

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
 Data File : VN067776.D
 Acq On : 16 Jul 2021 16:34
 Operator : JC/MD
 Sample : M3051-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-41257-59

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\82N070721W.M

Title : SW846 8260

Signal : TIC: VN067776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.296	840	860	879	rBV2	31539	98142	1.15%	0.272%
2	8.024	2227	2250	2261	rBV2	273791	654952	7.69%	1.817%
3	8.088	2261	2274	2300	rVB	492570	1130847	13.29%	3.138%
4	8.440	2380	2405	2434	rBV2	317732	744336	8.75%	2.065%
5	8.971	2582	2603	2630	rBV	760487	1585889	18.63%	4.400%
6	10.443	3133	3152	3196	rBV	1176425	2252145	26.46%	6.249%
7	11.747	3620	3638	3662	rBV	1101998	1992260	23.41%	5.527%
8	12.734	3990	4006	4033	rVB	824768	1415698	16.63%	3.928%
9	13.675	4341	4357	4376	rBV	1016769	1766759	20.76%	4.902%
10	13.771	4377	4393	4422	rBV	701071	1184509	13.92%	3.286%
11	13.997	4465	4477	4489	rBV2	217250	326790	3.84%	0.907%
12	14.477	4646	4656	4662	rBV8	62000	108940	1.28%	0.302%
13	14.555	4679	4685	4701	rVB3	104850	164133	1.93%	0.455%
14	14.622	4702	4710	4719	rBV2	101187	143736	1.69%	0.399%
15	14.847	4783	4794	4809	rBV	1283286	1829220	21.49%	5.075%
16	14.927	4814	4824	4829	rVV10	105733	179901	2.11%	0.499%
17	14.968	4831	4839	4856	rVB2	330639	601135	7.06%	1.668%
18	15.348	4975	4981	4988	rBV3	154872	205487	2.41%	0.570%
19	15.389	4990	4996	5013	rVB4	406362	692028	8.13%	1.920%
20	15.469	5015	5026	5044	rBV3	782507	1405605	16.51%	3.900%
21	15.705	5101	5114	5134	rVB	3709193	6167842	72.46%	17.112%
22	16.314	5334	5341	5361	rVB5	488665	1036699	12.18%	2.876%
23	16.467	5389	5398	5416	rVB	994893	1844315	21.67%	5.117%
24	16.681	5465	5478	5493	rBV	4503033	8511551	100.00%	23.615%

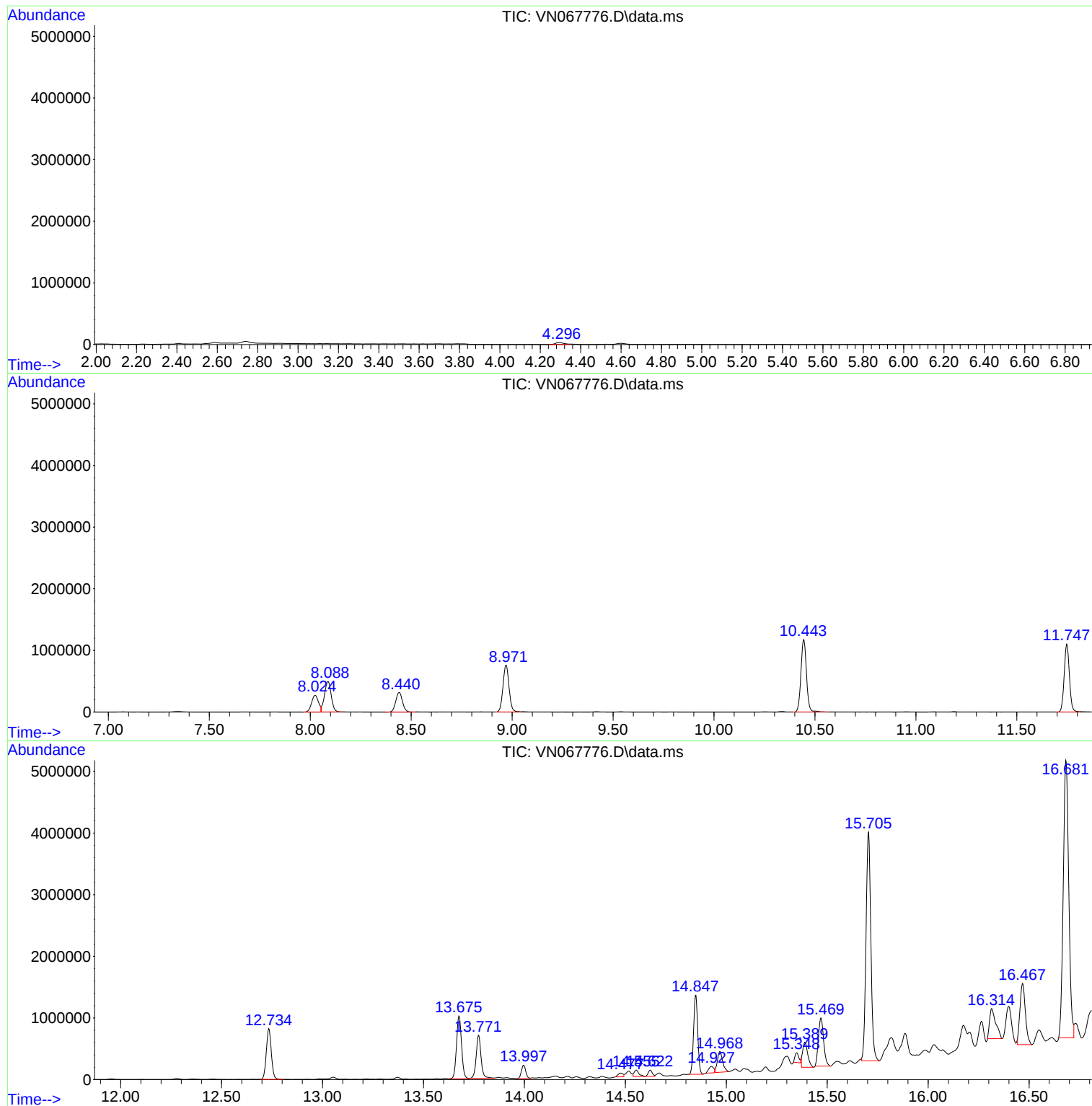
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Quant Title : SW846 8260

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



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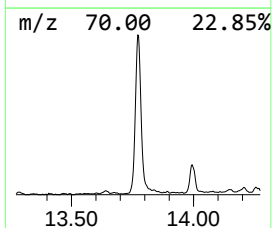
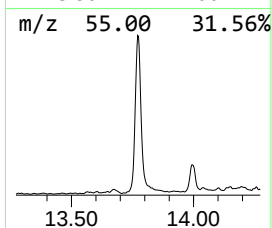
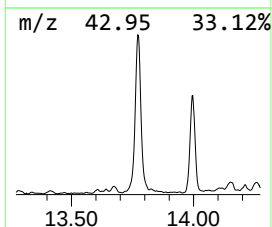
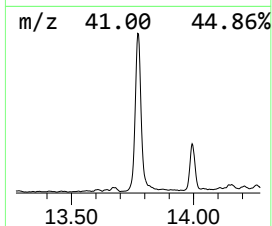
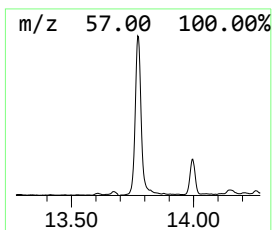
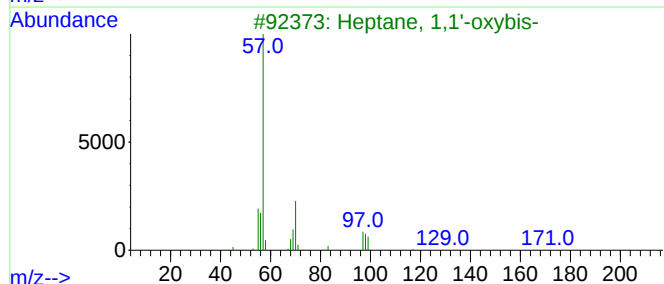
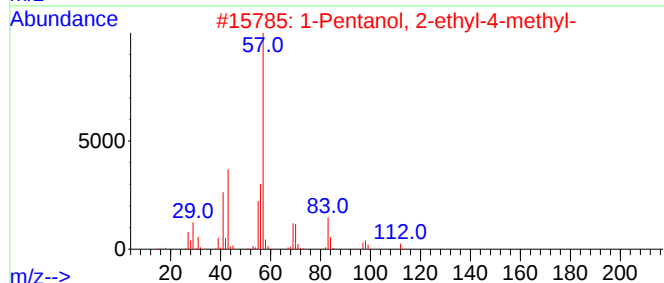
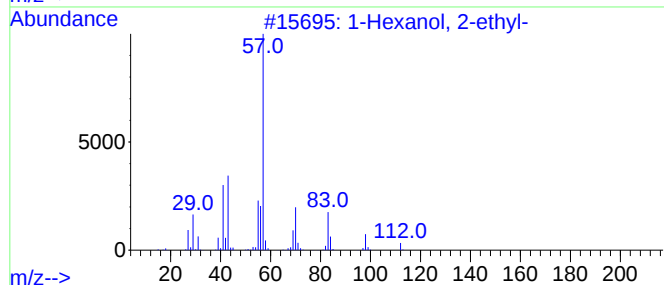
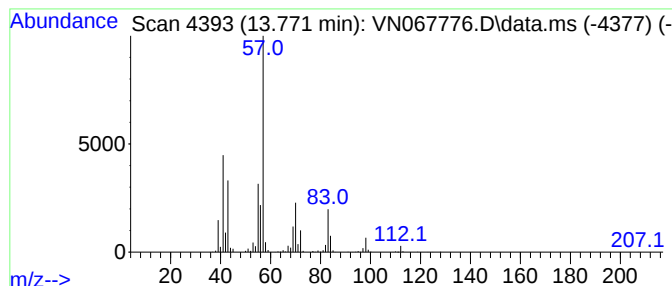
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070721W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.772	33.52 ug/l	1184510	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47



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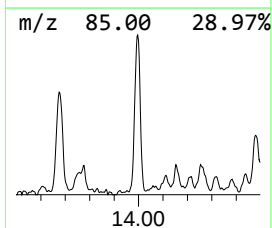
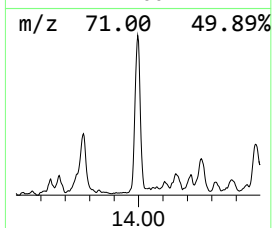
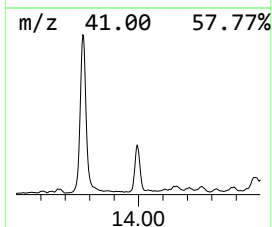
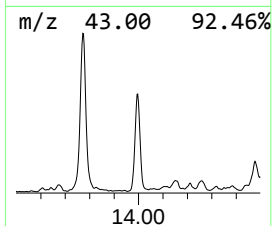
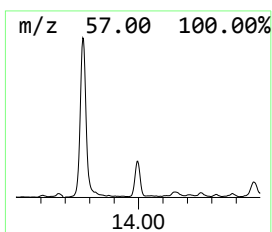
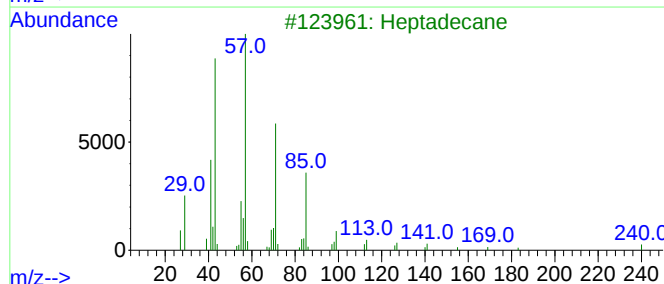
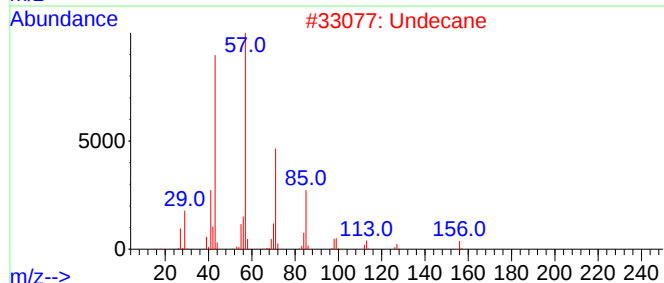
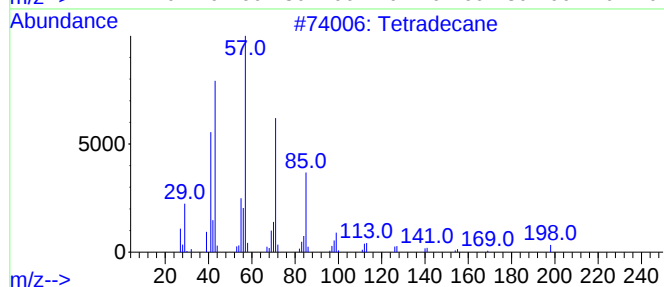
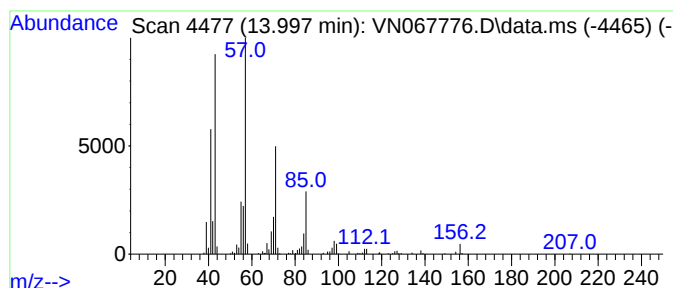
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070721W.M
Quant Title : SW846 8260

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

Peak Number 2 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	9.25 ug/l	326790	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	90
2		Undecane	156	C11H24	001120-21-4	80
3		Heptadecane	240	C17H36	000629-78-7	64
4		Tridecane	184	C13H28	000629-50-5	59
5		Hexadecane	226	C16H34	000544-76-3	59



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

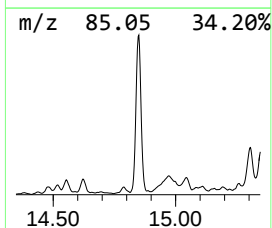
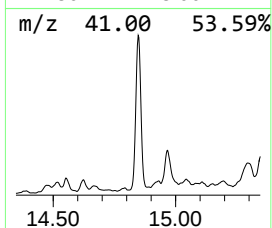
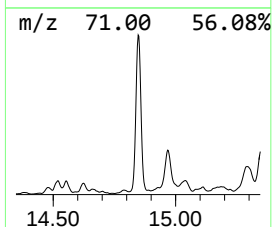
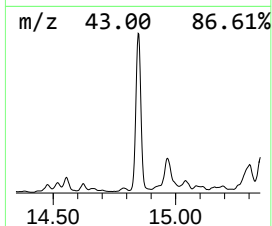
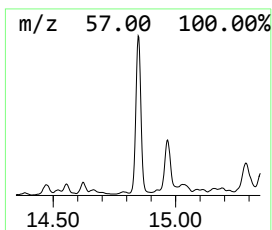
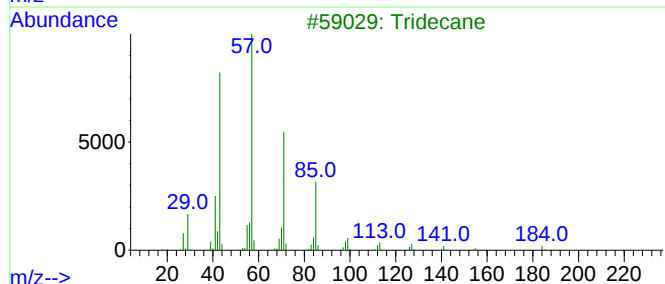
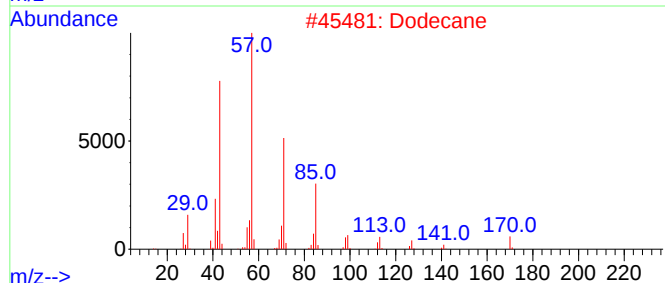
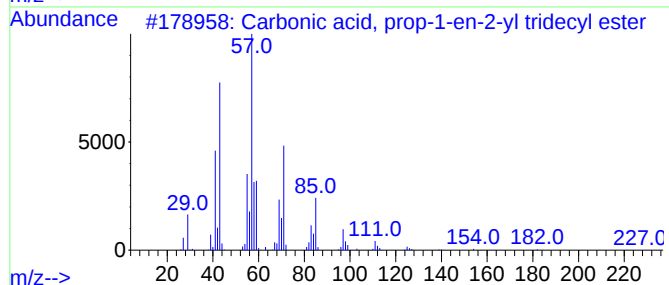
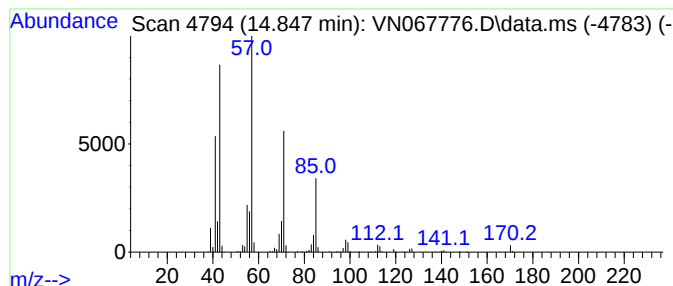
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Quant Title : SW846 8260

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

Peak Number 3 Carbonic acid, prop-1-en-2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	51.77 ug/l	1829220	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90
2			Dodecane	170	C12H26	000112-40-3	90
3			Tridecane	184	C13H28	000629-50-5	83
4			Tetradecane	198	C14H30	000629-59-4	83
5			1-Undecene, 4-methyl-	168	C12H24	074630-39-0	80



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ALS Vial : 11 Sample Multiplier: 1

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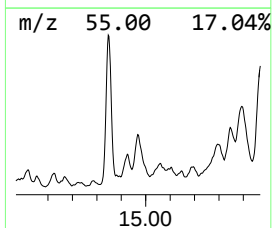
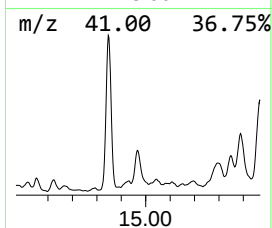
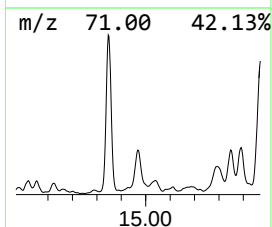
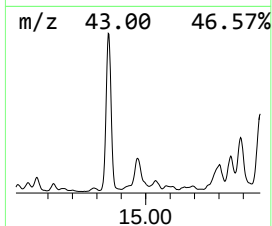
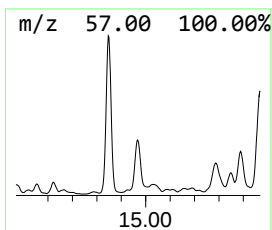
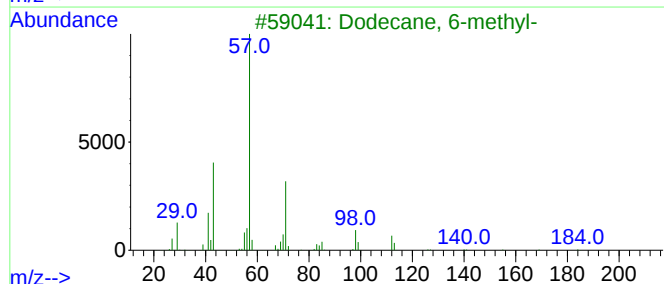
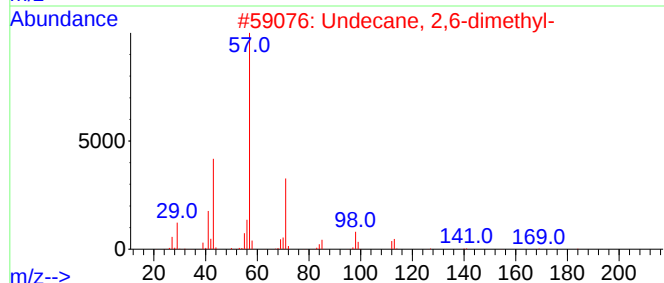
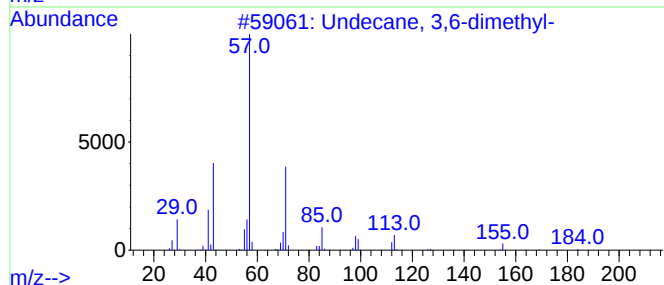
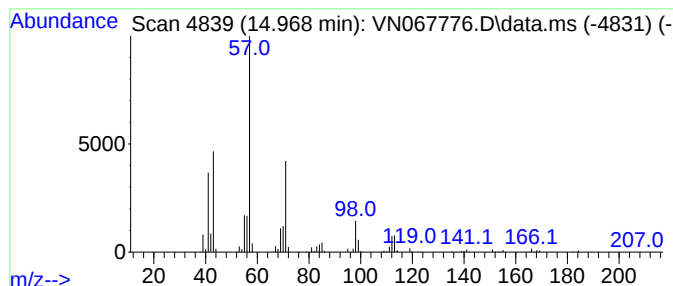
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	17.01 ug/l	601135	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	87
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	86
3			Dodecane, 6-methyl-	184	C13H28	006044-71-9	76
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
5			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	72



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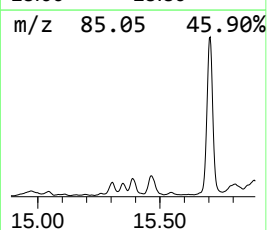
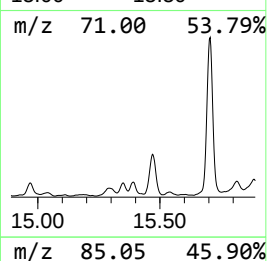
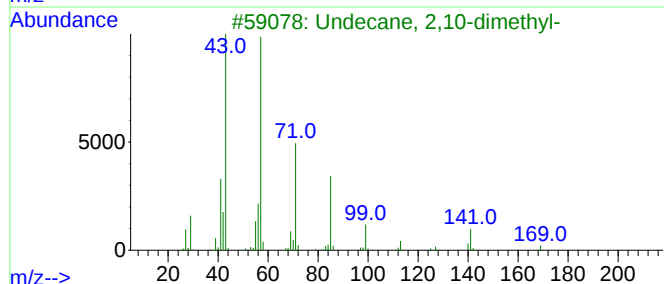
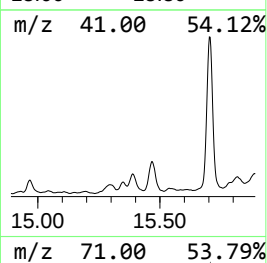
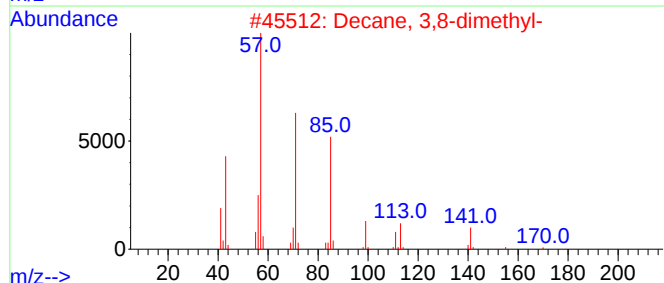
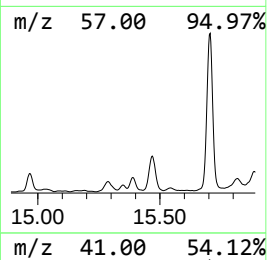
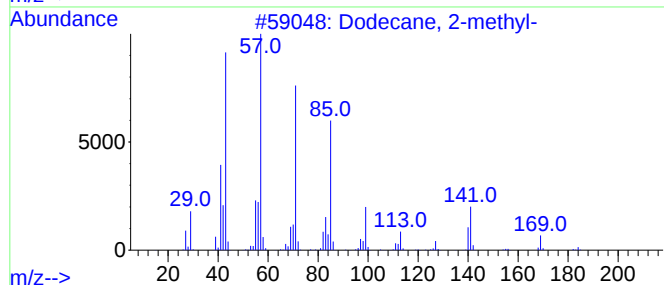
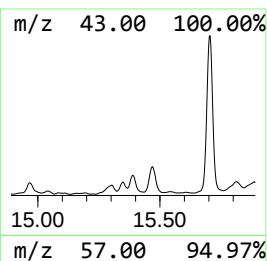
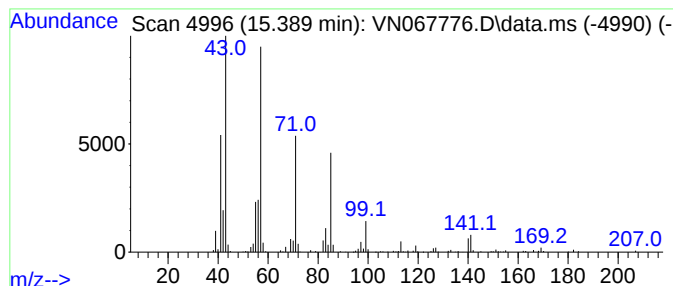
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070721W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.389	19.58 ug/l	692028	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	81
3			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	81
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	59
5			1-Iodoundecane	282	C11H23I	004282-44-4	58



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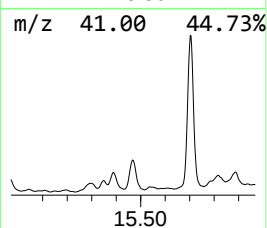
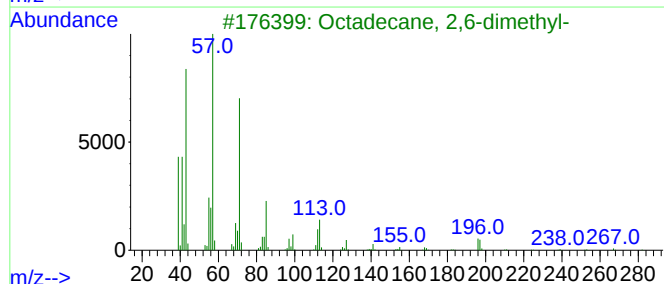
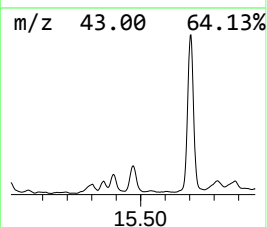
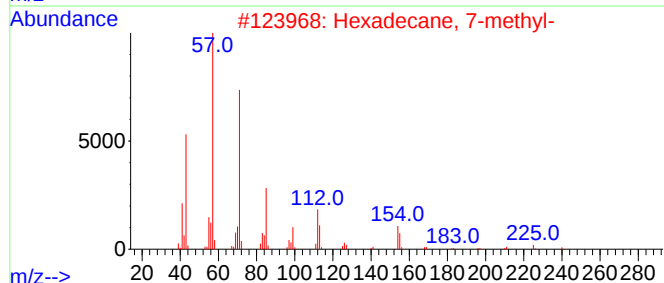
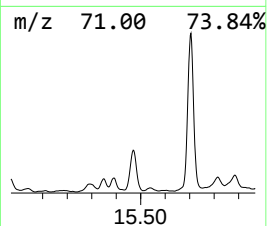
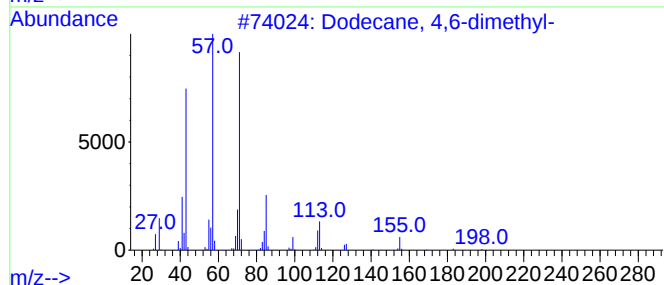
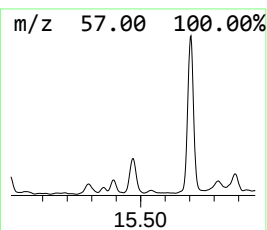
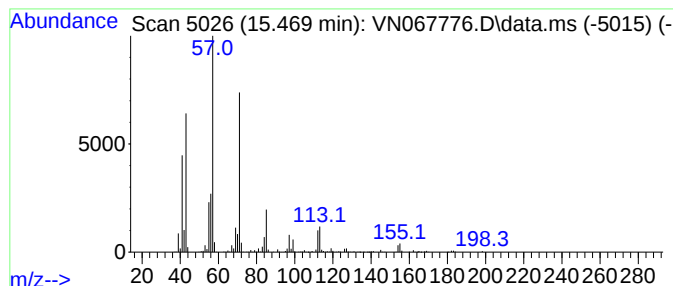
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane, 4,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	39.78 ug/l	1405610	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	91
2			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	86
3			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	86
4			Decane, 2-methyl-	156	C11H24	006975-98-0	83
5			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
Data File : VN067776.D
Acq On : 16 Jul 2021 16:34
Operator : JC/MD
Sample : M3051-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

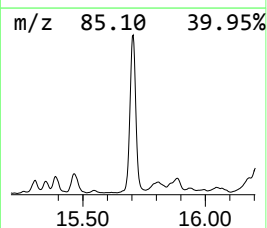
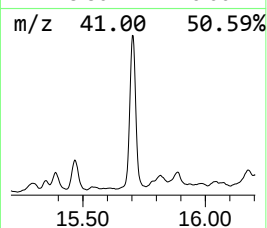
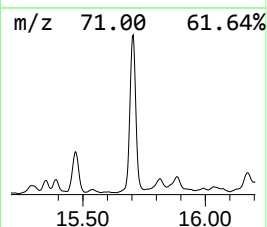
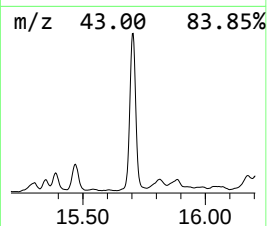
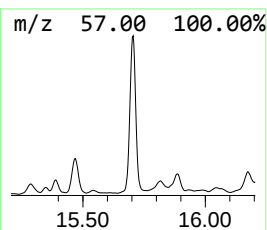
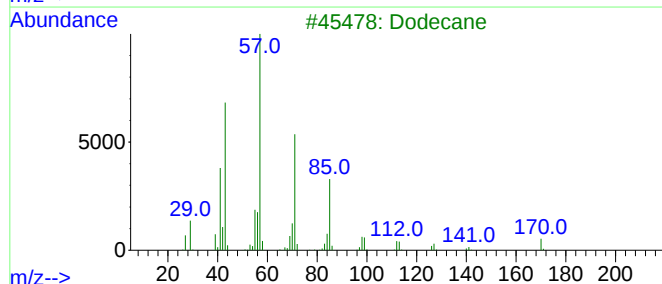
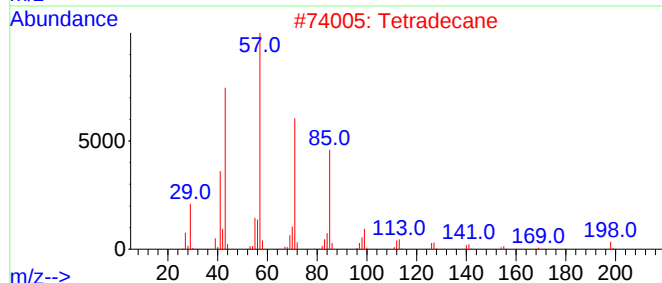
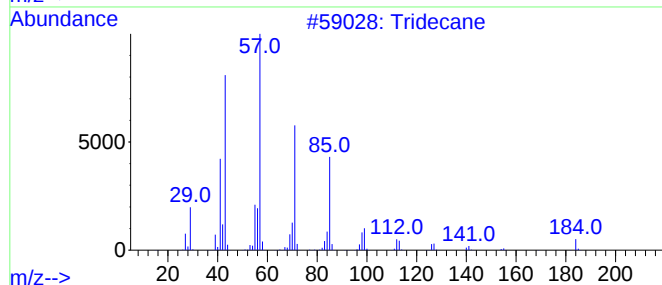
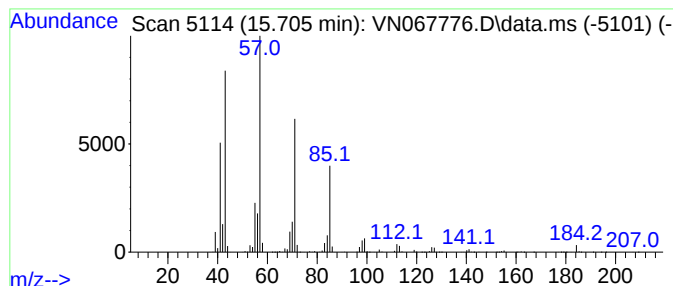
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.705	174.55 ug/l	6167840	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Tetradecane	198	C14H30	000629-59-4	86
3			Dodecane	170	C12H26	000112-40-3	86
4			Hexadecane	226	C16H34	000544-76-3	72
5			Decane, 3-bromo-	220	C10H21Br	030571-71-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
Data File : VN067776.D
Acq On : 16 Jul 2021 16:34
Operator : JC/MD
Sample : M3051-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

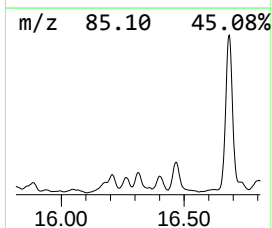
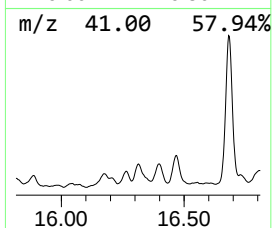
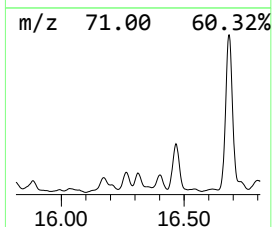
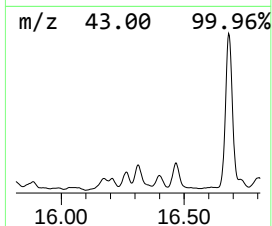
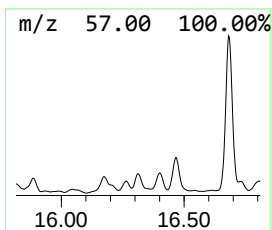
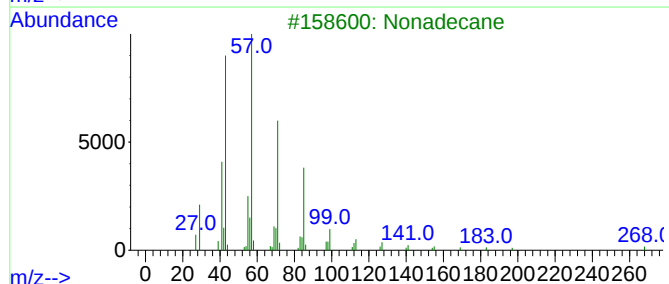
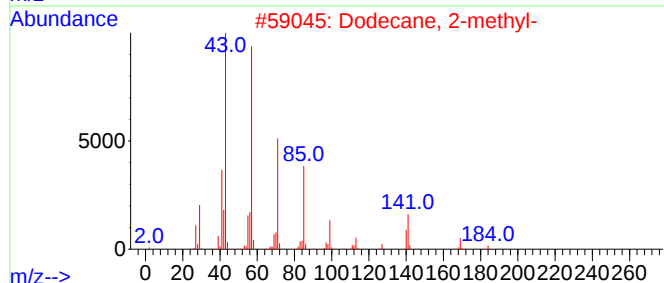
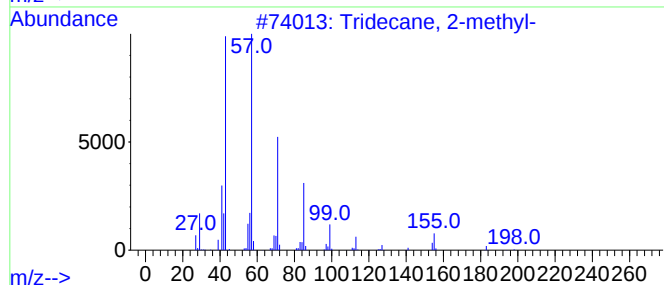
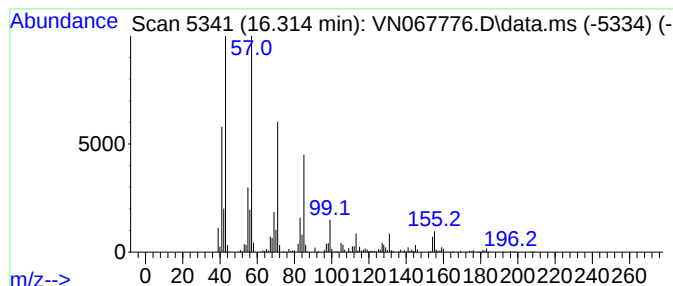
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	29.34 ug/l	1036700	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
3			Nonadecane	268	C19H40	000629-92-5	72
4			Heptadecane	240	C17H36	000629-78-7	72
5			Decane, 2-methyl-	156	C11H24	006975-98-0	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
Data File : VN067776.D
Acq On : 16 Jul 2021 16:34
Operator : JC/MD
Sample : M3051-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

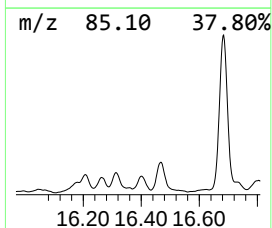
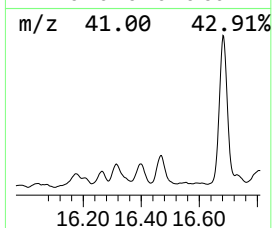
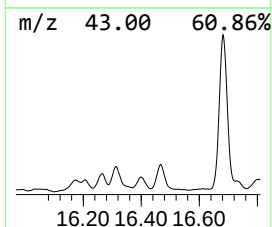
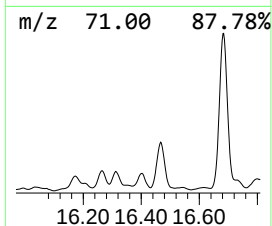
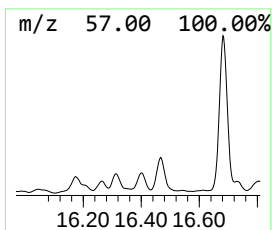
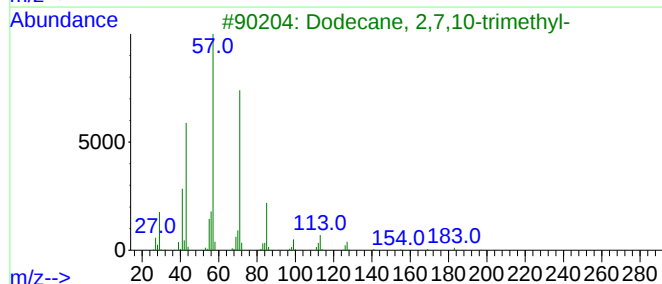
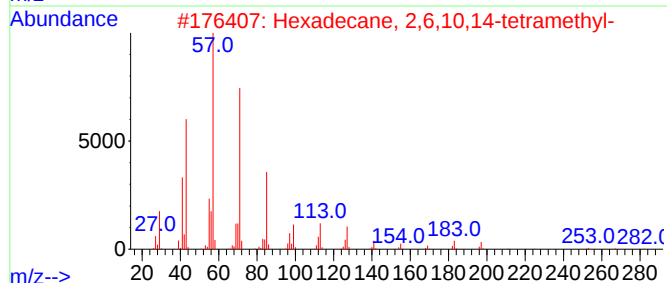
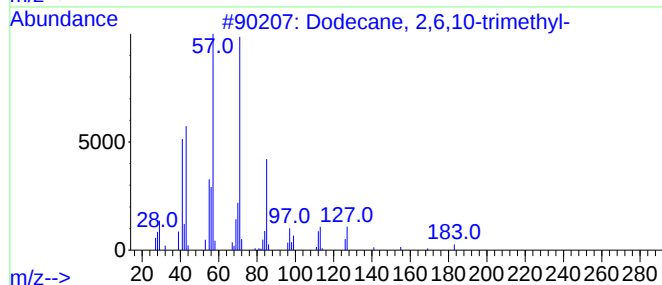
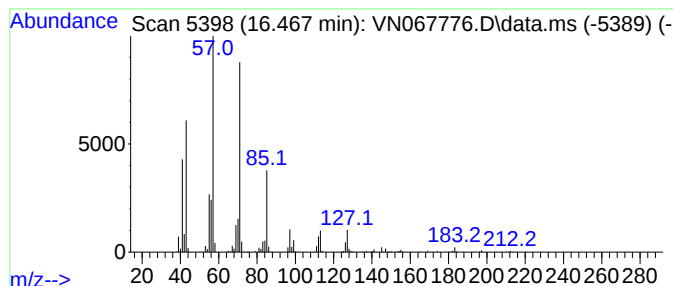
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,6,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.467	52.19 ug/l	1844320	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	91
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78
5			Octane, 2-methyl-	128	C9H20	003221-61-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
Data File : VN067776.D
Acq On : 16 Jul 2021 16:34
Operator : JC/MD
Sample : M3051-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

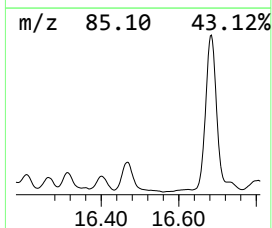
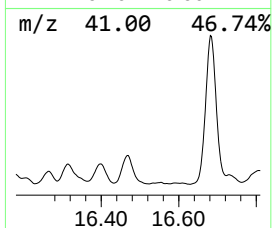
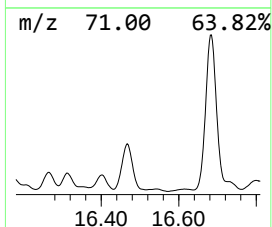
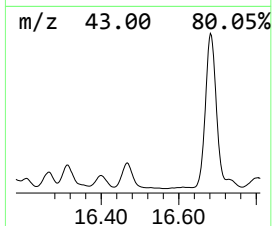
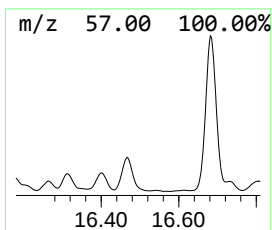
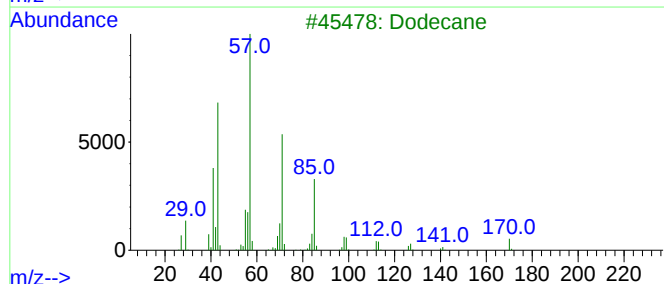
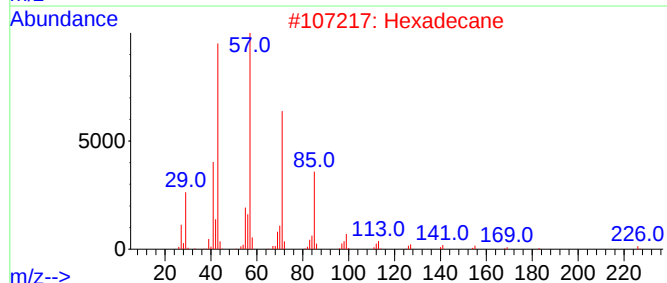
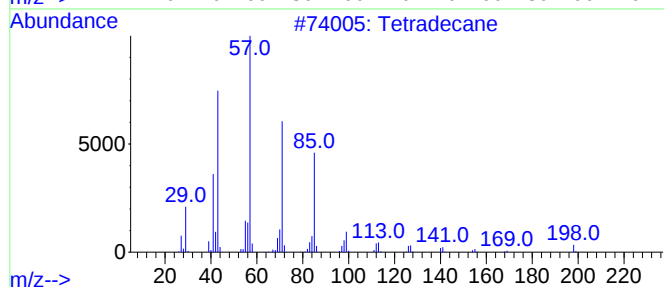
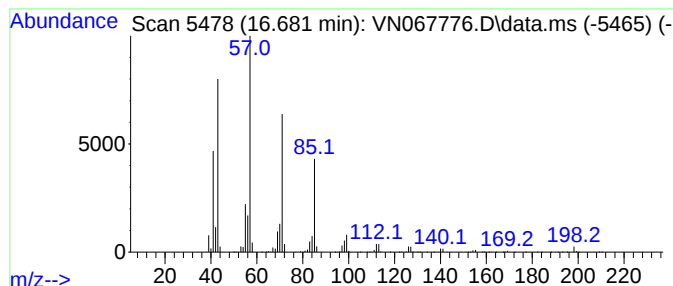
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Quant Title : SW846 8260

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

Peak Number 10 Hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.681	240.88 ug/l	8511550	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Hexadecane	226	C16H34	000544-76-3	91
3			Dodecane	170	C12H26	000112-40-3	81
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5			Decane, 3-bromo-	220	C10H21Br	030571-71-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071621\
Data File : VN067776.D
Acq On : 16 Jul 2021 16:34
Operator : JC/MD
Sample : M3051-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-41257-59

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070721W.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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Tetradecane	13.997	9.3	ug/l	326790	4	13.675	1766760	50.0
Carbonic acid, ...	14.847	51.8	ug/l	1829220	4	13.675	1766760	50.0
Undecane, 3,6-d...	14.968	17.0	ug/l	601135	4	13.675	1766760	50.0
Dodecane, 2-met...	15.389	19.6	ug/l	692028	4	13.675	1766760	50.0
Dodecane, 4,6-d...	15.469	39.8	ug/l	1405610	4	13.675	1766760	50.0
Tridecane	15.705	174.6	ug/l	6167840	4	13.675	1766760	50.0
Tridecane, 2-me...	16.314	29.3	ug/l	1036700	4	13.675	1766760	50.0
Dodecane, 2,6,1...	16.467	52.2	ug/l	1844320	4	13.675	1766760	50.0
Hexadecane	16.681	240.9	ug/l	8511550	4	13.675	1766760	50.0