

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081781.D
 Acq On : 18 Apr 2024 12:42
 Operator : JC\MD
 Sample : P2122-01
 Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 M-R-OILY-DEBRIS

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\82N041524W.M
 Title : SW846 8260

Signal : TIC: VN081781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.235	884	898	925	rBV	1021988	3709357	35.81%	6.168%
2	8.159	1044	1055	1060	rBV	157603	386198	3.73%	0.642%
3	8.218	1060	1065	1076	rVB	276832	617424	5.96%	1.027%
4	8.565	1112	1124	1135	rBV4	576235	1492417	14.41%	2.482%
5	9.100	1206	1215	1232	rVB	388492	822068	7.94%	1.367%
6	9.294	1237	1248	1275	rBV	5163899	10357929	100.00%	17.224%
7	9.665	1303	1311	1323	rVB2	155865	356582	3.44%	0.593%
8	10.565	1456	1464	1472	rBV	836287	1527566	14.75%	2.540%
9	10.965	1521	1532	1542	rBV	419030	798001	7.70%	1.327%
10	11.441	1605	1613	1620	rBV	320611	508137	4.91%	0.845%
11	11.870	1672	1686	1695	rBV3	684818	1687470	16.29%	2.806%
12	11.976	1696	1704	1710	rVV	2774823	4240756	40.94%	7.052%
13	12.041	1710	1715	1725	rVB2	101038	206798	2.00%	0.344%
14	12.412	1771	1778	1788	rBV	2196581	3258024	31.45%	5.418%
15	12.641	1811	1817	1823	rVB2	72988	118364	1.14%	0.197%
16	12.853	1846	1853	1862	rBV	470347	793653	7.66%	1.320%
17	13.006	1874	1879	1881	rVV	136334	221172	2.14%	0.368%
18	13.035	1881	1884	1890	rVV	219340	319662	3.09%	0.532%
19	13.117	1890	1898	1903	rVV2	138782	280454	2.71%	0.466%
20	13.341	1929	1936	1943	rBV	1257961	1929043	18.62%	3.208%
21	13.447	1946	1954	1958	rBV3	138788	308107	2.97%	0.512%
22	13.547	1963	1971	1980	rVB	371970	652557	6.30%	1.085%
23	13.688	1989	1995	2005	rBV	324080	609198	5.88%	1.013%
24	13.794	2007	2013	2021	rVB	598295	1033329	9.98%	1.718%
25	13.876	2021	2027	2035	rBV3	291995	586934	5.67%	0.976%
26	13.959	2037	2041	2049	rVV5	54953	108383	1.05%	0.180%
27	14.106	2061	2066	2073	rBV2	166131	294635	2.84%	0.490%
28	14.253	2083	2091	2099	rVV7	129660	278654	2.69%	0.463%
29	14.488	2127	2131	2139	rBV7	56621	123155	1.19%	0.205%
30	14.623	2141	2154	2158	rBV7	232661	613674	5.92%	1.020%
31	14.658	2158	2160	2164	rVB2	91552	107259	1.04%	0.178%
32	14.735	2169	2173	2176	rVV4	88729	127618	1.23%	0.212%
33	14.800	2176	2184	2189	rVV6	94983	248979	2.40%	0.414%
34	14.958	2202	2211	2217	rBV2	553342	1006485	9.72%	1.674%
35	15.047	2220	2226	2230	rVV3	594608	1188853	11.48%	1.977%
36	15.088	2230	2233	2243	rVB4	447494	899833	8.69%	1.496%

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37	15.347	2268	2277	2281	rBV3	901686	1803098	17.41%	2.998%
38	15.400	2281	2286	2288	rVV	711207	1252084	12.09%	2.082%
39	15.441	2288	2293	2300	rVV	2314008	3998571	38.60%	6.649%
40	15.511	2300	2305	2313	rVB2	270087	637661	6.16%	1.060%
41	15.588	2313	2318	2326	rBV3	409601	885388	8.55%	1.472%
42	15.664	2327	2331	2335	rBV5	176952	293234	2.83%	0.488%
43	15.829	2354	2359	2365	rVB	1183591	1949112	18.82%	3.241%
44	15.941	2372	2378	2385	rBV7	290934	718476	6.94%	1.195%
45	16.117	2404	2408	2412	rBV5	157096	282803	2.73%	0.470%
46	16.170	2412	2417	2424	rVB4	358038	661659	6.39%	1.100%
47	16.247	2426	2430	2433	rBV3	177402	305307	2.95%	0.508%
48	16.311	2433	2441	2452	rVB2	1475333	3671785	35.45%	6.106%
49	16.405	2454	2457	2462	rVB2	155174	224013	2.16%	0.372%
50	16.464	2462	2467	2469	rBV2	241188	459677	4.44%	0.764%
51	16.547	2478	2481	2487	rVB5	264836	450874	4.35%	0.750%
52	16.611	2488	2492	2497	rBV	277193	470982	4.55%	0.783%
53	16.717	2505	2510	2512	rBV4	128773	254294	2.46%	0.423%

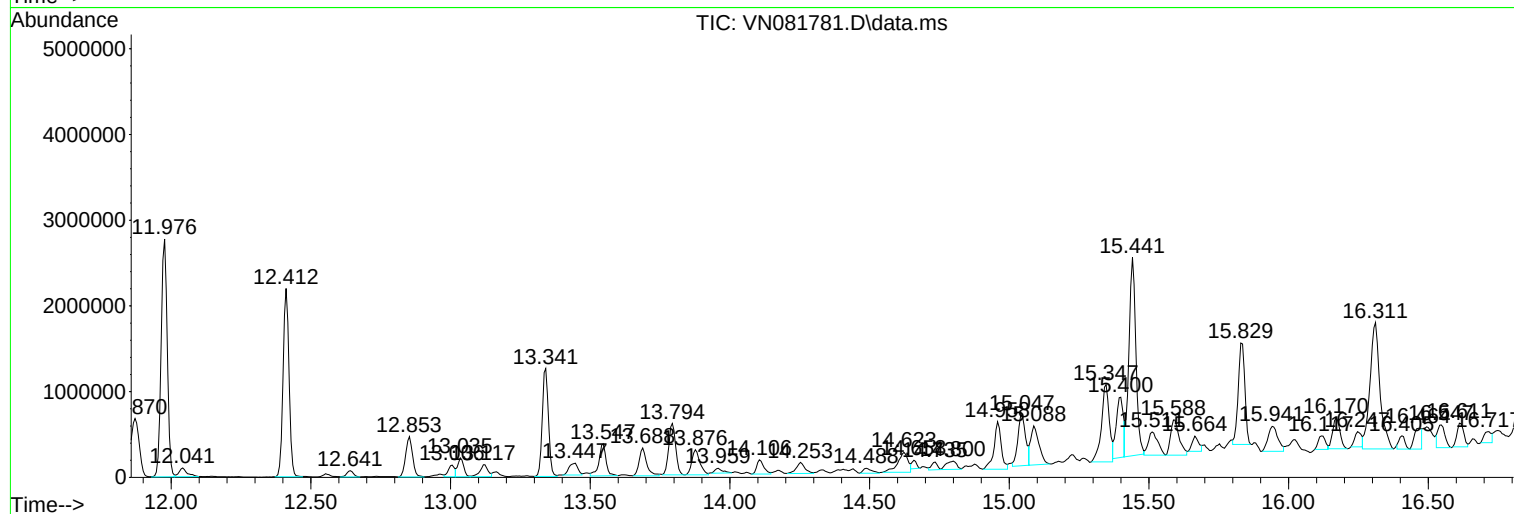
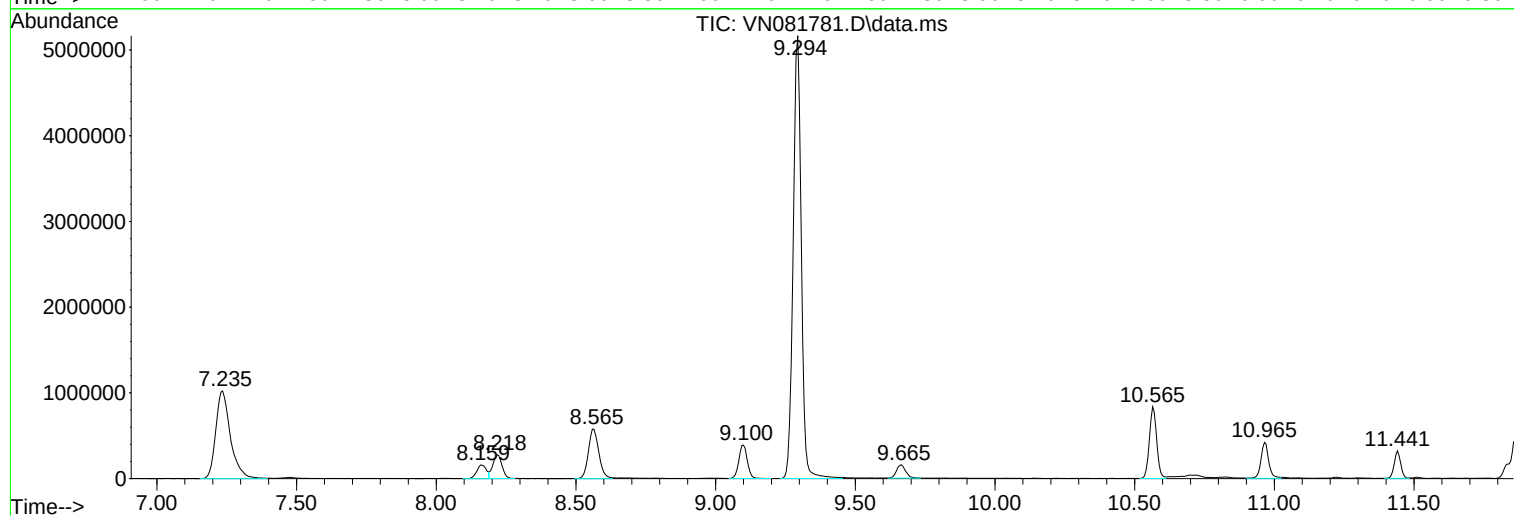
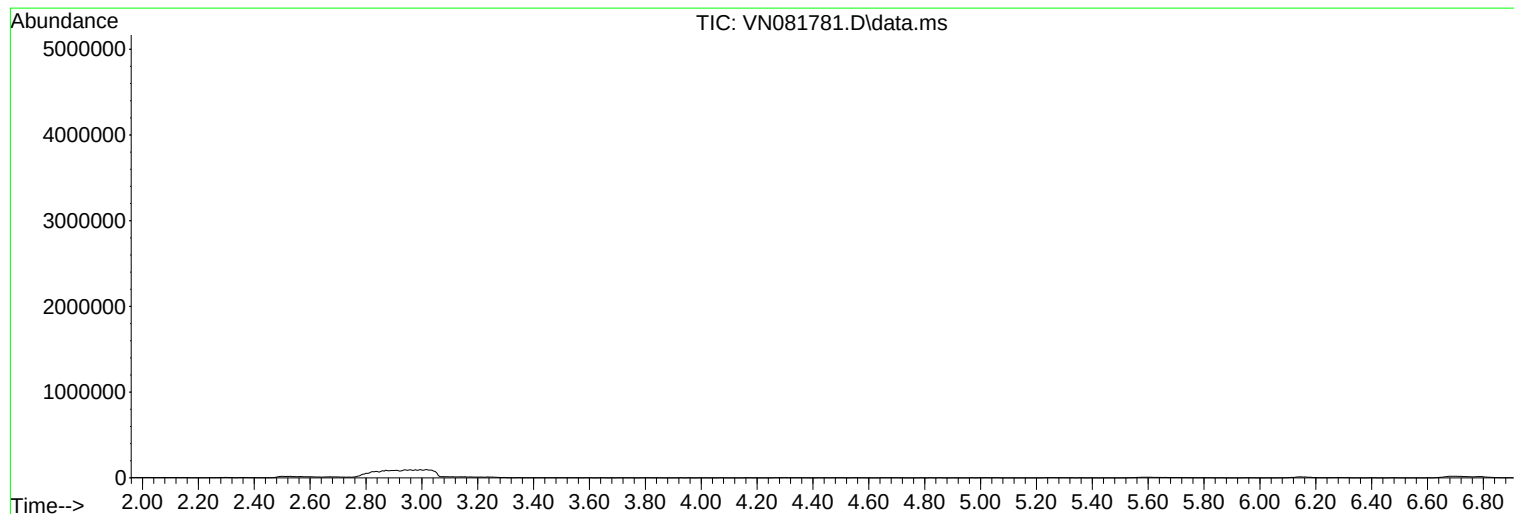
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Quant Title : SW846 8260

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



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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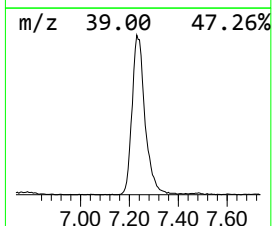
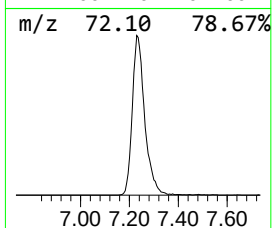
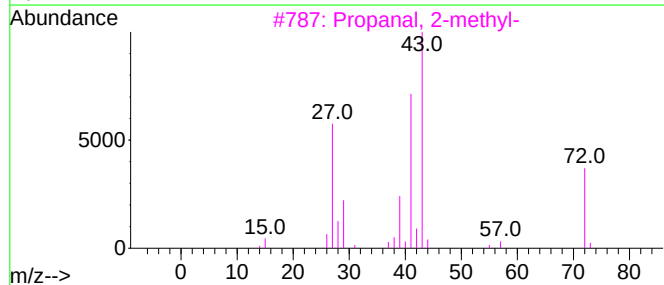
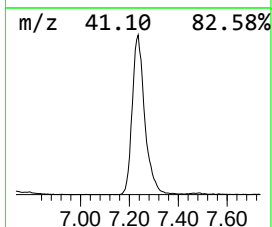
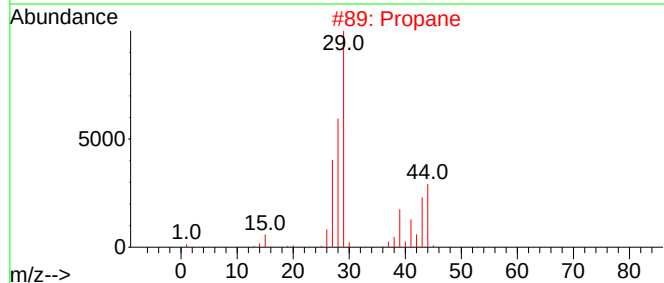
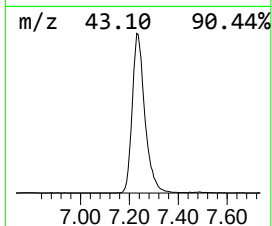
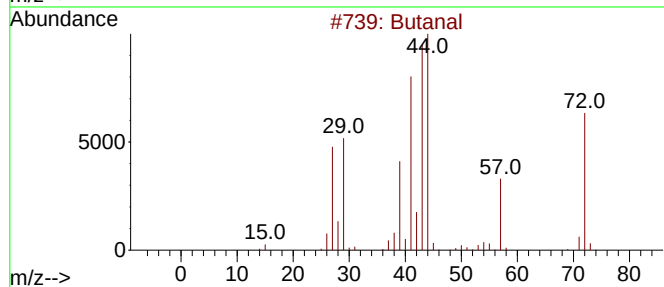
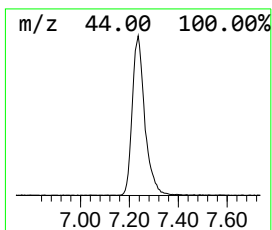
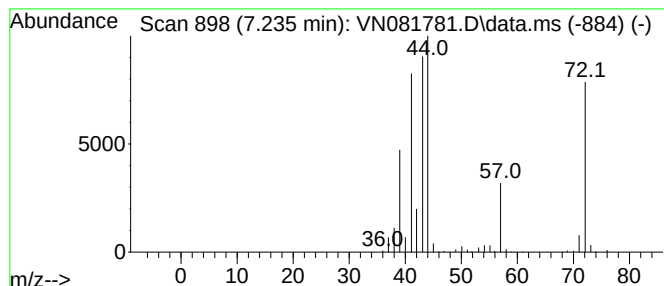
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Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.235	300.39 ug/l	3709360	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propane	44	C3H8	000074-98-6	50
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4		Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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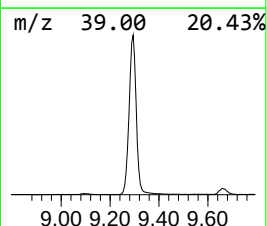
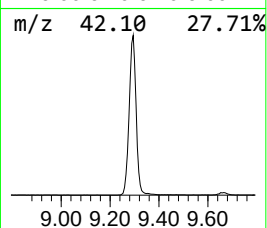
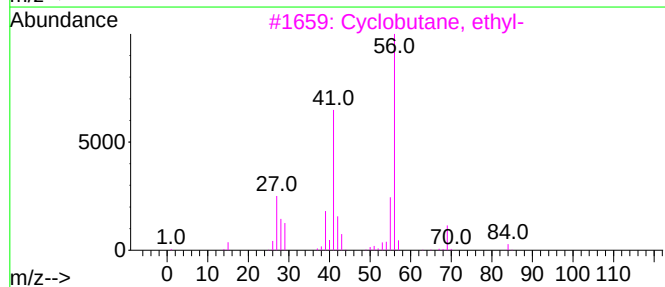
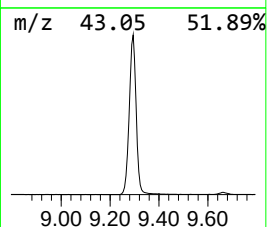
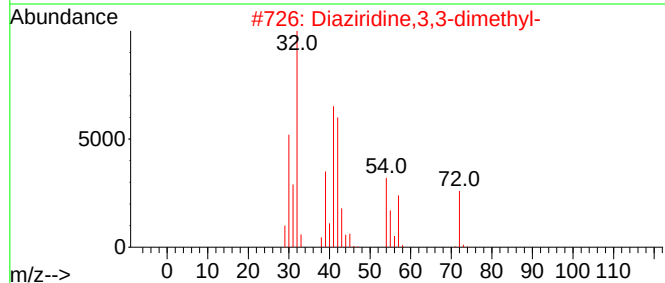
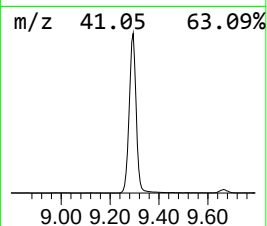
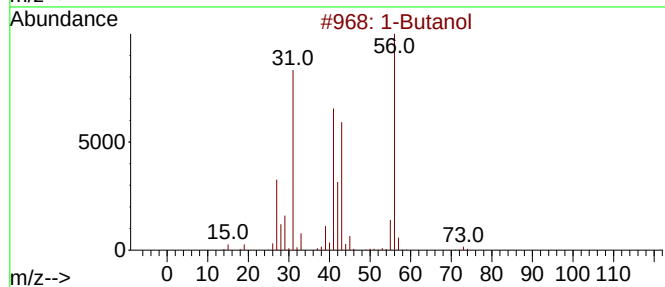
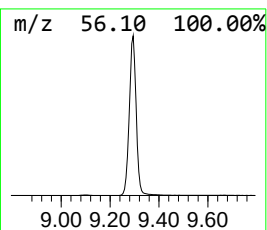
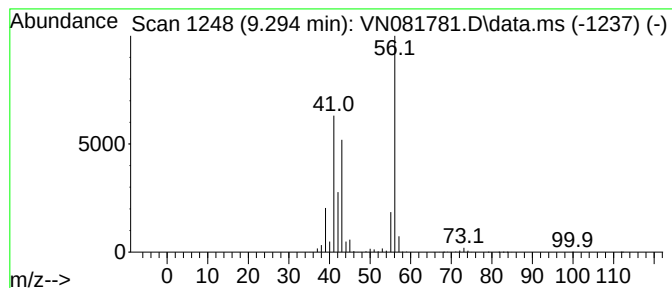
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.294	629.99 ug/l	10357900	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
4			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9



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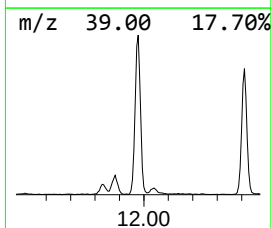
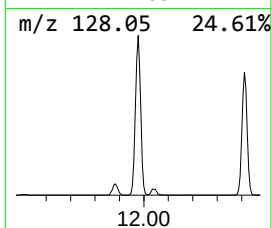
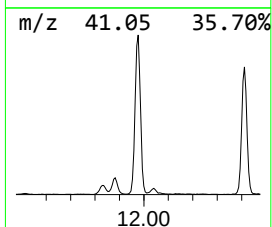
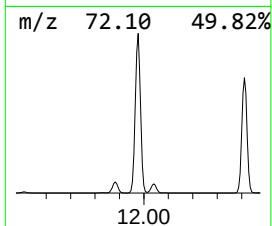
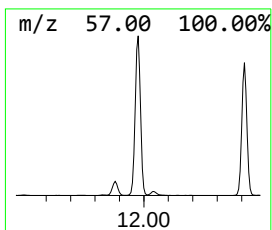
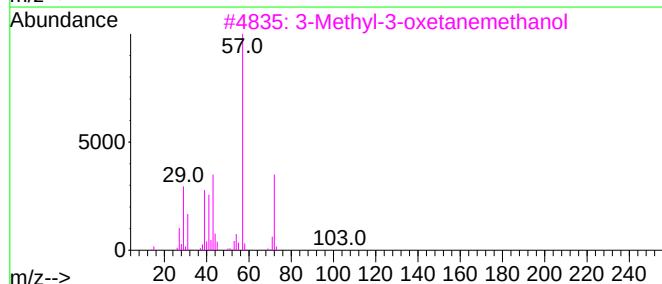
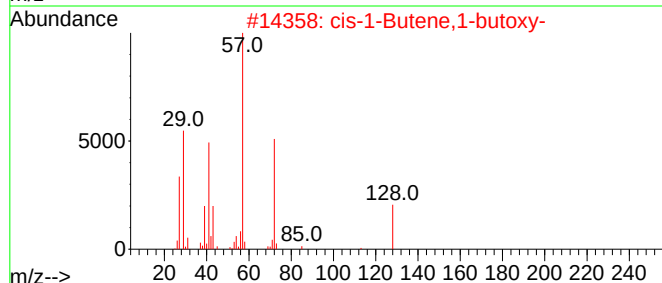
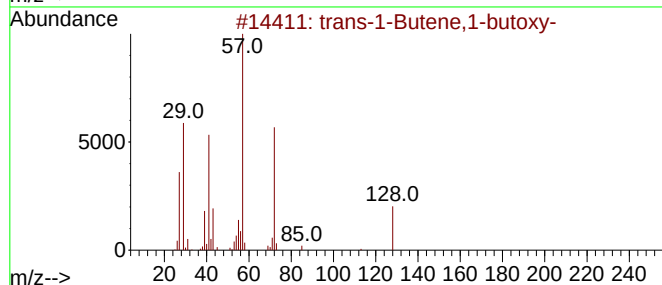
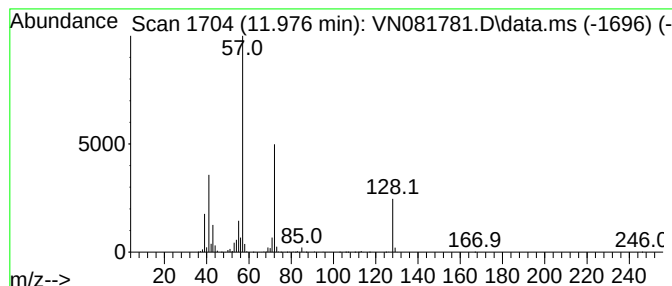
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 trans-1-Butene,1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.976	125.65 ug/l	4240760	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	86
2			cis-1-Butene,1-butoxy-	128	C8H16O	1000139-52-7	83
3			3-Methyl-3-oxetanemethanol	102	C5H10O2	003143-02-0	53
4			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	47
5			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	42



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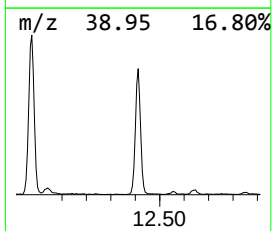
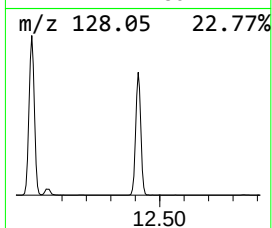
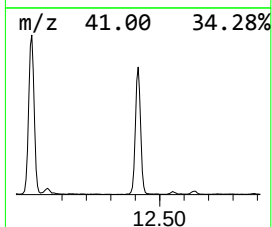
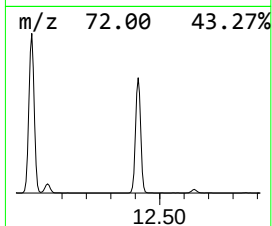
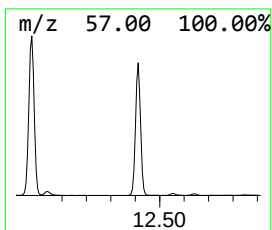
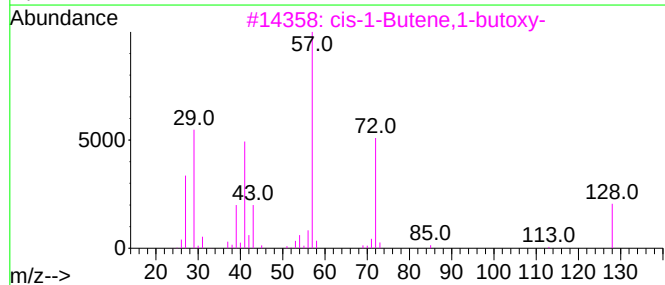
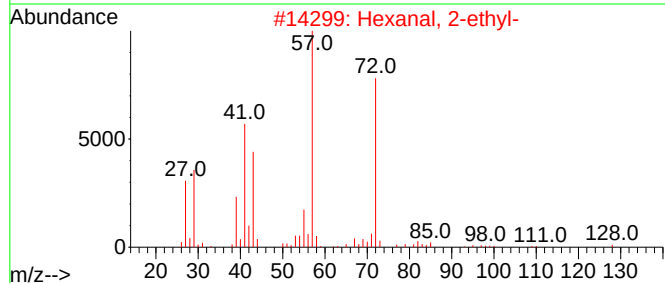
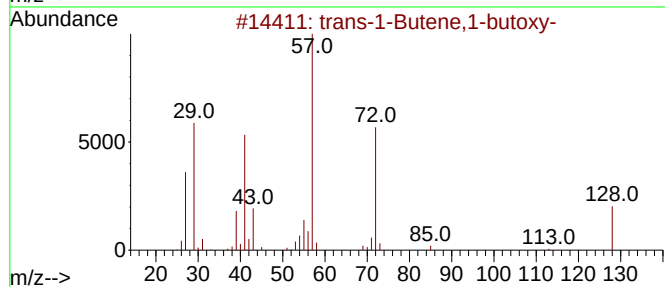
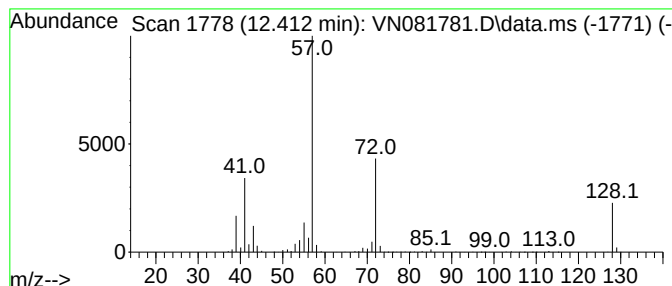
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 4 Hexanal, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.412	96.54 ug/l	3258020	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	64
2			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	59
3			cis-1-Butene,1-butoxy-	128	C8H16O	1000139-52-7	50
4			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	47
5			Hydrazine, 2-propenyl-	72	C3H8N2	007422-78-8	38



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M-R-OILY-DEBRIS

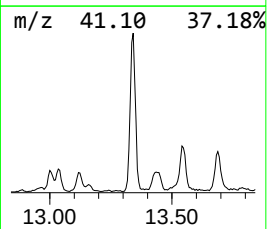
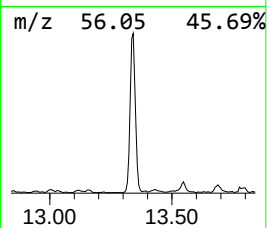
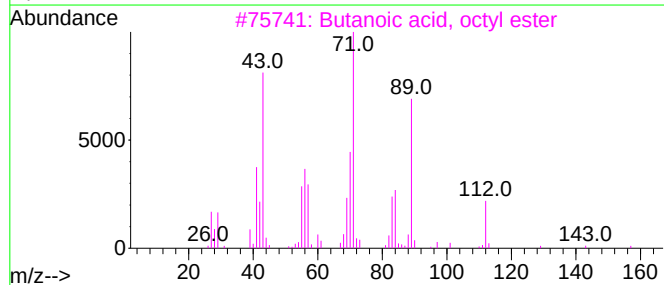
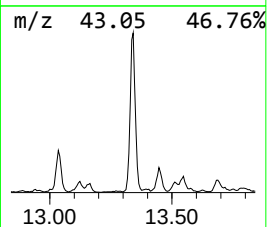
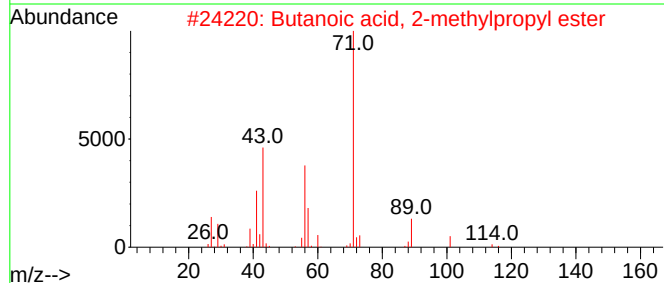
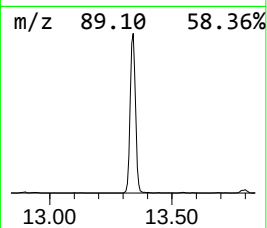
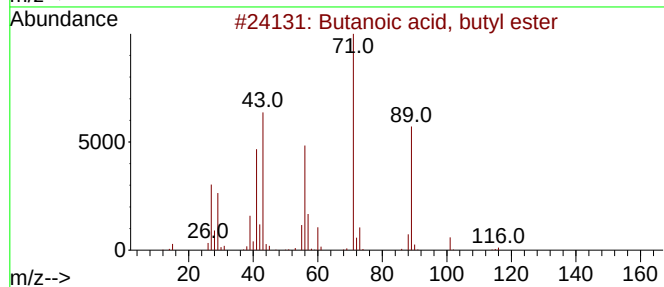
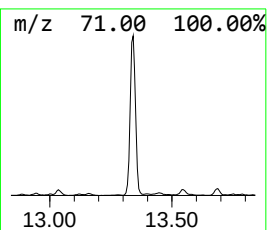
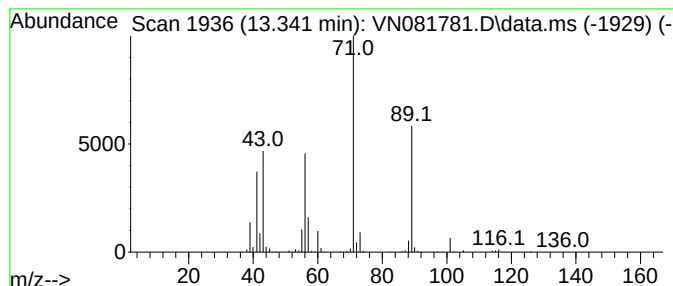
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Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	93.34 ug/l	1929040	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	64
4			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

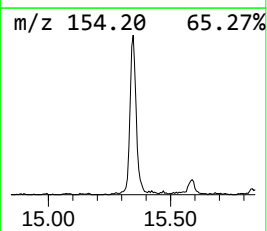
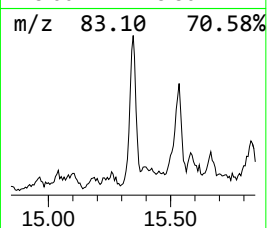
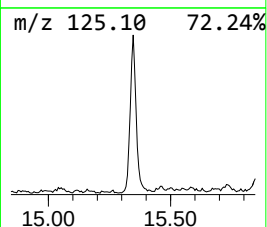
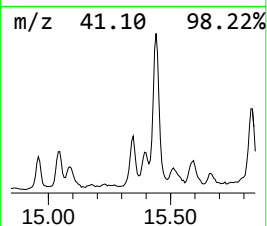
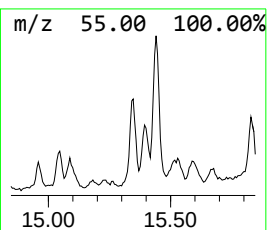
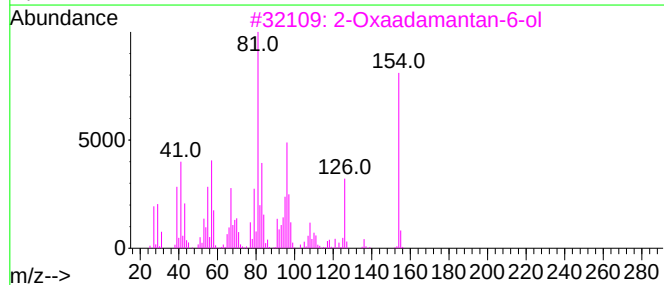
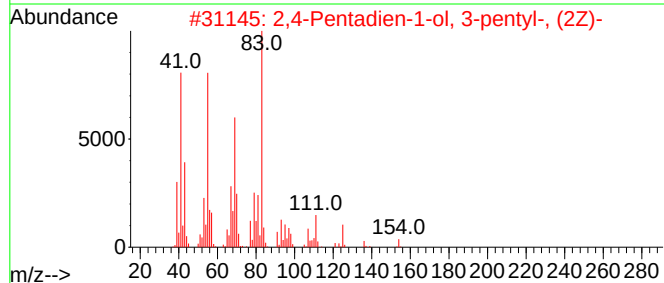
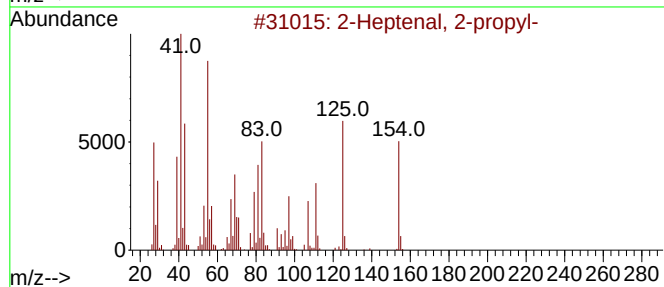
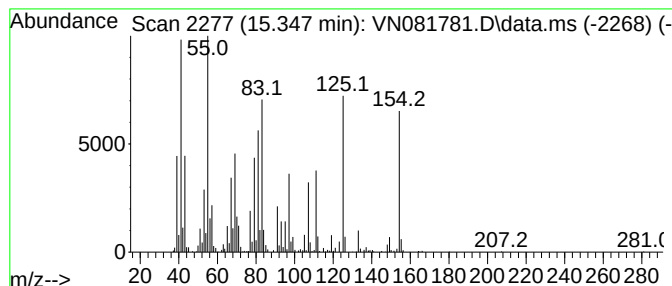
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Quant Title : SW846 8260

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

Peak Number 6 2-Heptenal, 2-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.347	87.25 ug/l	1803100	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, 2-propyl-	154	C10H18O	034880-43-8	96
2			2,4-Pentadien-1-ol, 3-pentyl-, (...)	154	C10H18O	1010142-19-7	52
3			2-Oxaadamantan-6-ol	154	C9H14O2	058512-55-3	30
4			Phenol, 3,5-dimethoxy-	154	C8H10O3	000500-99-2	30
5			Methyl pentyl ethylphosphonate	194	C8H19O3P	170275-31-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

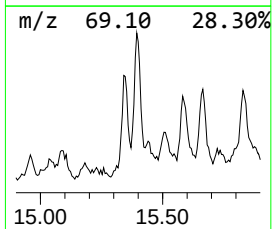
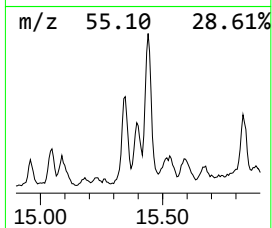
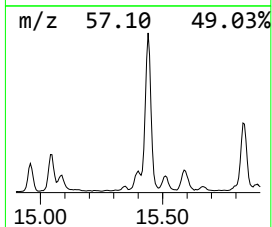
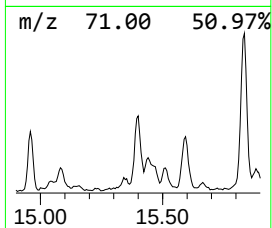
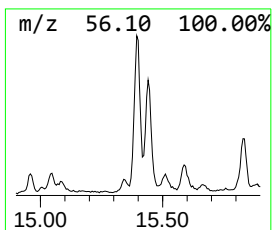
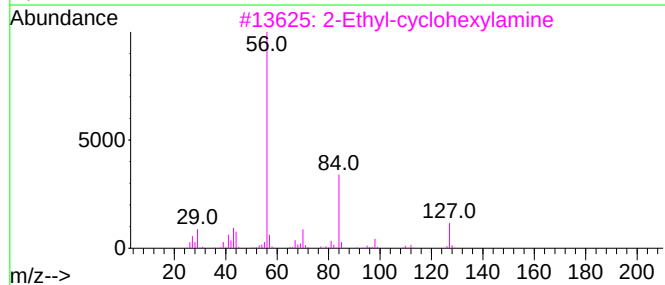
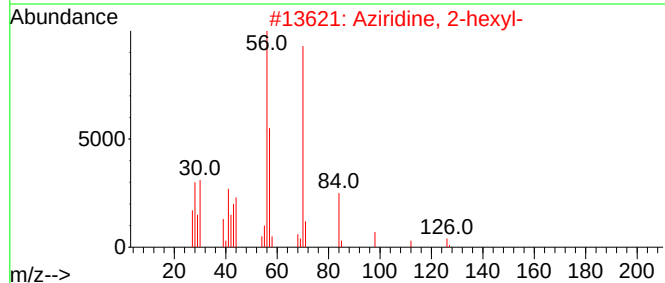
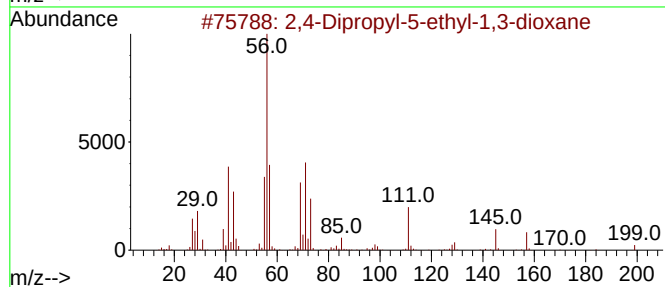
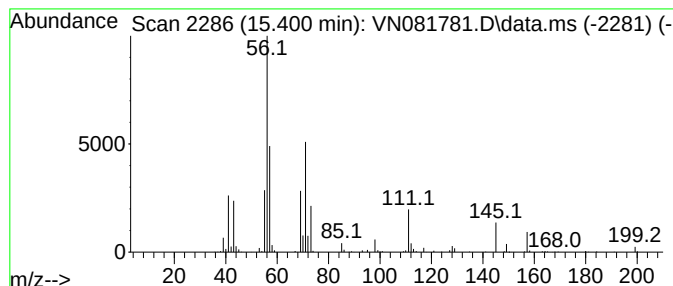
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Quant Title : SW846 8260

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

Peak Number 7 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.400	60.59 ug/l	1252080	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	78
2			Aziridine, 2-hexyl-	127	C8H17N	013906-89-3	32
3			2-Ethyl-cyclohexylamine	127	C8H17N	024216-90-8	25
4			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	25
5			Tridecane, 7-methylene-	196	C14H28	019780-80-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

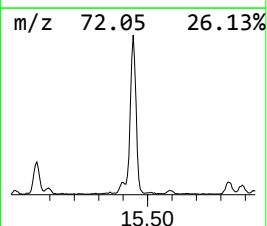
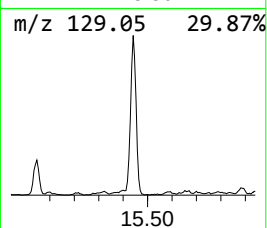
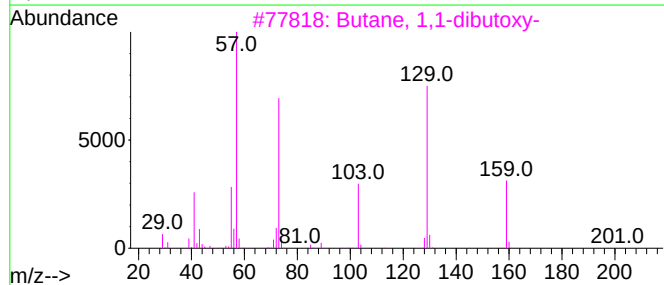
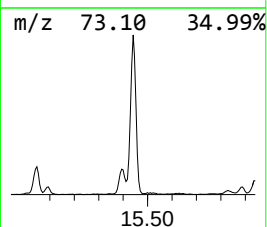
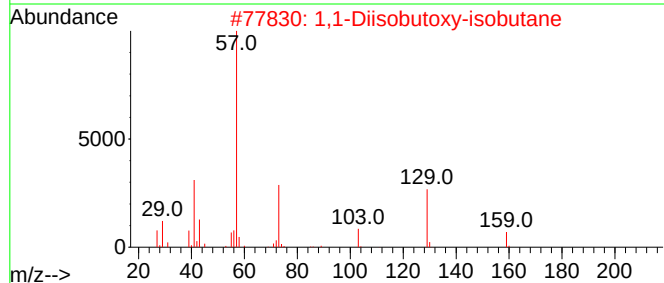
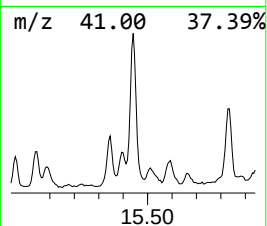
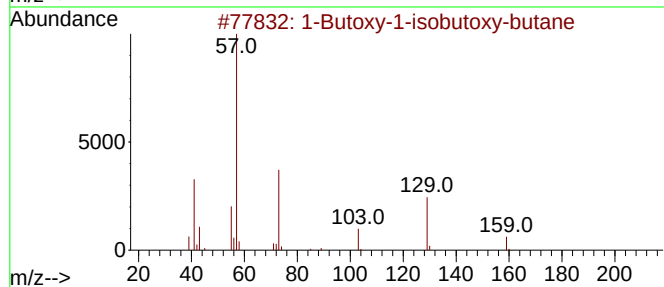
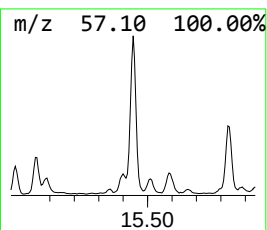
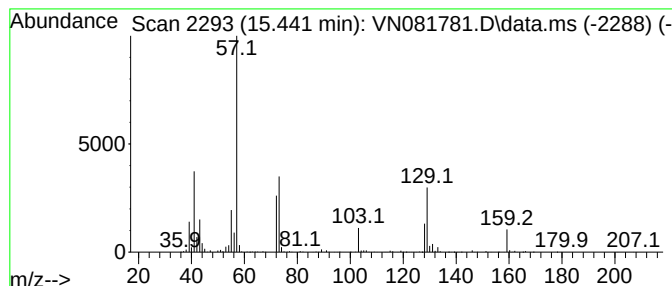
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Quant Title : SW846 8260

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

Peak Number 8 1-Butoxy-1-isobutoxy-butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	193.48 ug/l	3998570	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butoxy-1-isobutoxy-butane	202	C12H26O2	020266-12-0	53
2			1,1-Diisobutoxy-isobutane	202	C12H26O2	013262-24-3	50
3			Butane, 1,1-dibutoxy-	202	C12H26O2	005921-80-2	43
4			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	37
5			Nipecotic acid	129	C6H11NO2	000498-95-3	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

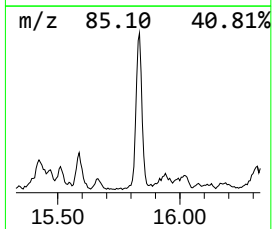
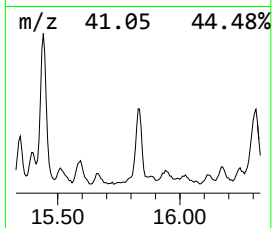
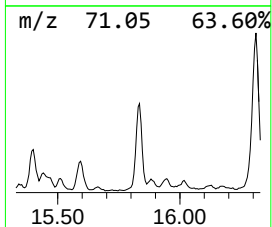
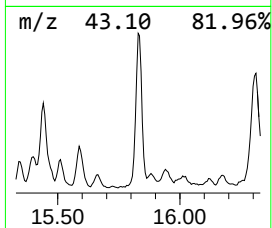
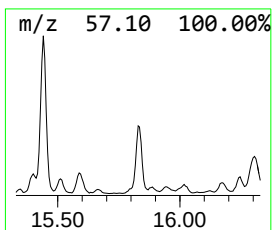
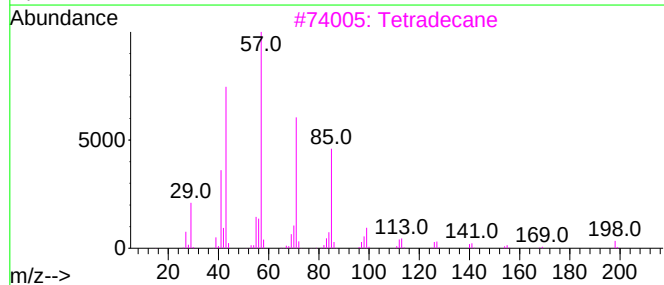
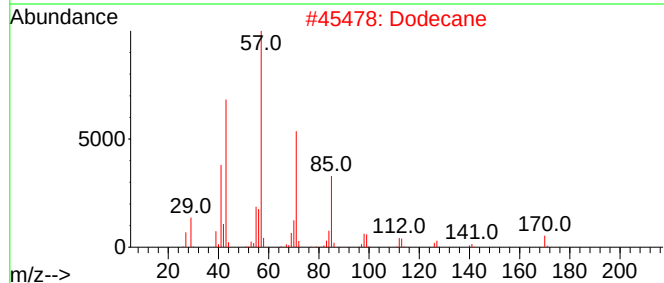
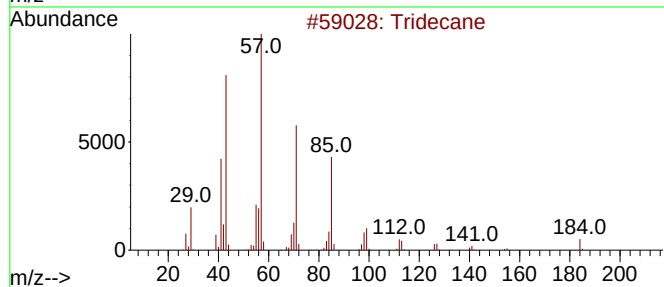
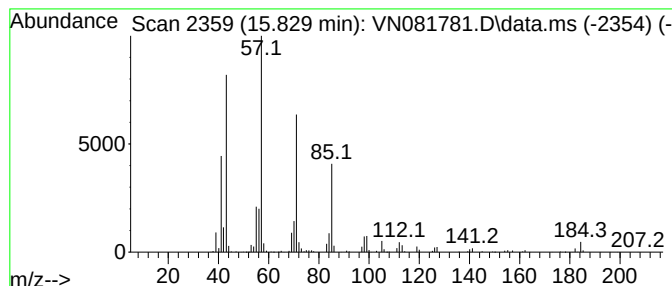
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	94.31 ug/l	1949110	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	86
3			Tetradecane	198	C14H30	000629-59-4	80
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	78
5			Hentriacontane	437	C31H64	000630-04-6	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

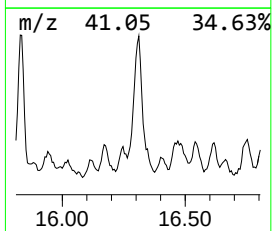
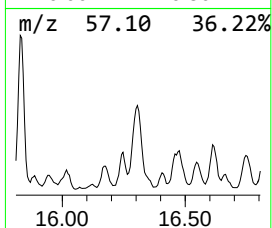
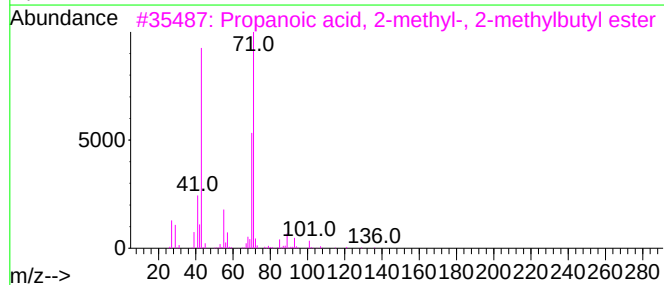
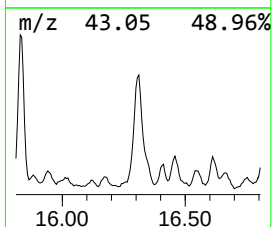
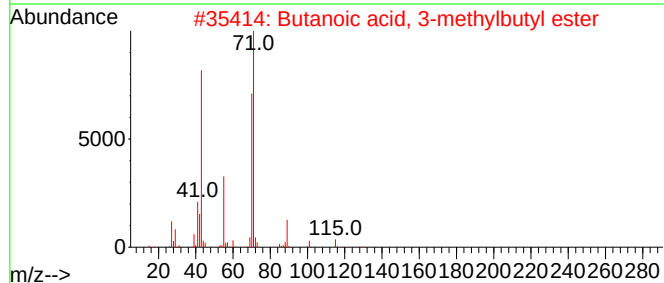
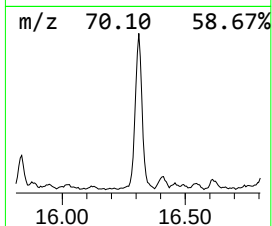
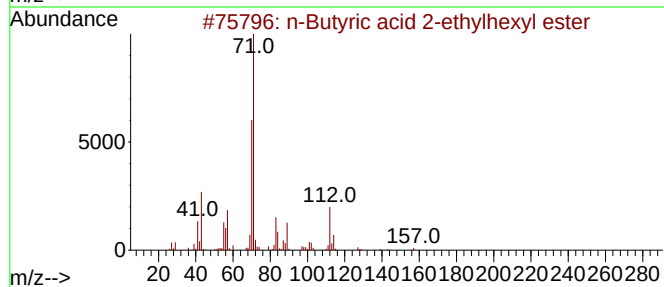
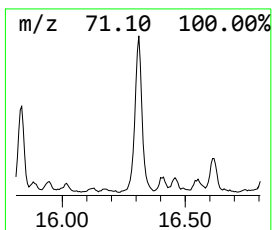
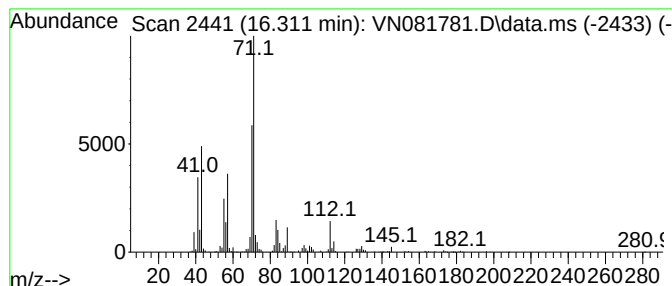
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Quant Title : SW846 8260

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

Peak Number 10 n-Butyric acid 2-ethylhexyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.311	177.67 ug/l	3671790	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	86
2			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	59
3			Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	59
4			2-Propyl-1-pentanol, 2-methylpro...	200	C12H24O2	1000447-36-4	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081781.D
Acq On : 18 Apr 2024 12:42
Operator : JC\MD
Sample : P2122-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
M-R-OILY-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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1-Butanol	9.294	630.0	ug/l	10357900	2	9.100	822068	50.0
trans-1-Butene,...	11.976	125.7	ug/l	4240760	3	11.865	1687470	50.0
Hexanal, 2-ethyl-	12.412	96.5	ug/l	3258020	3	11.865	1687470	50.0
Butanoic acid, ...	13.341	93.3	ug/l	1929040	4	13.794	1033330	50.0
2-Heptenal, 2-p...	15.347	87.3	ug/l	1803100	4	13.794	1033330	50.0
2,4-Dipropyl-5-...	15.400	60.6	ug/l	1252080	4	13.794	1033330	50.0
1-Butoxy-1-isob...	15.441	193.5	ug/l	3998570	4	13.794	1033330	50.0
Tridecane	15.829	94.3	ug/l	1949110	4	13.794	1033330	50.0
n-Butyric acid ...	16.311	177.7	ug/l	3671790	4	13.794	1033330	50.0