

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122419\
 Data File : VX014245.D
 Acq On : 24 Dec 2019 15:15
 Operator : JC/SP
 Sample : K6406-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C-WATER_12.20.19

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	43	rBV	929590	1132949	36.21%	4.095%
2	1.277	59	64	69	rBV2	163538	208898	6.68%	0.755%
3	1.607	109	118	122	rVB2	35914	79860	2.55%	0.289%
4	2.436	249	254	259	rVB	23654	42286	1.35%	0.153%
5	5.490	743	755	765	rBV	282440	808032	25.83%	2.920%
6	5.648	770	781	793	rBV	513142	1428784	45.67%	5.164%
7	6.051	834	847	858	rBV	317810	841651	26.90%	3.042%
8	6.849	969	978	990	rBV	789981	1824957	58.33%	6.596%
9	8.709	1277	1283	1291	rBV	1641933	2527574	80.79%	9.135%
10	9.434	1394	1402	1407	rBV	116511	174140	5.57%	0.629%
11	10.105	1505	1512	1523	rBV	1559305	2195113	70.17%	7.933%
12	10.709	1604	1611	1614	rBV2	28158	44798	1.43%	0.162%
13	11.135	1675	1681	1687	rBV	1252354	1665301	53.23%	6.019%
14	11.282	1701	1705	1711	rVV	23811	33663	1.08%	0.122%
15	12.074	1830	1835	1848	rBV	1656739	2052896	65.62%	7.419%
16	12.263	1862	1866	1879	rBV	251602	400838	12.81%	1.449%
17	12.385	1879	1886	1890	rVV7	21668	50601	1.62%	0.183%
18	12.434	1890	1894	1898	rVV2	26508	41705	1.33%	0.151%
19	12.507	1902	1906	1913	rVB3	52415	93874	3.00%	0.339%
20	12.605	1918	1922	1927	rVB3	29197	43466	1.39%	0.157%
21	12.672	1928	1933	1936	rBV7	22869	35539	1.14%	0.128%
22	12.787	1947	1952	1953	rBV	68736	87494	2.80%	0.316%
23	12.836	1953	1960	1964	rVV2	346856	744592	23.80%	2.691%
24	12.909	1964	1972	1978	rVV	1377193	2400959	76.75%	8.677%
25	12.958	1978	1980	1987	rVV6	117750	286768	9.17%	1.036%
26	13.019	1987	1990	1992	rVV	201536	274656	8.78%	0.993%
27	13.043	1992	1994	1997	rVV2	247830	350315	11.20%	1.266%
28	13.074	1997	1999	2001	rVV	234141	285470	9.12%	1.032%
29	13.117	2001	2006	2008	rVV3	392146	757927	24.23%	2.739%
30	13.153	2008	2012	2014	rVV	1587109	2261899	72.30%	8.175%
31	13.178	2014	2016	2027	rVV2	1793583	3128464	100.00%	11.307%
32	13.263	2027	2030	2037	rVB	477427	665449	21.27%	2.405%
33	13.470	2058	2064	2068	rBV2	63631	113414	3.63%	0.410%
34	13.604	2079	2086	2088	rBV7	29127	70358	2.25%	0.254%

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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

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Title : SW846 8260

35	13.635	2089	2091	2095	rVV3	44818	56563	1.81%	0.204%
36	13.745	2106	2109	2113	rBV3	27008	47029	1.50%	0.170%
37	13.806	2114	2119	2129	rVB2	168207	378039	12.08%	1.366%
38	14.086	2162	2165	2169	rVB	26614	32983	1.05%	0.119%

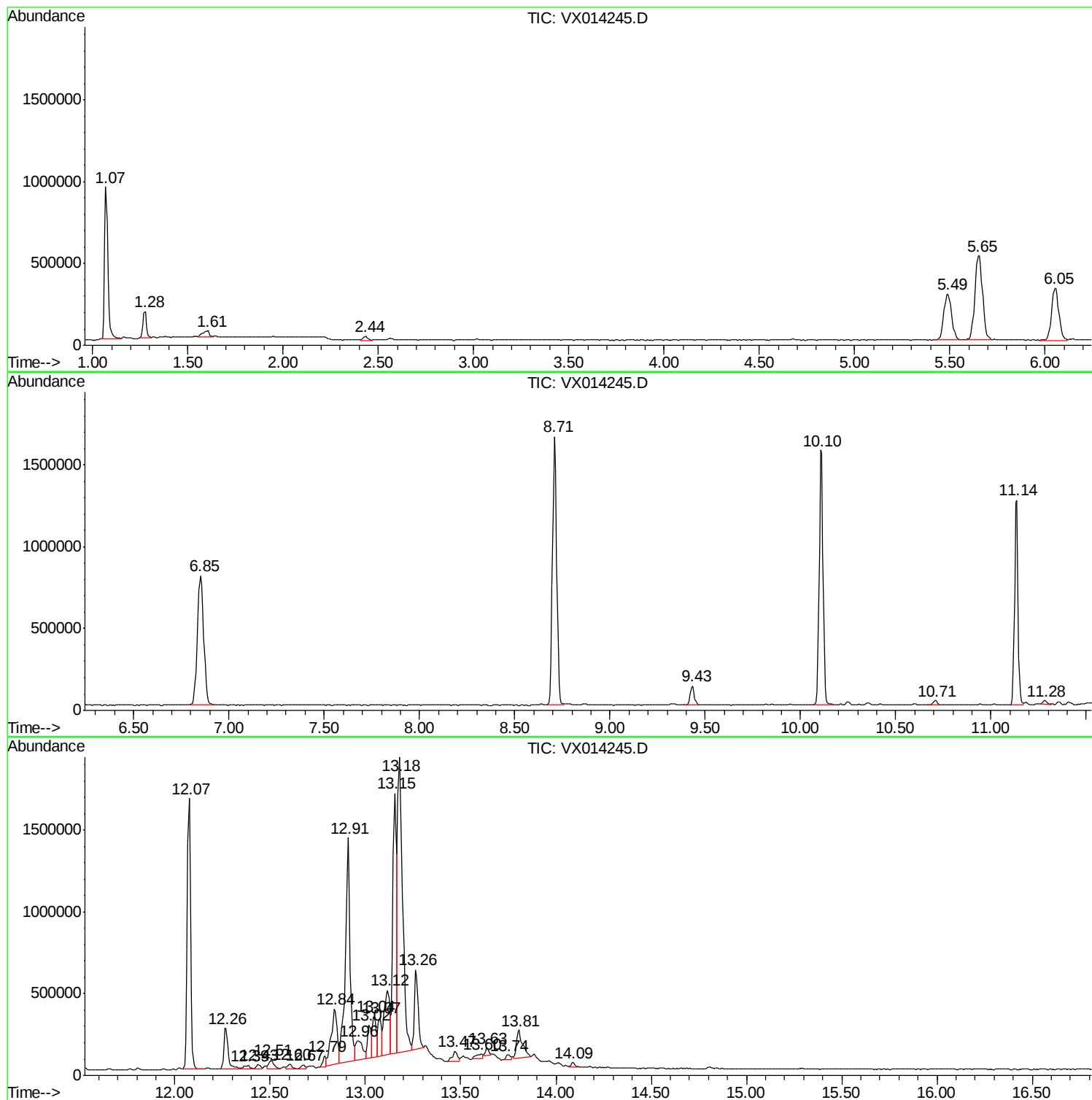
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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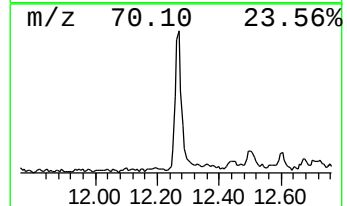
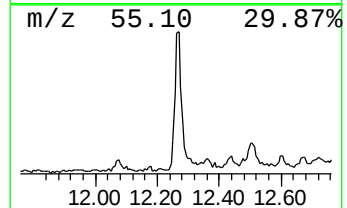
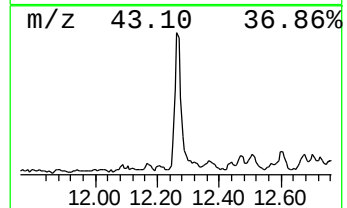
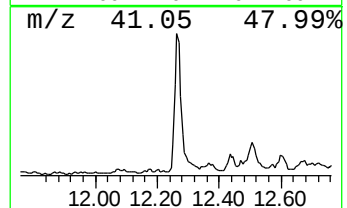
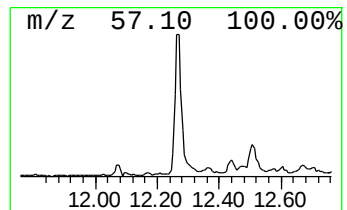
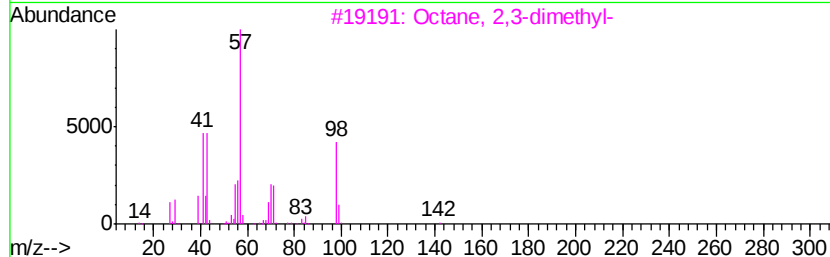
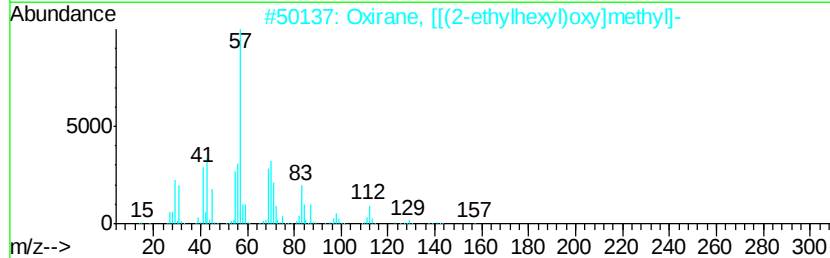
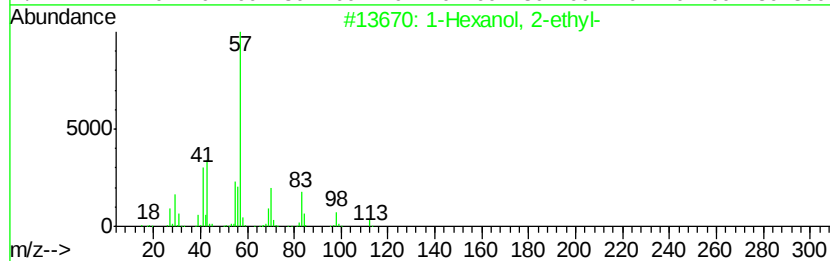
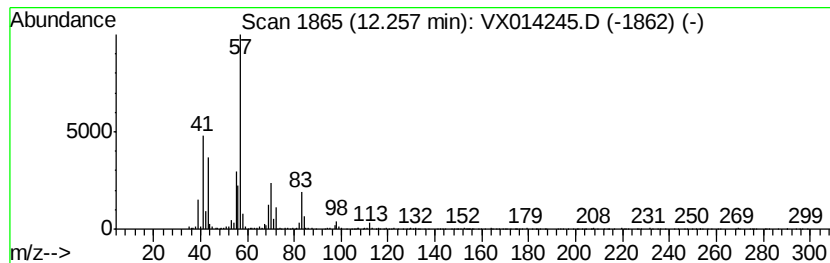
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	9.76 ug/l	400838	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2		Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	64
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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Instrument :
MSVOA_X
ClientSampleId :
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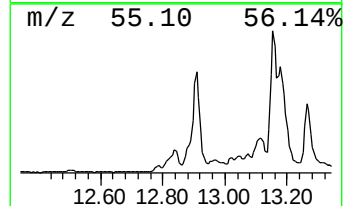
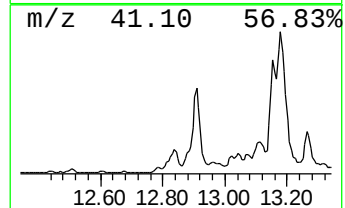
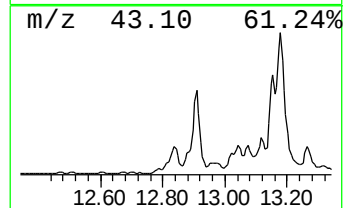
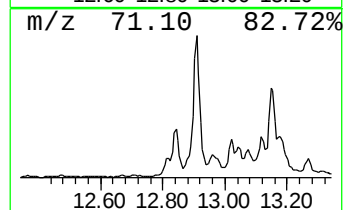
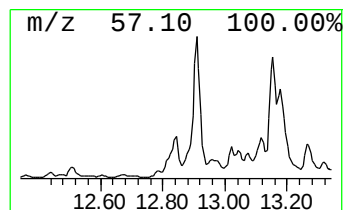
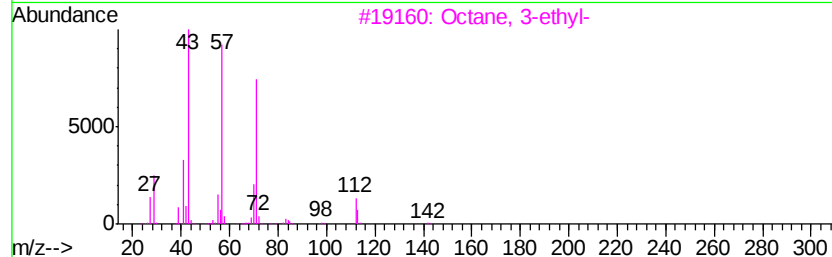
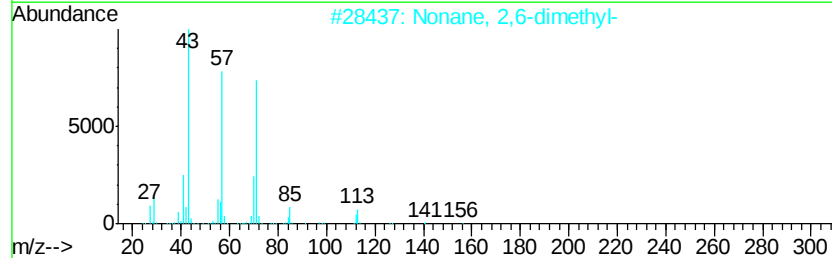
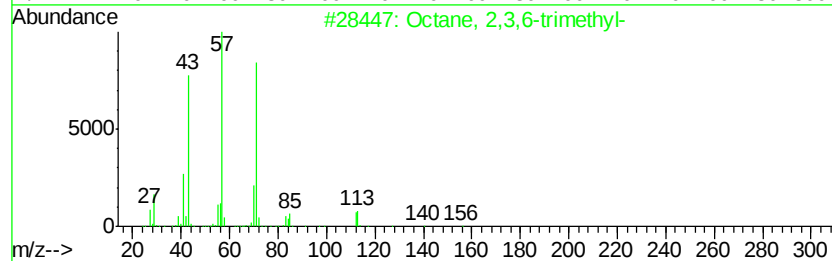
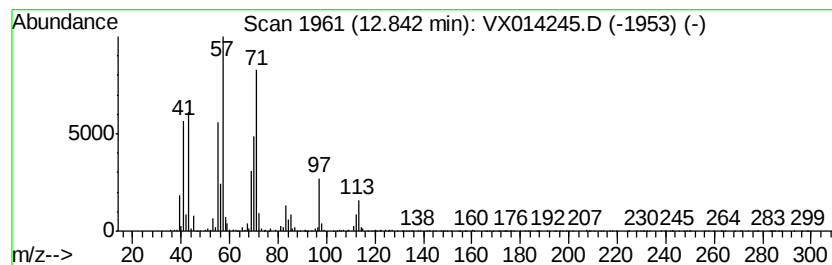
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane, 2,3,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	18.14 ug/l	744592	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	53
2		Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	50
3		Octane, 3-ethyl-	142	C10H22	005881-17-4	49
4		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	47
5		Decane, 4-methyl-	156	C11H24	002847-72-5	47



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C-WATER_12.20.19

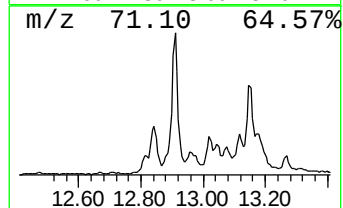
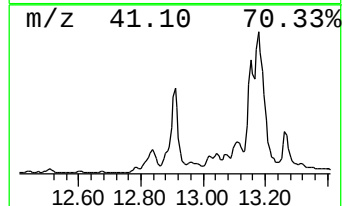
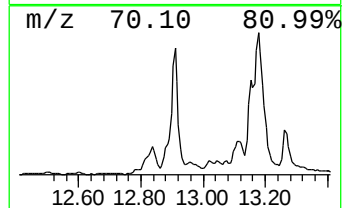
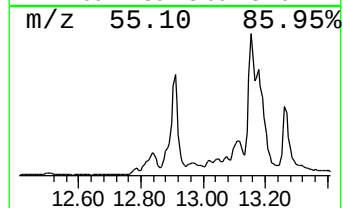
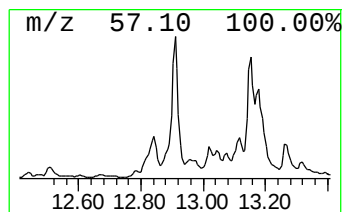
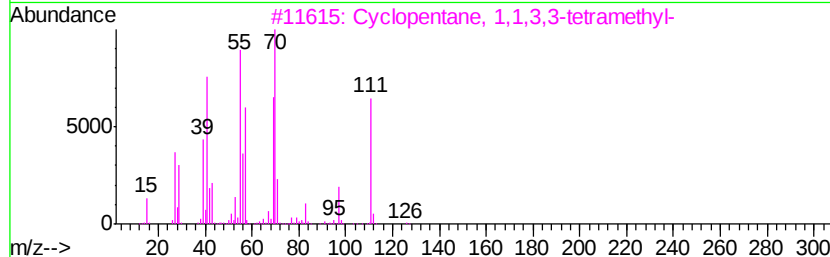
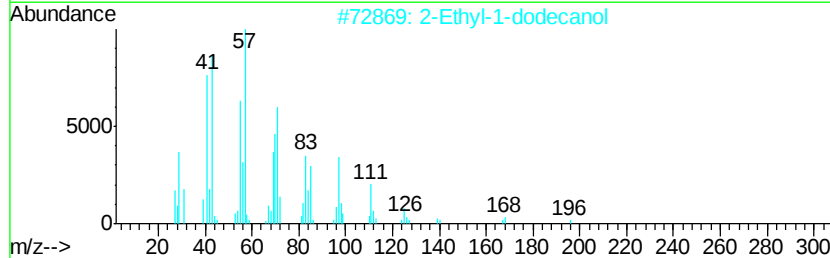
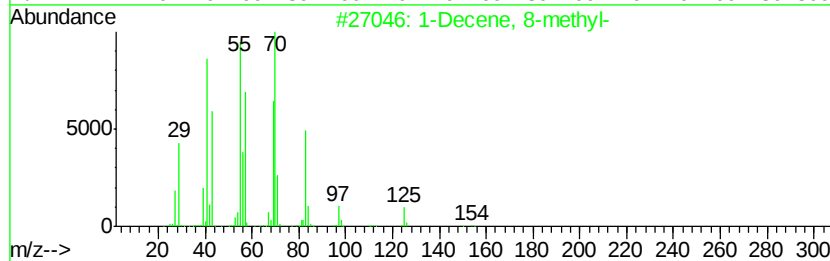
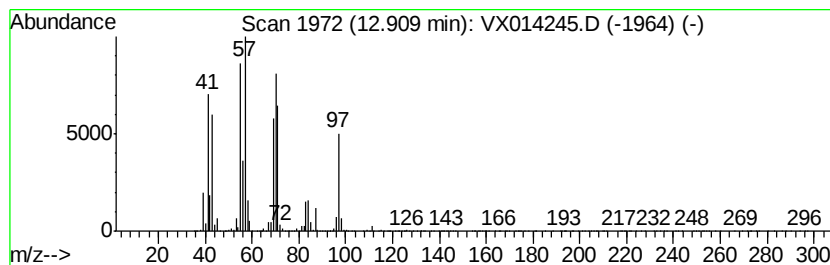
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Decene, 8-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	58.48 ug/l	2400960	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decene, 8-methyl-	154	C11H22	061142-79-8	50
2		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	47
3		Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	47
4		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	47
5		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47



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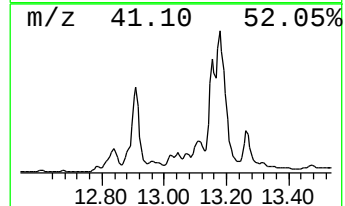
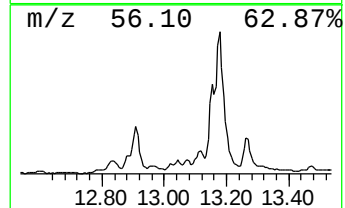
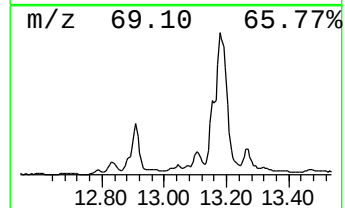
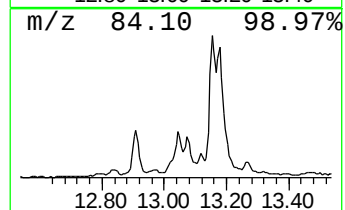
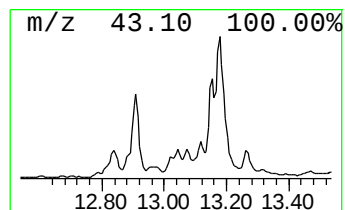
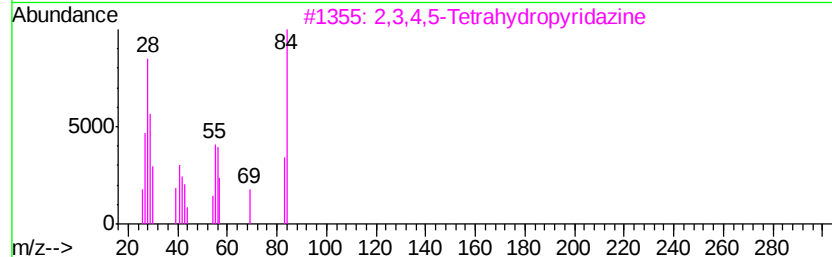
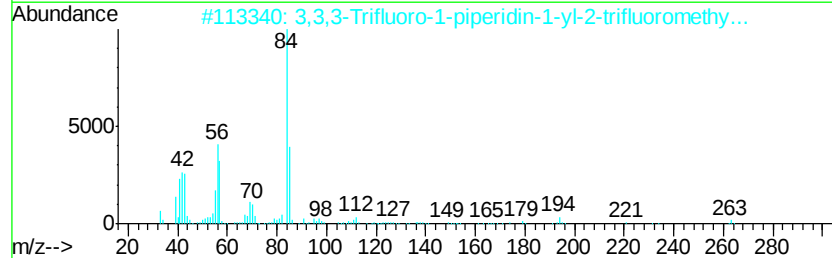
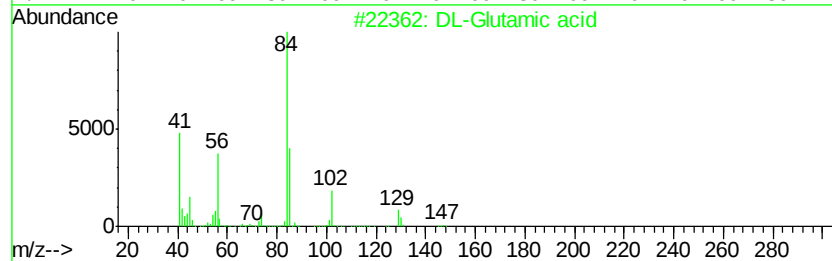
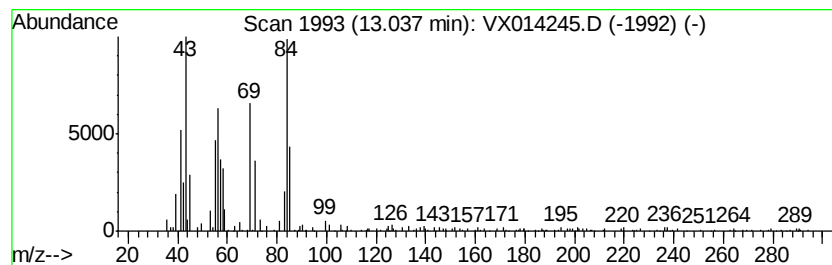
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 DL-Glutamic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.04	8.53 ug/l	350315	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		DL-Glutamic acid	147 C5H9NO4	000617-65-2 53
2		3,3,3-Trifluoro-1-piperidin-1-yl...	263 C9H11F6NO	1000300-43-7 50
3		2,3,4,5-Tetrahydrovridazine	84 C4H8N2	000694-06-4 43
4		Piperidine	85 C5H11N	000110-89-4 43
5		Acetic acid, 2-acetoxymethyl-1,2...	230 C12H22O4	1000187-50-7 38



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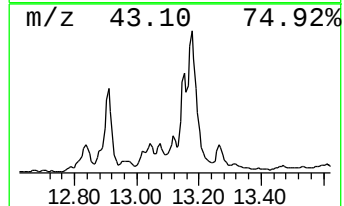
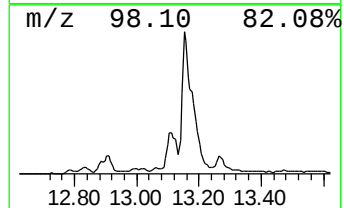
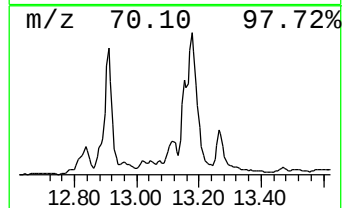
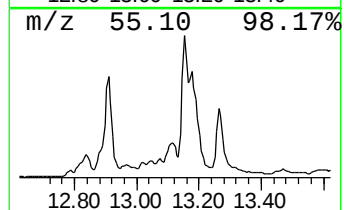
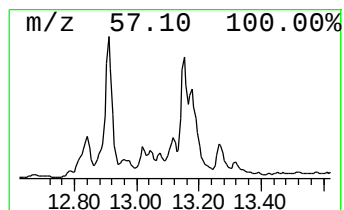
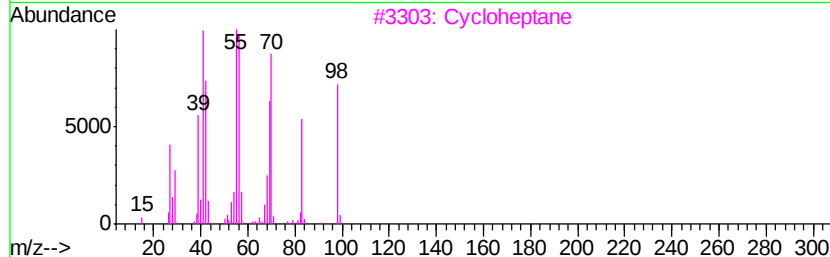
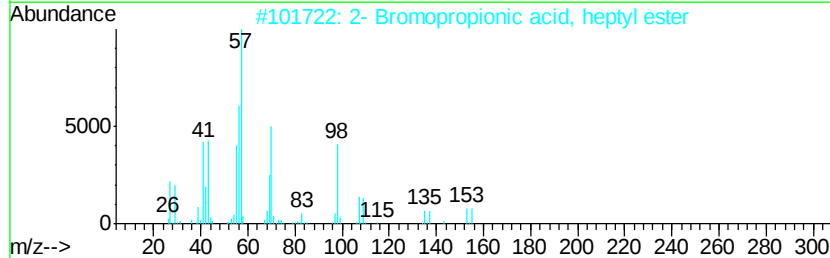
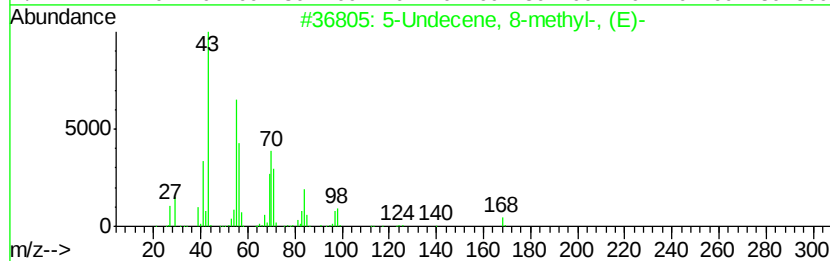
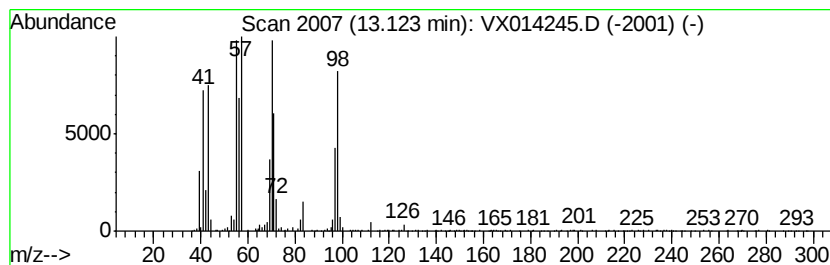
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5-Undecene, 8-methyl-, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	18.46 ug/l	757927	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Undecene, 8-methyl-, (E)-	168	C12H24	039546-85-5	50
2		2- Bromopropionic acid, heptyl e...	250	C10H19BrO2	038674-99-6	50
3		Cycloheptane	98	C7H14	000291-64-5	49
4		1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	47
5		Isopropylcyclobutane	98	C7H14	000872-56-0	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122419\
Data File : VX014245.D
Acq On : 24 Dec 2019 15:15
Operator : JC/SP
Sample : K6406-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C-WATER_12.20.19

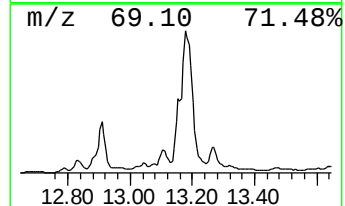
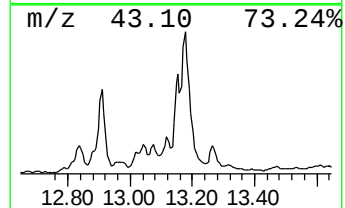
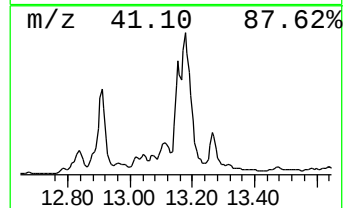
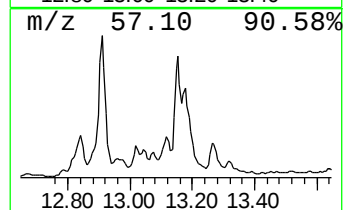
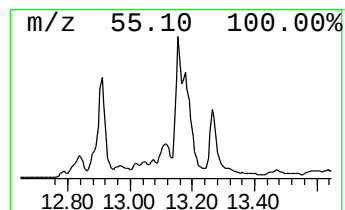
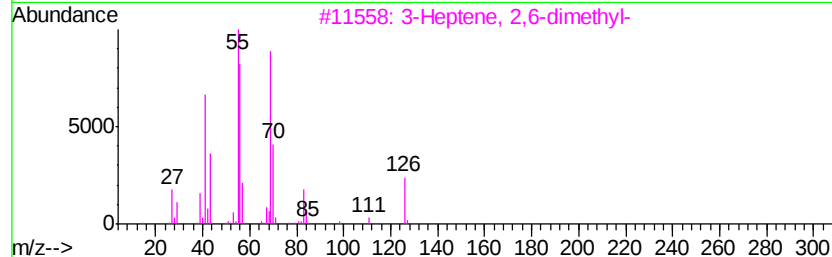
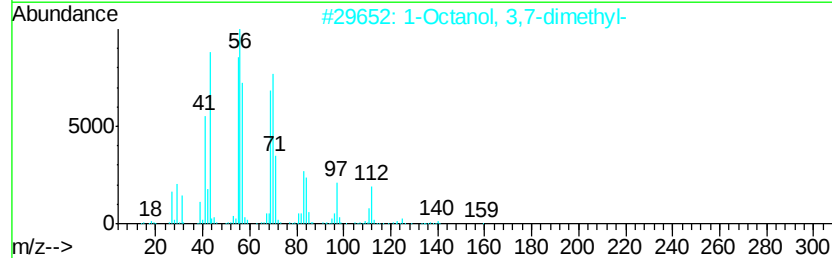
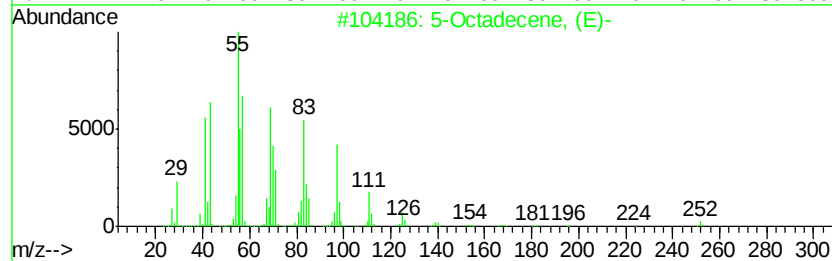
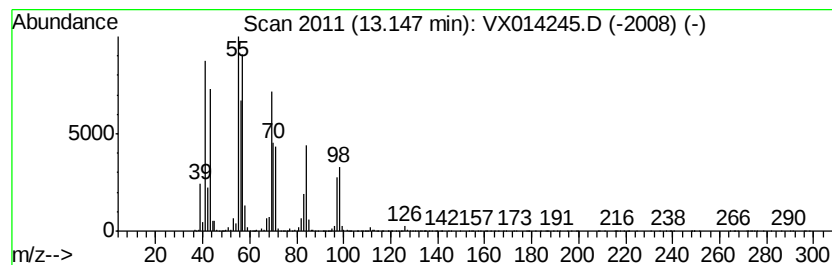
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	55.09 ug/l	2261900	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-		252	C18H36	007206-21-5	50
2	1-Octanol, 3,7-dimethyl-		158	C10H22O	000106-21-8	47
3	3-Heptene, 2,6-dimethyl-		126	C9H18	002738-18-3	45
4	1-Heptanol, 6-methyl-		130	C8H18O	001653-40-3	43
5	2-Hexene, 4-methyl-, (E)-		98	C7H14	003683-22-5	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122419\
 Data File : VX014245.D
 Acq On : 24 Dec 2019 15:15
 Operator : JC/SP
 Sample : K6406-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C-WATER_12.20.19

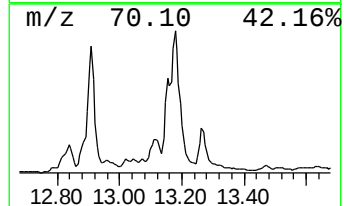
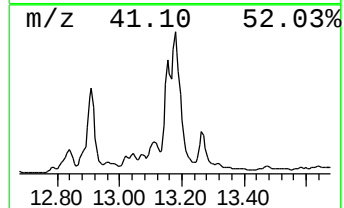
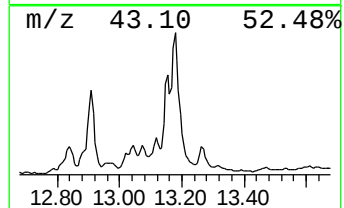
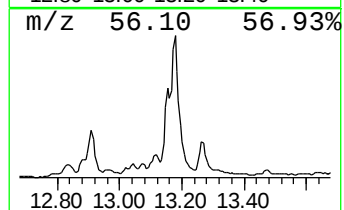
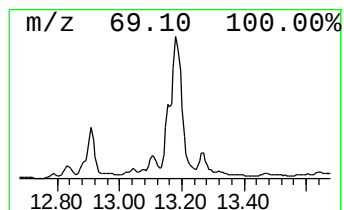
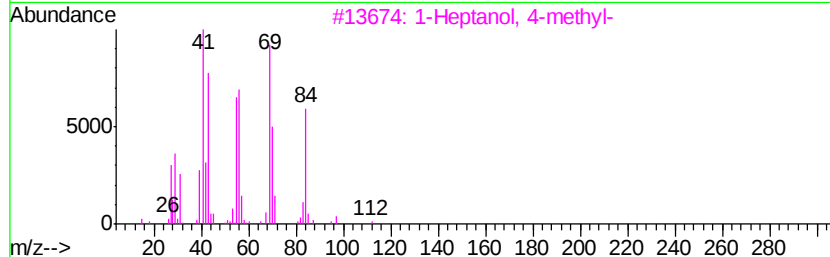
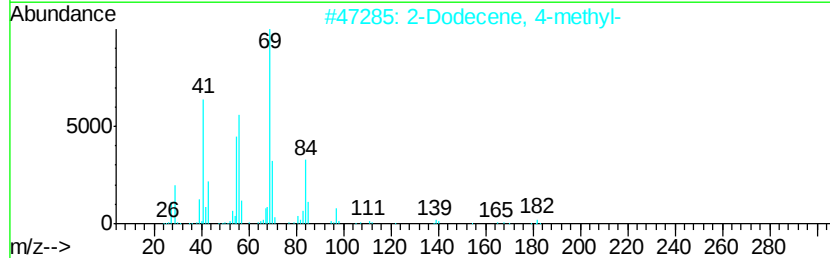
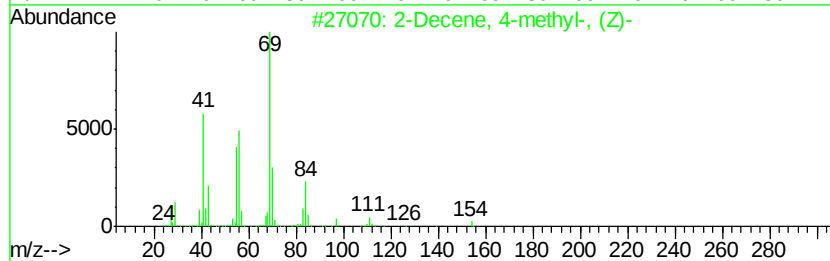
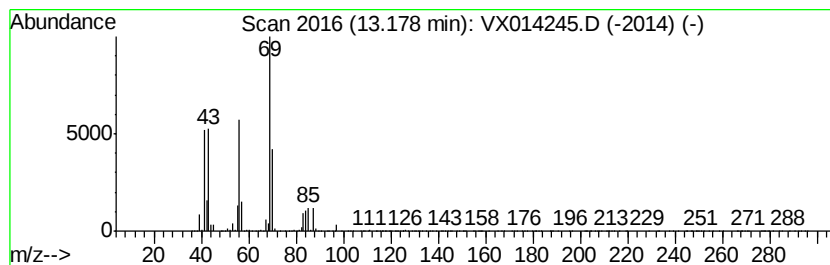
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 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 9 2-Decene, 4-methyl-, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	76.20 ug/l	3128460	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	56
2		2-Dodecene, 4-methyl-	182	C13H26	056851-45-7	56
3		1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	56
4		1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	45
5		2-Undecene, 4-methyl-	168	C12H24	091695-32-8	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122419\
Data File : VX014245.D
Acq On : 24 Dec 2019 15:15
Operator : JC/SP
Sample : K6406-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

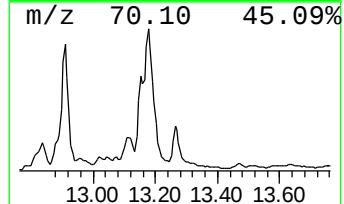
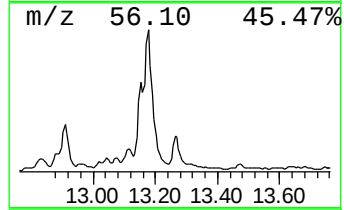
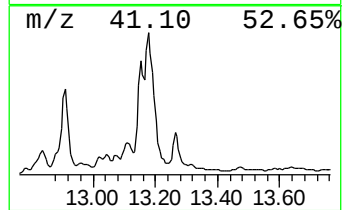
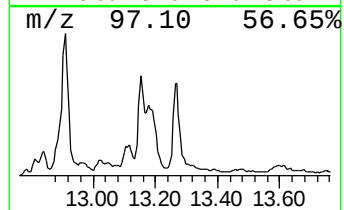
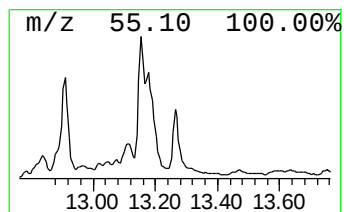
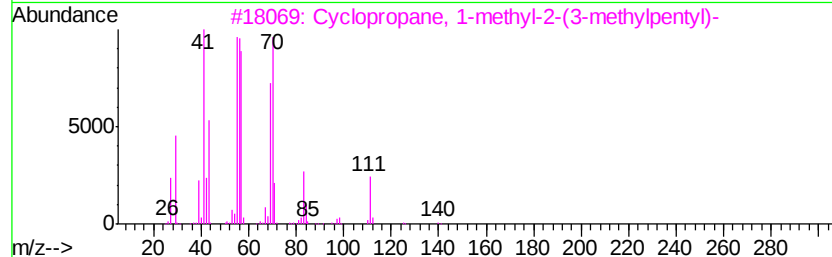
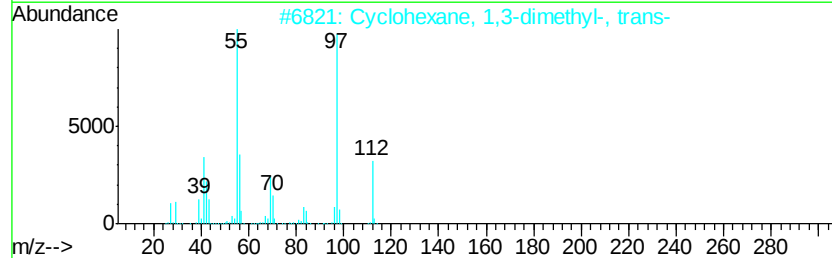
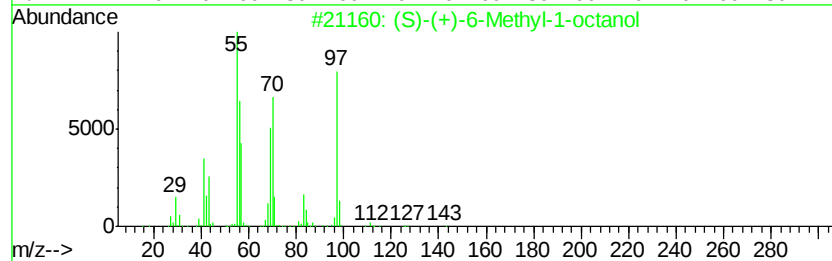
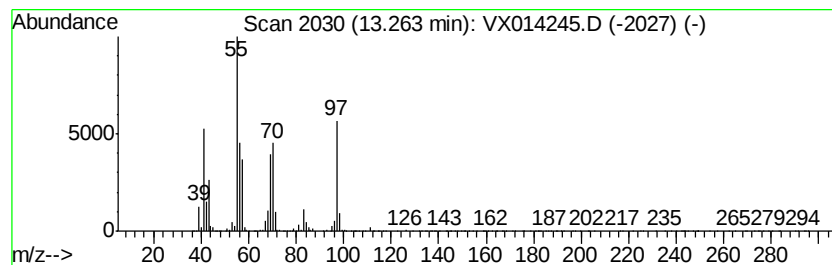
Instrument :
MSVOA_X
ClientSampleId :
C-WATER_12.20.19

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 (S)-(+)-6-Methyl-1-octanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.26	16.21 ug/l	665449	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	86
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	53
3	Cyclopropane, 1-methyl-2-(3-meth...	140	C10H20	062238-07-7	50
4	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	47
5	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122419\
Data File : VX014245.D
Acq On : 24 Dec 2019 15:15
Operator : JC/SP
Sample : K6406-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C-WATER_12.20.19

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-ethyl-	12.26	9.8	ug/l	400838	4	12.07	2052900	50.0
Octane, 2,3,6-tri...	12.84	18.1	ug/l	744592	4	12.07	2052900	50.0
1-Decene, 8-methyl-	12.91	58.5	ug/l	2400960	4	12.07	2052900	50.0
DL-Glutamic acid	13.04	8.5	ug/l	350315	4	12.07	2052900	50.0
5-Undecene, 8-met...	13.12	18.5	ug/l	757927	4	12.07	2052900	50.0
5-Octadecene, (E)-	13.15	55.1	ug/l	2261900	4	12.07	2052900	50.0
2-Decene, 4-methy...	13.18	76.2	ug/l	3128460	4	12.07	2052900	50.0
(S)-(+)-6-Methyl-...	13.26	16.2	ug/l	665449	4	12.07	2052900	50.0