

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
 Data File : VN083233.D
 Acq On : 12 Aug 2024 13:23
 Operator : JC\MD
 Sample : P3545-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 BUR-1295

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\82N080724W.M
 Title : SW846 8260

Signal : TIC: VN083233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.424	410	420	440	rBV	151910	447407	25.17%	3.047%
2	5.530	596	608	620	rVB2	7313	25053	1.41%	0.171%
3	7.483	934	940	950	rVB2	33757	87635	4.93%	0.597%
4	7.847	994	1002	1014	rVB3	18566	52600	2.96%	0.358%
5	8.171	1046	1057	1061	rBV	135966	329511	18.54%	2.244%
6	8.224	1061	1066	1080	rVB	228724	530758	29.86%	3.614%
7	8.583	1117	1127	1136	rBV	142298	324894	18.28%	2.212%
8	8.859	1168	1174	1185	rVB3	10337	22265	1.25%	0.152%
9	8.994	1185	1197	1207	rBV3	69587	164418	9.25%	1.120%
10	9.100	1207	1215	1221	rVV	391458	810098	45.57%	5.517%
11	9.159	1221	1225	1236	rVB	88694	177057	9.96%	1.206%
12	9.359	1249	1259	1275	rBV2	68006	142548	8.02%	0.971%
13	9.530	1282	1288	1297	rVB2	10030	19300	1.09%	0.131%
14	9.665	1304	1311	1318	rBV4	9035	21023	1.18%	0.143%
15	9.906	1347	1352	1360	rVB3	8691	18080	1.02%	0.123%
16	10.153	1388	1394	1405	rBV2	8454	18790	1.06%	0.128%
17	10.447	1436	1444	1454	rVB	31273	59533	3.35%	0.405%
18	10.565	1456	1464	1473	rBV	535595	1021315	57.45%	6.955%
19	10.929	1519	1526	1533	rBV2	25713	45875	2.58%	0.312%
20	11.088	1543	1553	1563	rVB3	21090	43554	2.45%	0.297%
21	11.865	1675	1685	1697	rBV	556518	989017	55.63%	6.735%
22	12.071	1715	1720	1727	rVB2	14549	27985	1.57%	0.191%
23	12.376	1761	1772	1782	rBV	402476	685587	38.56%	4.669%
24	12.488	1782	1791	1797	rVV2	104908	188344	10.59%	1.283%
25	12.606	1806	1811	1818	rVB4	21078	40931	2.30%	0.279%
26	12.741	1827	1834	1838	rBV	832739	1326522	74.62%	9.033%
27	12.788	1838	1842	1848	rVV	843990	1392524	78.33%	9.483%
28	12.847	1848	1852	1864	rVB	480866	802801	45.16%	5.467%
29	13.118	1889	1898	1904	rBV2	95523	181534	10.21%	1.236%
30	13.300	1919	1929	1933	rBV6	11314	26229	1.48%	0.179%
31	13.341	1933	1936	1947	rVB4	13807	27914	1.57%	0.190%
32	13.488	1955	1961	1967	rBV4	32091	72595	4.08%	0.494%
33	13.547	1967	1971	1974	rVV2	22925	39386	2.22%	0.268%
34	13.588	1974	1978	1984	rVB	55247	87873	4.94%	0.598%
35	13.794	2001	2013	2020	rBV	557296	988108	55.58%	6.729%
36	13.876	2020	2027	2040	rVV	1086690	1777758	100.00%	12.106%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Title : SW846 8260

37	13.988	2043	2046	2049	rVV3	18343	31652	1.78%	0.216%
38	14.047	2050	2056	2064	rVB2	106822	203134	11.43%	1.383%
39	14.382	2108	2113	2119	rBV	113354	187431	10.54%	1.276%
40	15.035	2219	2224	2241	rVB	679163	1218129	68.52%	8.295%
41	15.641	2320	2327	2333	rVB2	13253	27564	1.55%	0.188%

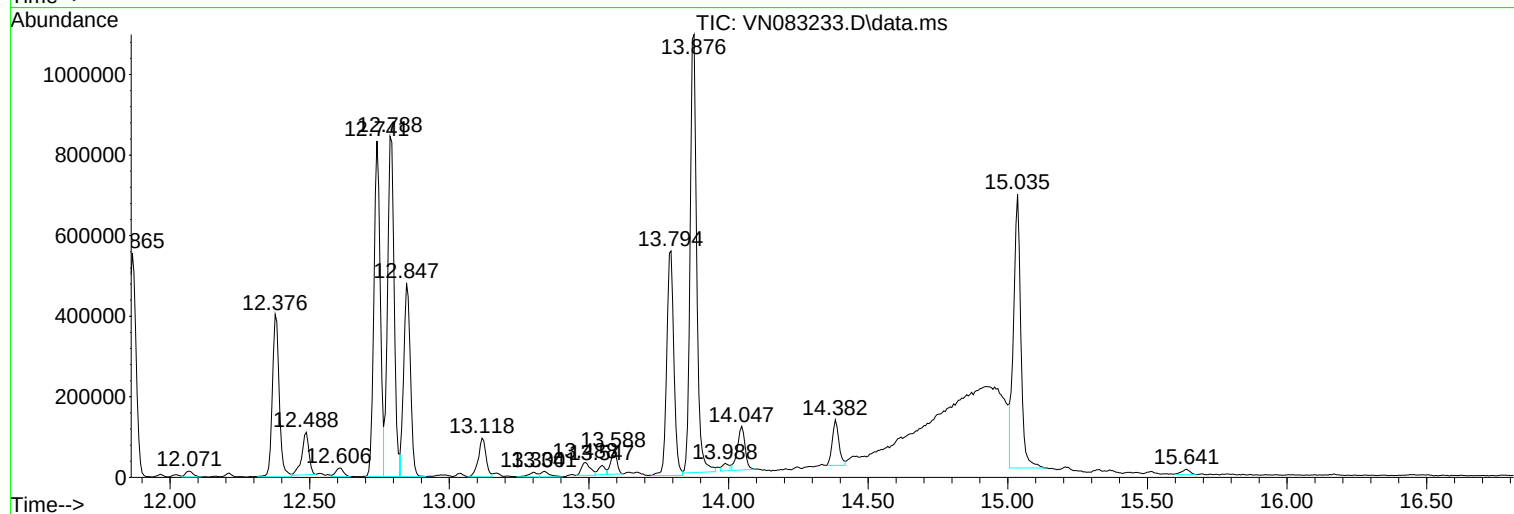
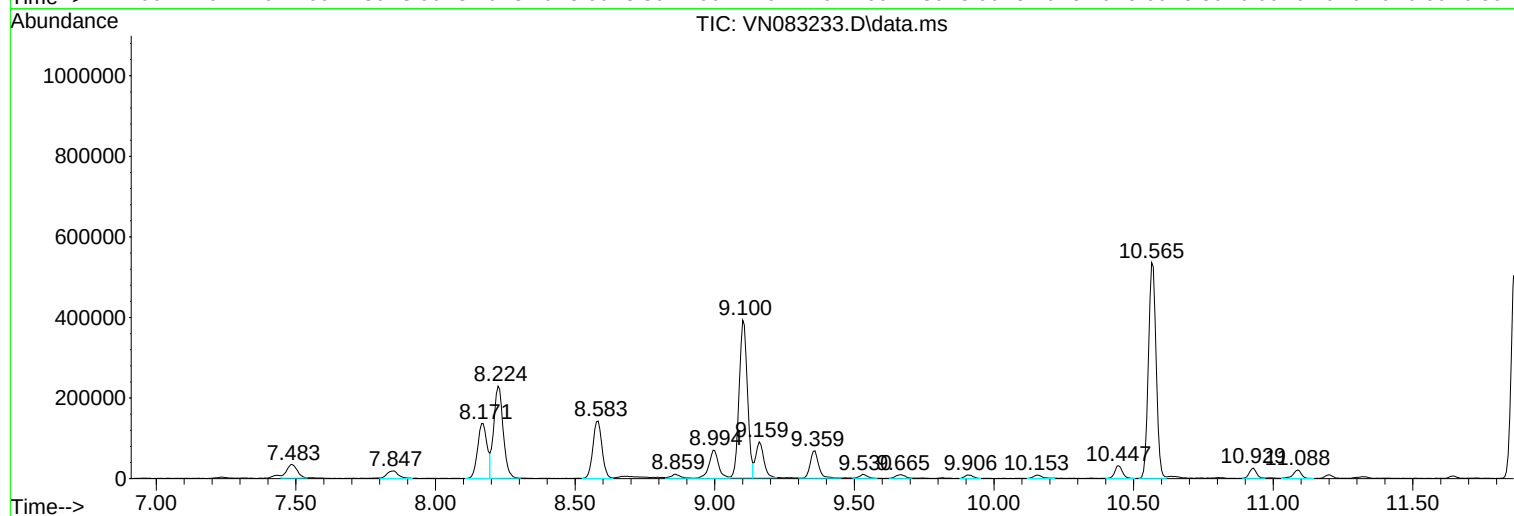
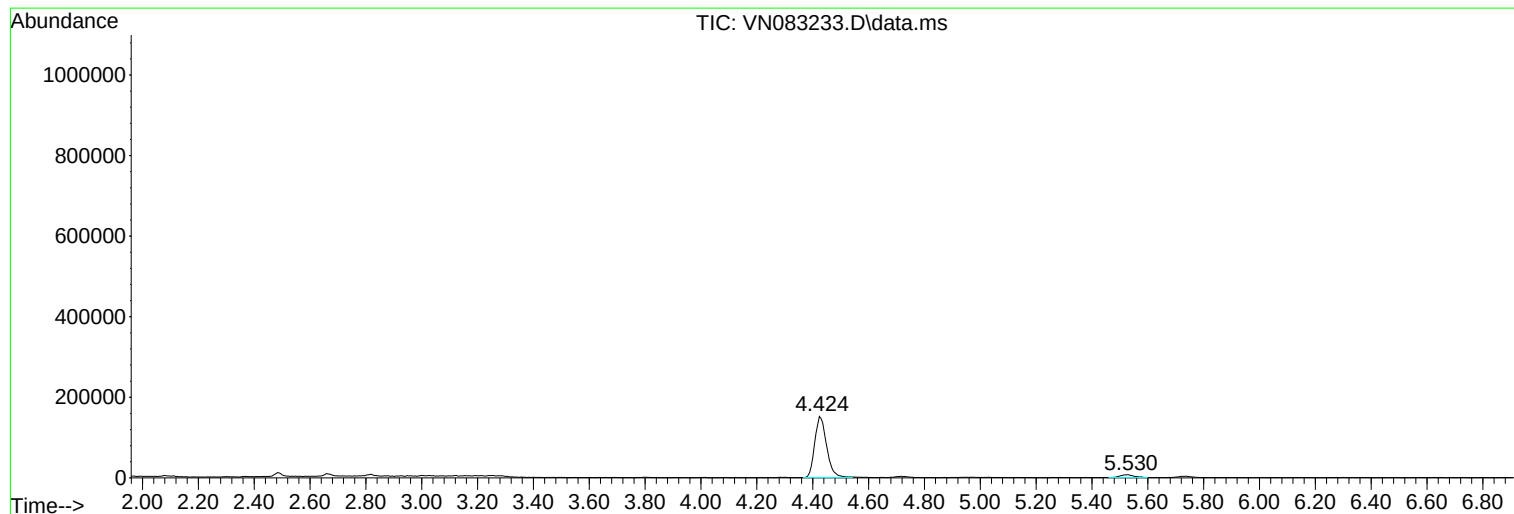
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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



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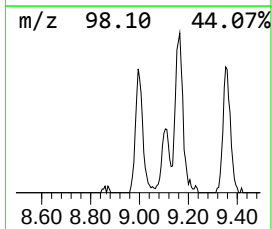
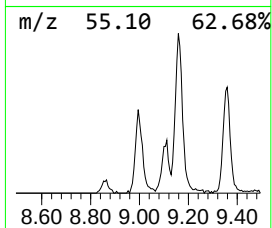
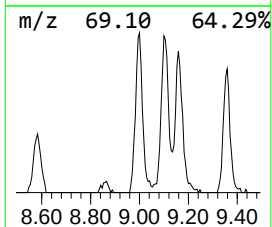
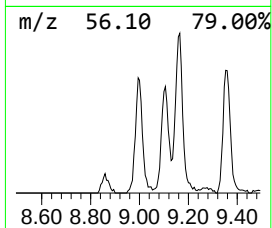
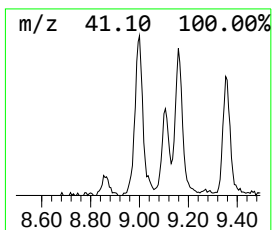
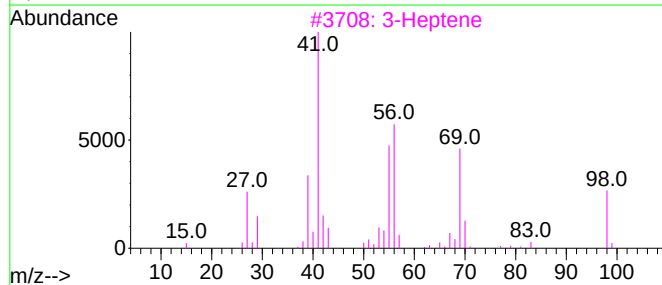
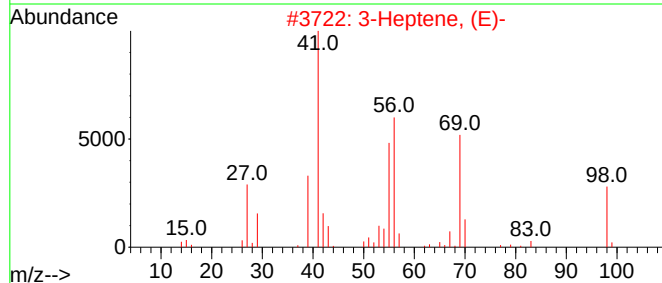
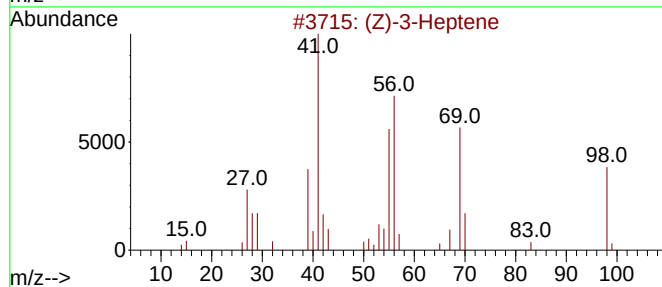
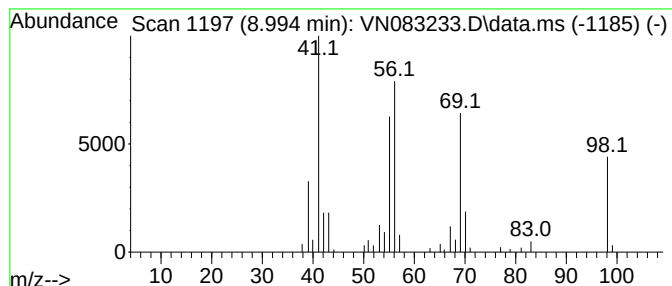
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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

Peak Number 1 (Z)-3-Heptene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.994	10.15 ug/l	164418	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-3-Heptene			98	C7H14	007642-10-6	97
2	3-Heptene, (E)-			98	C7H14	014686-14-7	96
3	3-Heptene			98	C7H14	000592-78-9	95
4	(Z)-2-Heptene			98	C7H14	006443-92-1	91
5	2-Heptene			98	C7H14	000592-77-8	87



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
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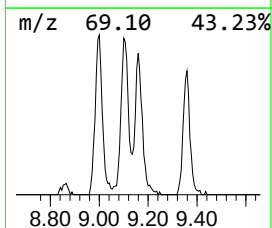
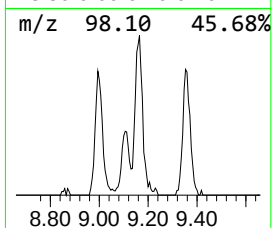
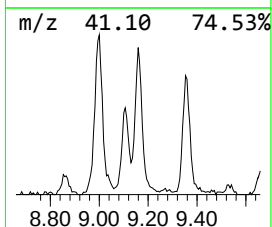
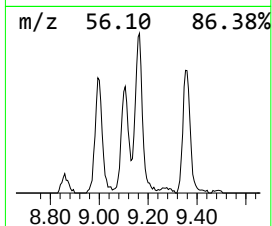
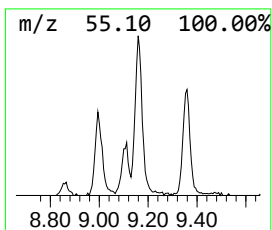
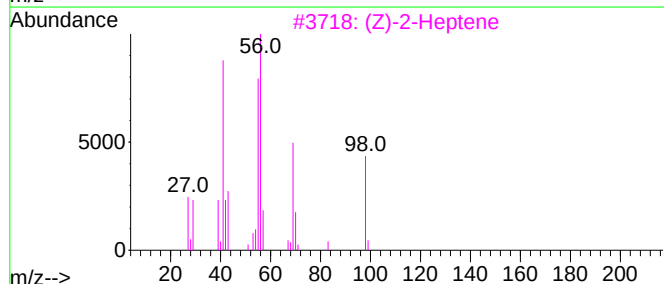
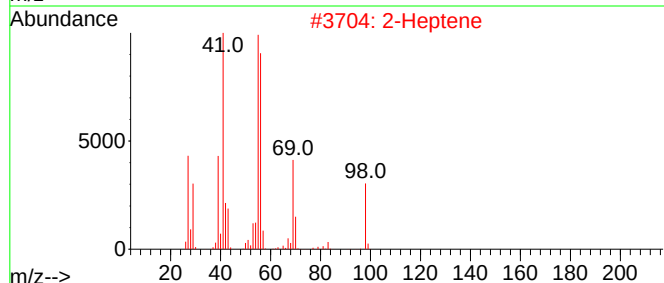
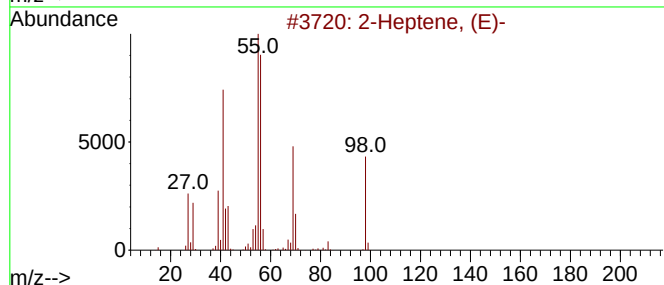
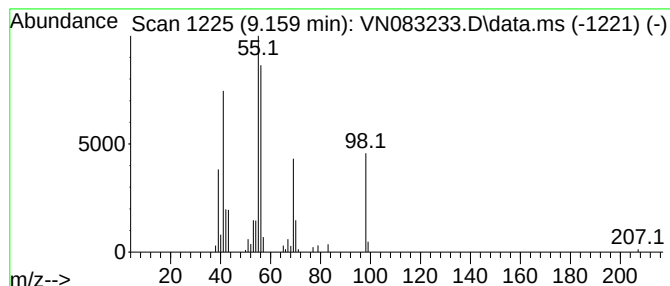
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Heptene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	10.93 ug/l	177057	1,4-Difluorobenzene	9.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptene, (E)-	98	C7H14	014686-13-6	96
2		2-Heptene	98	C7H14	000592-77-8	87
3		(Z)-2-Heptene	98	C7H14	006443-92-1	76
4		Cyclobutanone, 2,3-dimethyl-, cis-	98	C6H10O	028113-36-2	64
5		3-Heptene, (E)-	98	C7H14	014686-14-7	58



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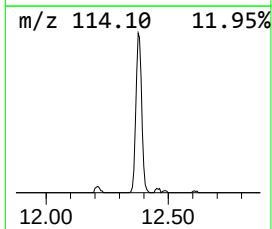
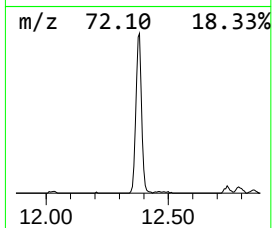
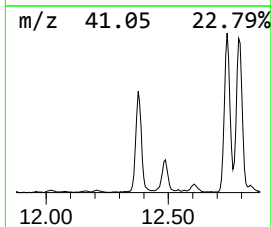
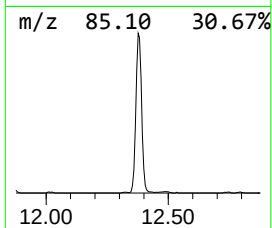
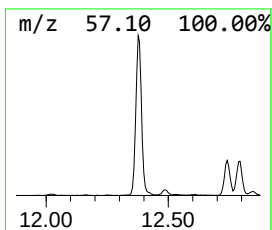
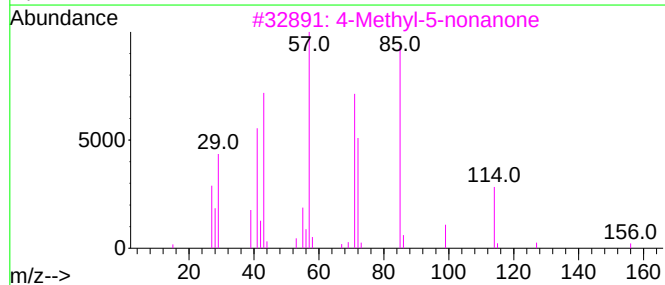
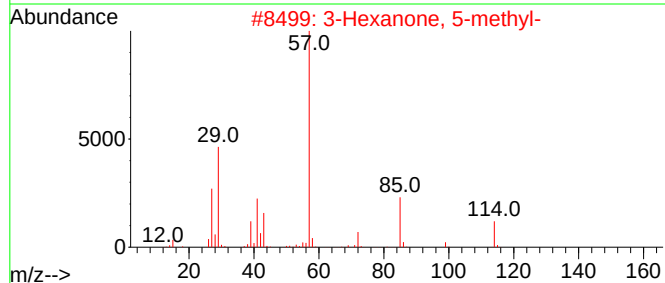
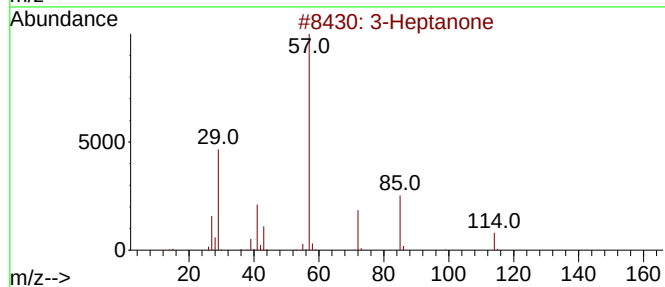
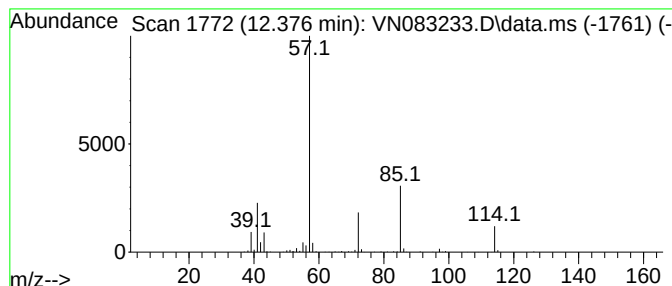
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.376	34.66 ug/l	685587	Chlorobenzene-d5	11.865

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptanone	114	C7H14O	000106-35-4	91
2		3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	78
3		4-Methyl-5-nonanone	156	C10H20O	035900-26-6	53
4		3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	47
5		3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	47



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Instrument :
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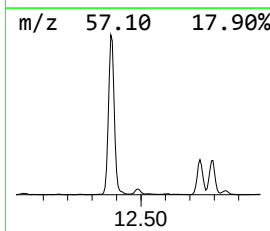
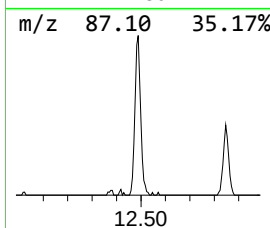
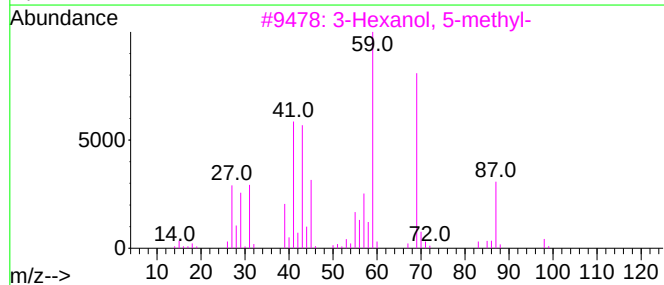
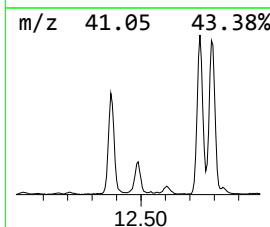
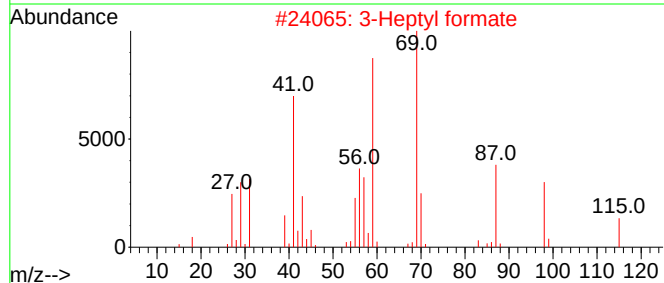
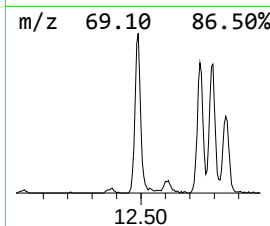
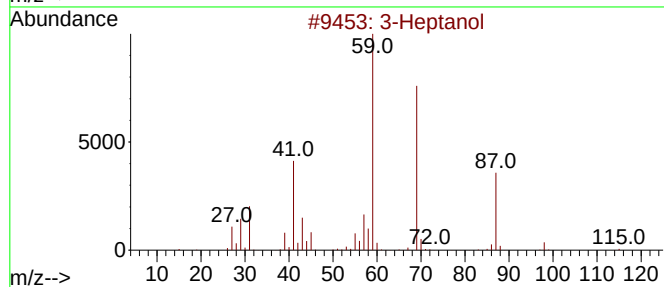
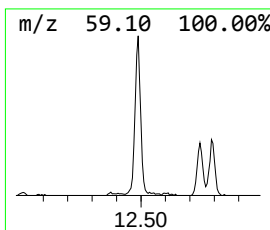
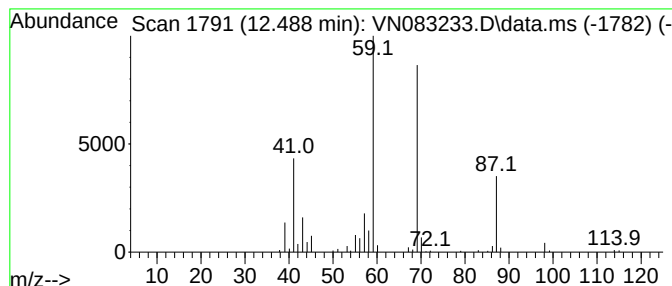
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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

Peak Number 4 3-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.488	9.52 ug/l	188344	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol	116	C7H16O	000589-82-2	90
2			3-Heptyl formate	144	C8H16O2	1000368-76-5	64
3			3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	64
4			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	43
5			5-Nonanol	144	C9H20O	000623-93-8	43



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ALS Vial : 11 Sample Multiplier: 1

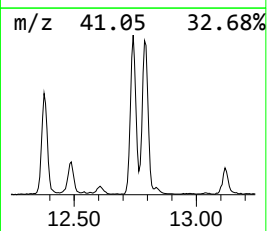
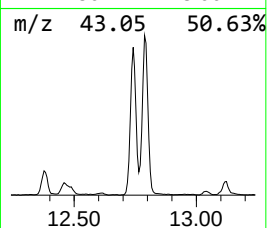
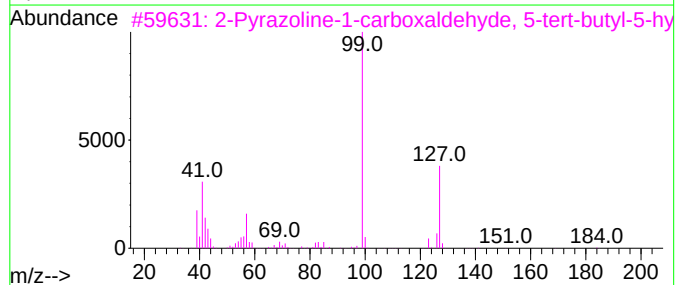
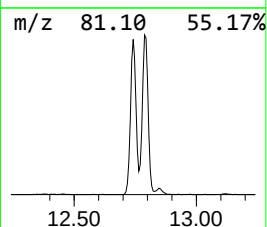
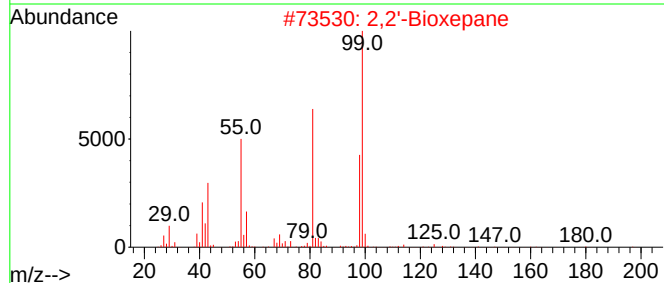
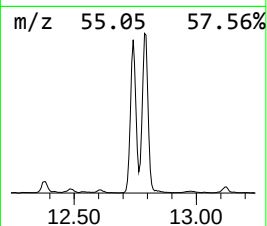
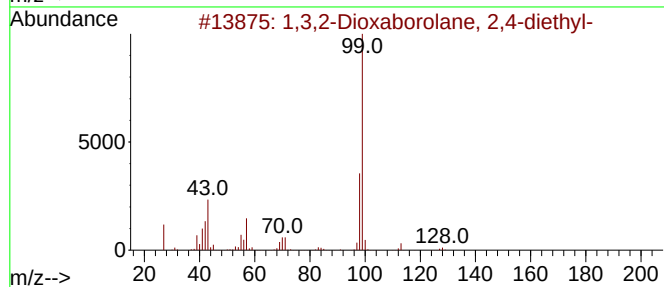
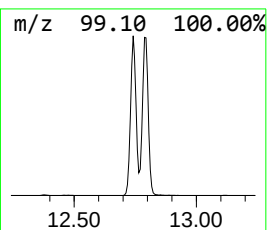
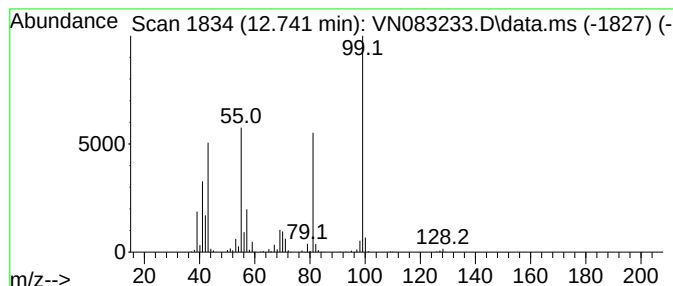
Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3,2-Dioxaborolane, 2,4-di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.741	67.06 ug/l	1326520	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13B02	057633-63-3	72
2	2,2'-Bioxepane	198	C12H22O2	074793-02-5	72
3	2-Pyrazoline-1-carboxaldehyde, 5...	184	C9H16N2O2	103214-44-4	59
4	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	53
5	4-Methyl-2-(4-methyl-6-oxo-1-oxa...	214	C12H22O3	101153-83-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

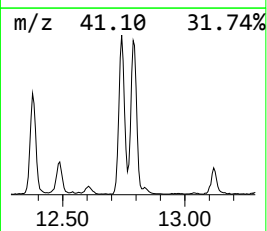
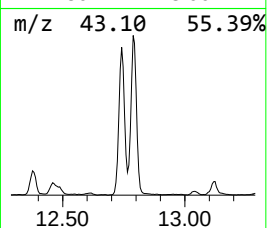
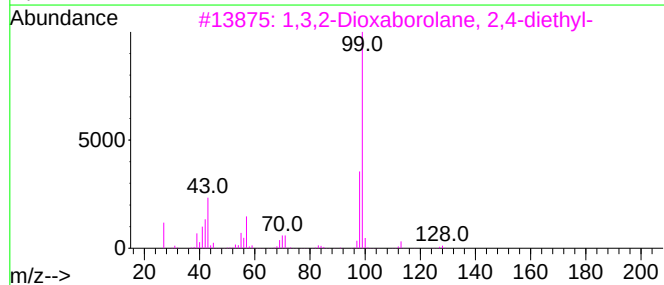
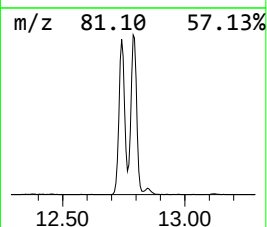
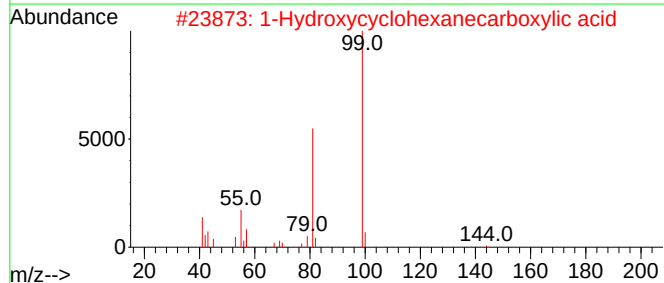
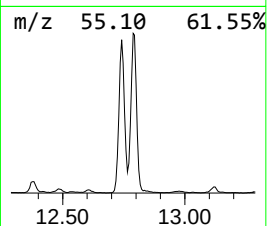
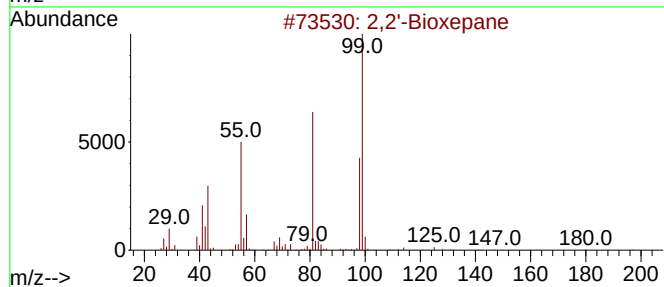
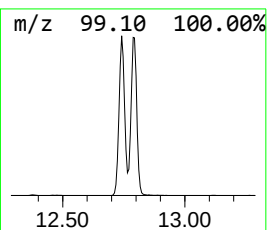
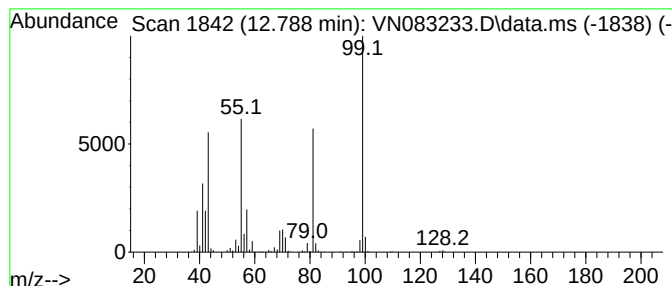
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Quant Title : SW846 8260

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

Peak Number 6 2,2'-Bioxepane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.788	70.40 ug/l	1392520	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2'-Bioxepane	198	C12H22O2	074793-02-5	72
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	64
3			1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	59
4			2-Pyrazoline-1-carboxaldehyde, 5...	184	C9H16N2O2	103214-44-4	59
5			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

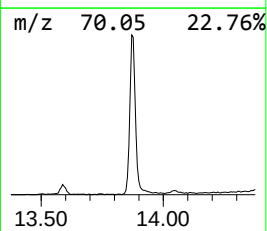
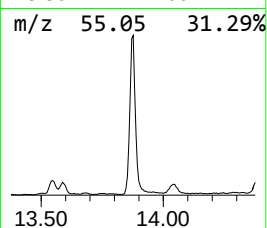
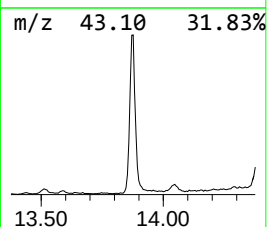
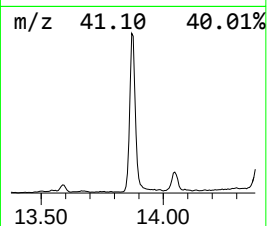
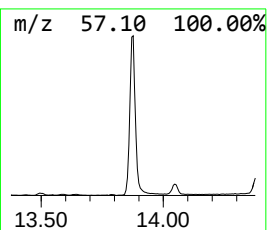
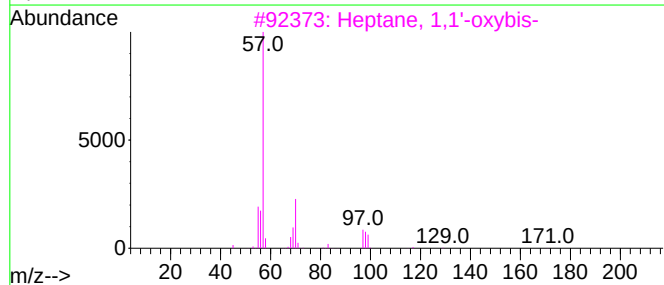
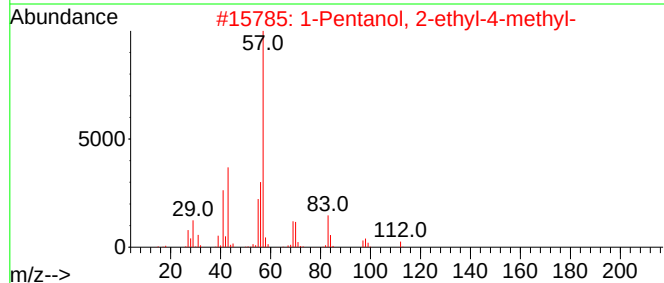
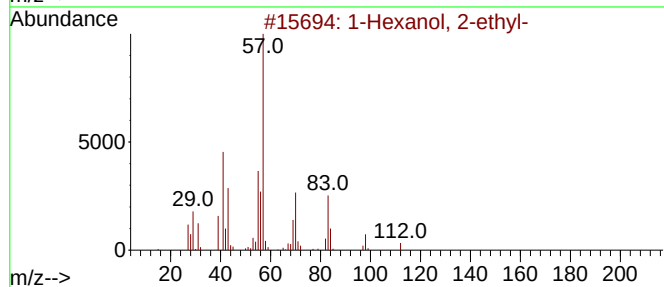
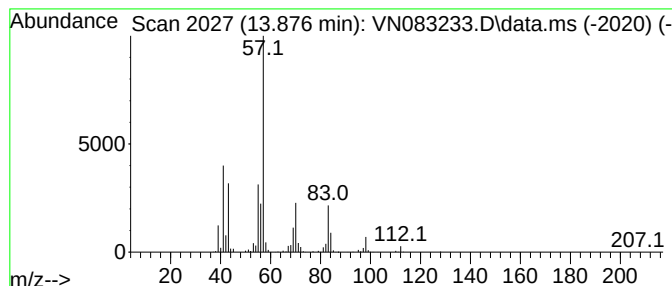
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	89.96 ug/l	1777760	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

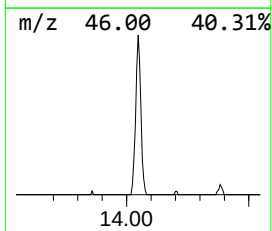
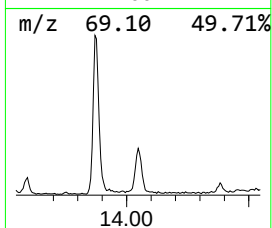
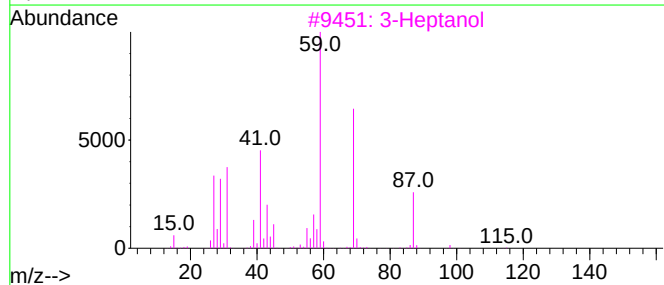
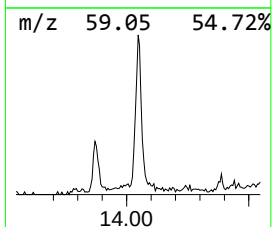
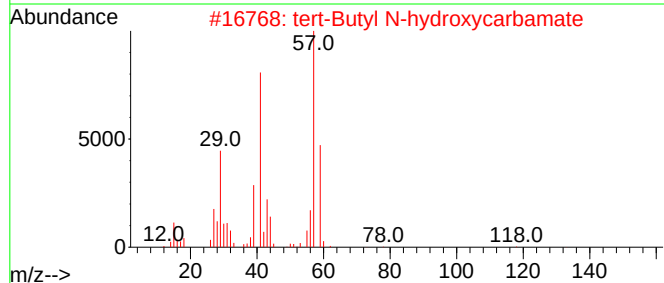
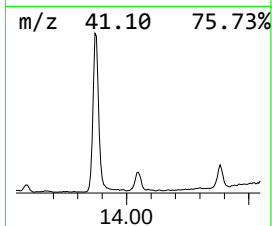
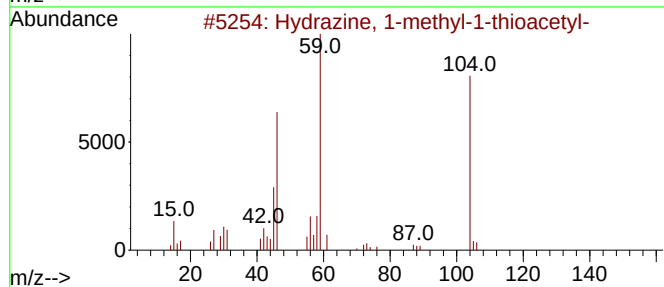
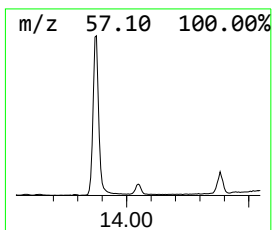
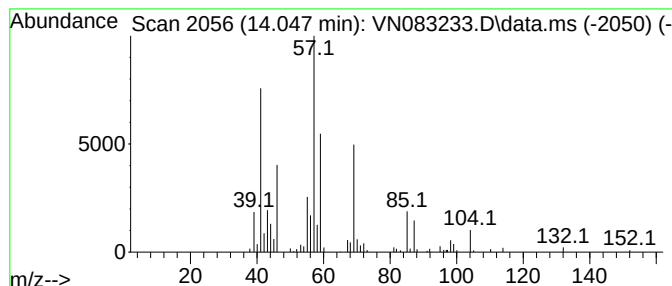
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.047 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.047	10.28 ug/l	203134	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1-methyl-1-thioacetyl-	104	C3H8N2S	018389-73-6	38
2			tert-Butyl N-hydroxycarbamate	133	C5H11NO3	036016-38-3	27
3			3-Heptanol	116	C7H16O	000589-82-2	22
4			(4S)-4-BOC-aminoxolan-2-one	201	C9H15NO4	104227-71-6	17
5			Propane, 2,2'-[methylenebis(oxy)...	160	C9H20O2	002568-93-6	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

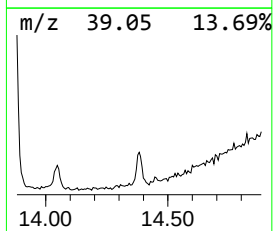
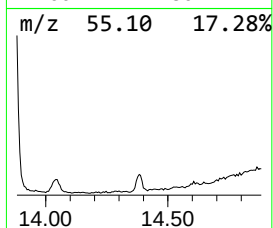
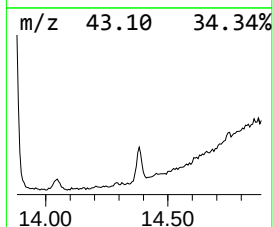
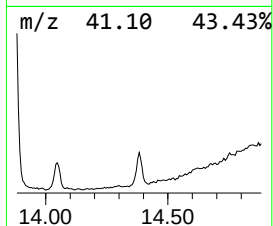
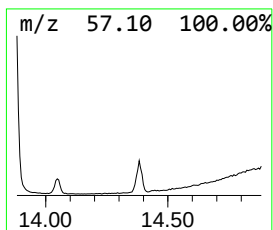
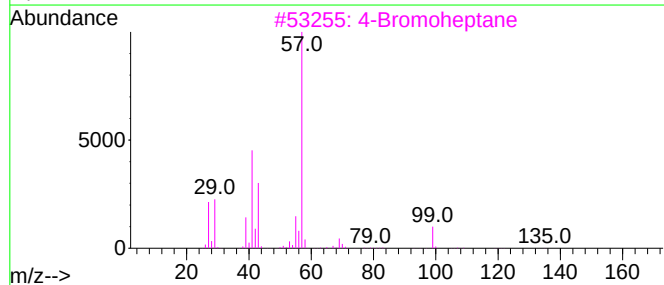
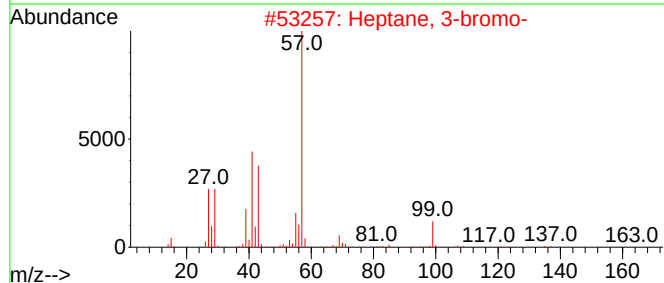
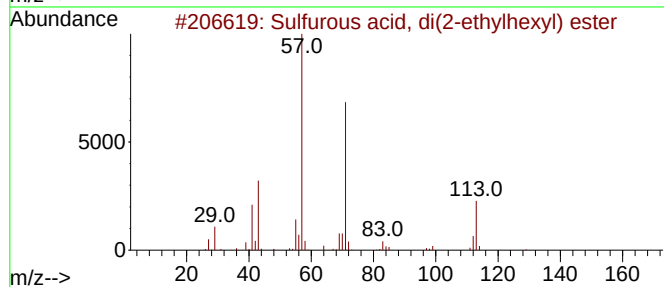
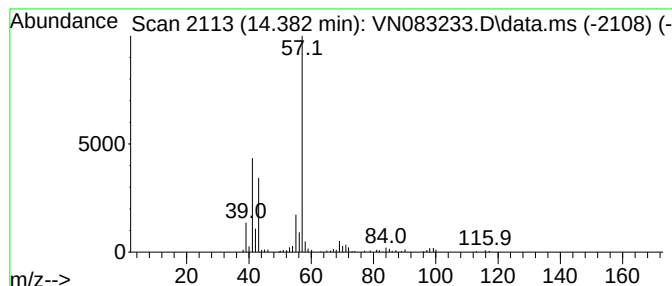
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Quant Title : SW846 8260

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

Peak Number 9 Sulfurous acid, di(2-ethylh... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.382	9.48 ug/l	187431	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	53
2			Heptane, 3-bromo-	178	C7H15Br	001974-05-6	53
3			4-Bromoheptane	178	C7H15Br	000998-93-6	53
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50
5			Sulfurous acid, 2-propyl heptyl ...	222	C10H22O3S	1000309-11-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

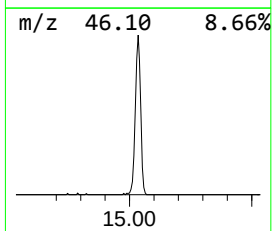
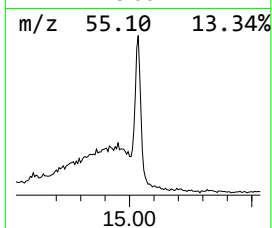
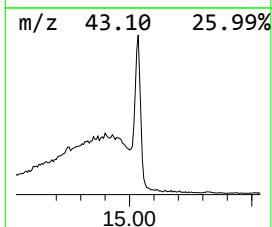
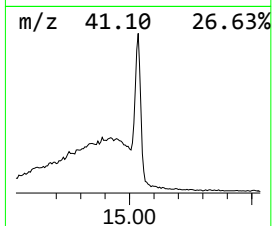
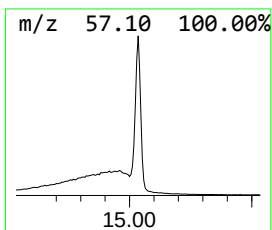
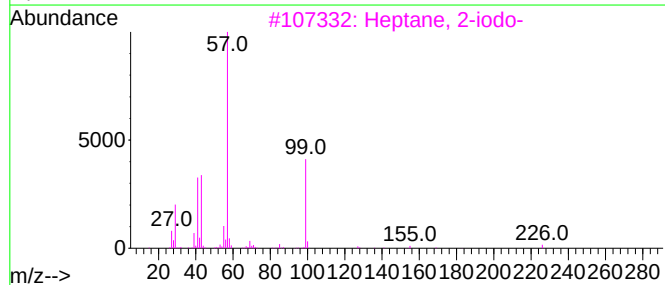
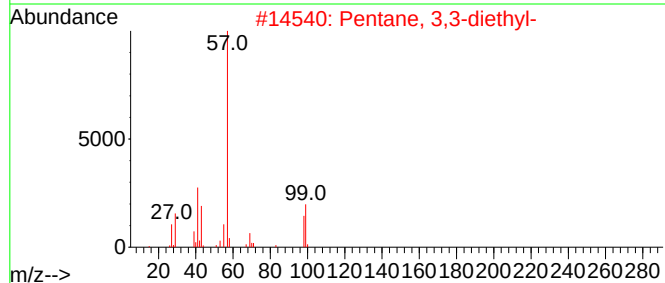
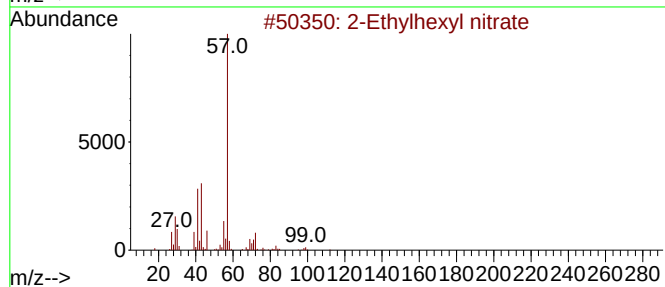
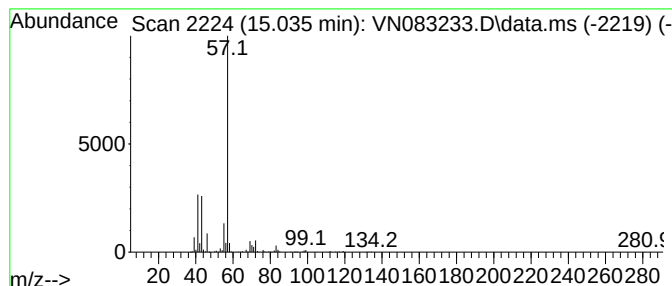
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Quant Title : SW846 8260

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

Peak Number 10 2-Ethylhexyl nitrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	61.64 ug/l	1218130	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl nitrate	175	C8H17NO3	027247-96-7	59
2			Pentane, 3,3-diethyl-	128	C9H20	001067-20-5	47
3			Heptane, 2-iodo-	226	C7H15I	018589-29-2	42
4			4-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055534-69-5	40
5			Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081224\
Data File : VN083233.D
Acq On : 12 Aug 2024 13:23
Operator : JC\MD
Sample : P3545-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BUR-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N080724W.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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2-Heptene, (E)-	9.159	10.9	ug/l	177057	2	9.100	810098	50.0
3-Heptanone	12.376	34.7	ug/l	685587	3	11.865	989017	50.0
3-Heptanol	12.488	9.5	ug/l	188344	3	11.865	989017	50.0
1,3,2-Dioxaboro...	12.741	67.1	ug/l	1326520	3	11.865	989017	50.0
2,2'-Bioxepane	12.788	70.4	ug/l	1392520	3	11.865	989017	50.0
1-Hexanol, 2-et...	13.876	90.0	ug/l	1777760	4	13.794	988108	50.0
unknown14.047	14.047	10.3	ug/l	203134	4	13.794	988108	50.0
Sulfurous acid,...	14.382	9.5	ug/l	187431	4	13.794	988108	50.0
2-Ethylhexyl ni...	15.035	61.6	ug/l	1218130	4	13.794	988108	50.0