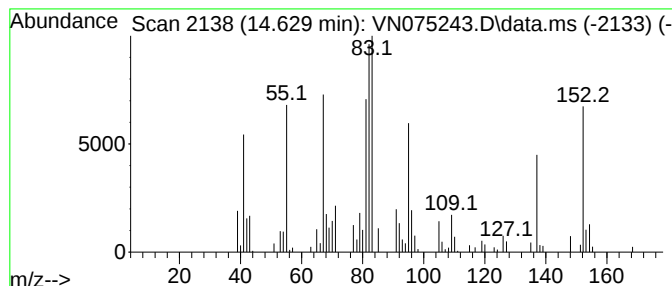
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Quant Title : SW846 8260

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

Peak Number 8 Bicyclo(3.3.1)nonane-2,6-dione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	9.33 ug/l	112469	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo(3.3.1)nonane-2,6-dione	152	C9H12O2	016473-11-3	58
2			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	43
3			Cyclohexane, pentyl-	154	C11H22	004292-92-6	43
4			3-Amino-4-acetyl-5-methylene-pyr...	152	C7H8N2O2	092220-23-0	35
5			3-Isopropylidene-5-methyl-hex-4-...	152	C10H16O	064149-32-2	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

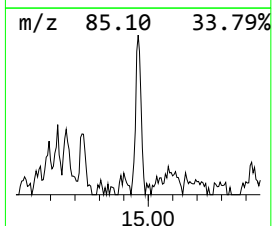
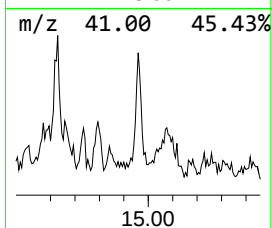
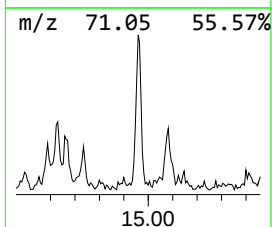
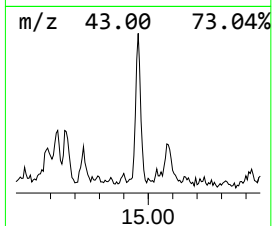
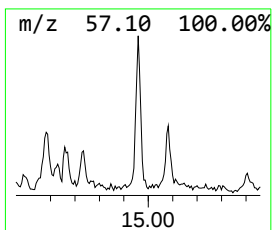
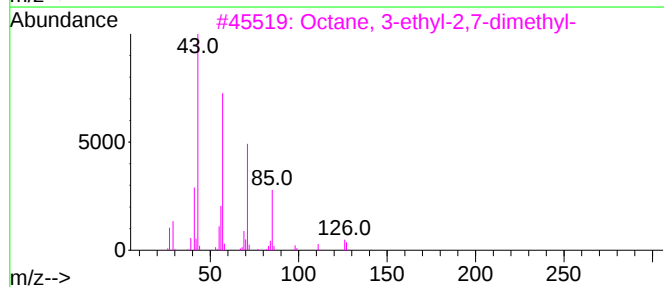
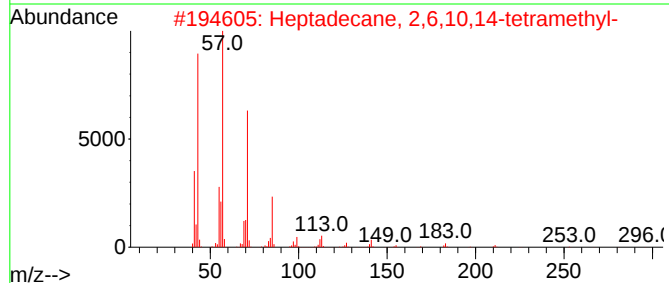
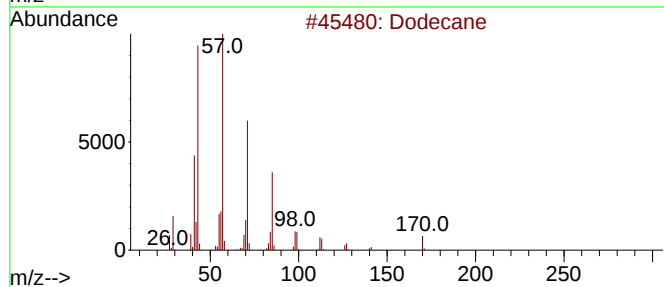
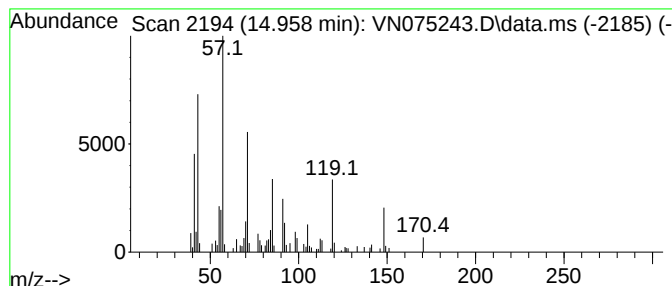
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	13.71 ug/l	165369	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	92
2			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	49
3			Octane, 3-ethyl-2,7-dimethyl-	170	C12H26	062183-55-5	47
4			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	47
5			Nonane	128	C9H20	000111-84-2	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

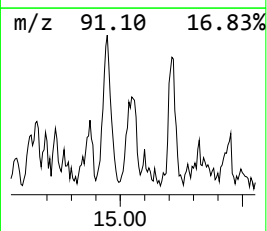
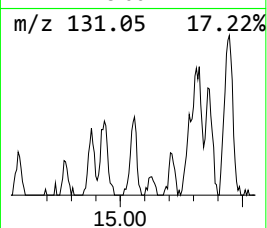
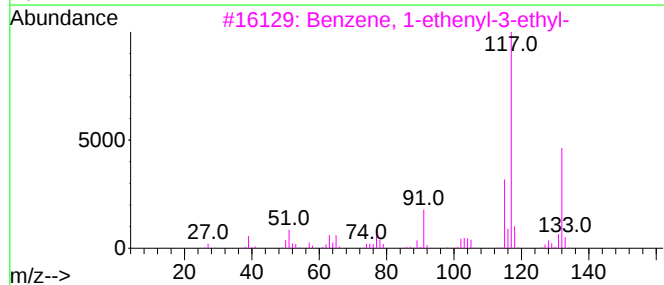
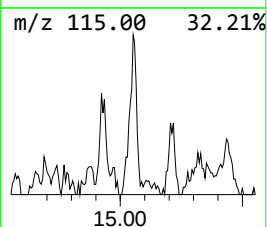
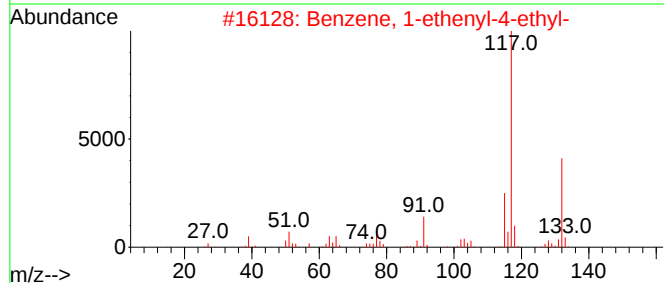
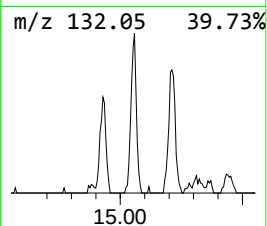
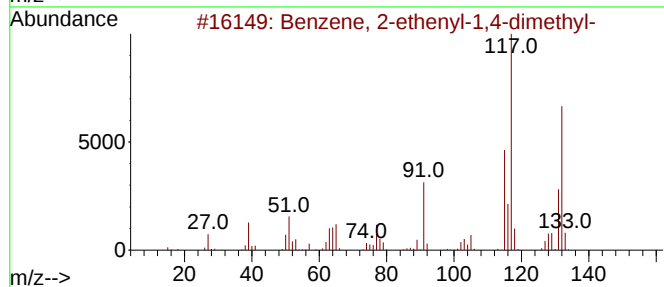
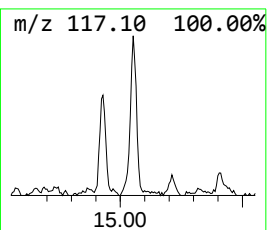
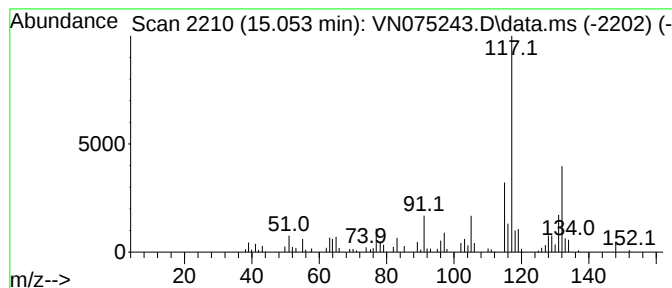
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	13.01 ug/l	156875	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111122\
Data File : VN075243.D
Acq On : 11 Nov 2022 13:17
Operator : JC\MD
Sample : N5487-01
Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FMC-0612

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.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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Heptane	8.965	29.5	ug/l	280332	2	9.100	475558	50.0
Benzene, 1-ethy...	13.100	24.0	ug/l	289707	4	13.794	602986	50.0
Benzene, 1-ethy...	13.335	13.5	ug/l	162519	4	13.794	602986	50.0
o-Cymene	13.676	10.9	ug/l	131217	4	13.794	602986	50.0
Benzene, 2-prop...	13.988	11.6	ug/l	139897	4	13.794	602986	50.0
Undecane	14.111	21.4	ug/l	258419	4	13.794	602986	50.0
Bicyclo(3.3.1)n...	14.629	9.3	ug/l	112469	4	13.794	602986	50.0
Dodecane	14.959	13.7	ug/l	165369	4	13.794	602986	50.0
Benzene, 2-ethe...	15.053	13.0	ug/l	156875	4	13.794	602986	50.0