

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062718\
 Data File : VX002936.D
 Acq On : 27 Jun 2018 15:11
 Operator : JC/MD
 Sample : J3707-02
 Misc : 5.97µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WP021SB488-23-25-180622

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\82X062518W.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	1.069	75	79	93	rBV	512853	702494	2.22%	0.420%
2	1.410	130	135	147	rVB	754966	1154055	3.65%	0.690%
3	5.507	795	807	823	rBV4	148188	562094	1.78%	0.336%
4	5.659	823	832	854	rVB	239862	745049	2.36%	0.446%
5	6.068	888	899	907	rBV	164762	448618	1.42%	0.268%
6	6.860	1018	1029	1046	rBV	335139	814416	2.58%	0.487%
7	7.458	1115	1127	1137	rBV	147758	342011	1.08%	0.205%
8	8.720	1329	1334	1339	rVB	793407	1240820	3.93%	0.742%
9	8.787	1339	1345	1359	rVB	3342054	5206185	16.48%	3.114%
10	8.970	1370	1375	1381	rBV	228835	321763	1.02%	0.192%
11	9.963	1533	1538	1544	rVB	721732	1037253	3.28%	0.620%
12	10.067	1549	1555	1559	rBV	572828	768284	2.43%	0.460%
13	10.116	1559	1563	1579	rVV	731184	1275312	4.04%	0.763%
14	10.256	1579	1586	1591	rVV	202789	316157	1.00%	0.189%
15	10.360	1591	1603	1608	rVV2	716322	1422380	4.50%	0.851%
16	10.415	1608	1612	1623	rVB	3718528	4842880	15.33%	2.897%
17	10.646	1643	1650	1655	rBV3	765159	1086349	3.44%	0.650%
18	10.701	1655	1659	1661	rVV	423627	564521	1.79%	0.338%
19	10.726	1661	1663	1667	rVV	697070	872371	2.76%	0.522%
20	10.768	1667	1670	1674	rVB	375552	472963	1.50%	0.283%
21	10.835	1674	1681	1685	rVB	1514884	2152512	6.81%	1.287%
22	10.884	1685	1689	1691	rBV	393201	533142	1.69%	0.319%
23	10.915	1691	1694	1697	rVV	1123223	1485583	4.70%	0.889%
24	10.951	1697	1700	1705	rVB	640581	859634	2.72%	0.514%
25	11.006	1705	1709	1714	rVB3	181823	363910	1.15%	0.218%
26	11.085	1714	1722	1725	rBV2	1371377	2353261	7.45%	1.408%
27	11.140	1725	1731	1733	rVV2	3331174	5330919	16.87%	3.189%
28	11.165	1733	1735	1741	rVB	3589348	4081764	12.92%	2.441%
29	11.219	1741	1744	1745	rBV	462817	459360	1.45%	0.275%
30	11.250	1745	1749	1752	rVV	2998961	3789542	11.99%	2.267%
31	11.280	1752	1754	1757	rVV2	424610	441858	1.40%	0.264%
32	11.360	1763	1767	1770	rBV3	236976	339292	1.07%	0.203%
33	11.402	1770	1774	1777	rBV2	280999	372221	1.18%	0.223%
34	11.439	1777	1780	1785	rVV2	724737	1131712	3.58%	0.677%

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 Stop Thrs : 0 Peak Location: TOP

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35	11.488	1785	1788	1791	rVV	1110968	1645263	5.21%	0.984%
36	11.536	1791	1796	1801	rVB	25123483	31596621	100.00%	18.898%
37	11.689	1814	1821	1825	rBV5	1466874	2440935	7.73%	1.460%
38	11.744	1826	1830	1832	rBV	1411697	1725325	5.46%	1.032%
39	11.774	1832	1835	1838	rVB	4787059	5124030	16.22%	3.065%
40	11.811	1838	1841	1844	rBV	1764962	2510212	7.94%	1.501%
41	11.896	1851	1855	1858	rBV	1617892	2270346	7.19%	1.358%
42	11.945	1858	1863	1868	rVV5	1503297	3144134	9.95%	1.881%
43	12.006	1868	1873	1875	rVV	2237356	3246369	10.27%	1.942%
44	12.030	1875	1877	1880	rVV3	1187418	1672642	5.29%	1.000%
45	12.097	1883	1888	1891	rVV2	3892884	6125519	19.39%	3.664%
46	12.128	1891	1893	1895	rVV	2819428	3337801	10.56%	1.996%
47	12.158	1895	1898	1902	rVV2	4707200	5808245	18.38%	3.474%
48	12.201	1902	1905	1906	rVV2	517868	577744	1.83%	0.346%
49	12.231	1906	1910	1918	rVB	3439194	4421279	13.99%	2.644%
50	12.329	1918	1926	1929	rBV2	736568	1501743	4.75%	0.898%
51	12.372	1929	1933	1941	rBV4	1669032	3718989	11.77%	2.224%
52	12.487	1946	1952	1956	rVV	19321601	23821220	75.39%	14.248%
53	12.524	1956	1958	1964	rVB3	860624	1416186	4.48%	0.847%
54	12.615	1970	1973	1975	rBV	334447	407398	1.29%	0.244%
55	12.640	1975	1977	1980	rVB2	652701	664580	2.10%	0.397%
56	12.670	1980	1982	1985	rVB	439958	414661	1.31%	0.248%
57	12.743	1990	1994	1996	rBV	460865	529473	1.68%	0.317%
58	12.774	1996	1999	2005	rVB4	532190	967344	3.06%	0.579%
59	12.878	2005	2016	2019	rBV5	670521	1370553	4.34%	0.820%
60	12.945	2024	2027	2031	rBV3	803288	1451164	4.59%	0.868%
61	13.024	2037	2040	2048	rVB3	1011422	1680128	5.32%	1.005%
62	13.097	2048	2052	2056	rBV3	463496	577331	1.83%	0.345%
63	13.323	2083	2089	2092	rBV	2206315	2695077	8.53%	1.612%
64	13.353	2092	2094	2099	rVB3	575026	679450	2.15%	0.406%
65	13.481	2111	2115	2126	rVB7	220081	603265	1.91%	0.361%
66	13.835	2169	2173	2180	rVB	570279	830389	2.63%	0.497%
67	14.097	2212	2216	2219	rVB	315324	325210	1.03%	0.195%

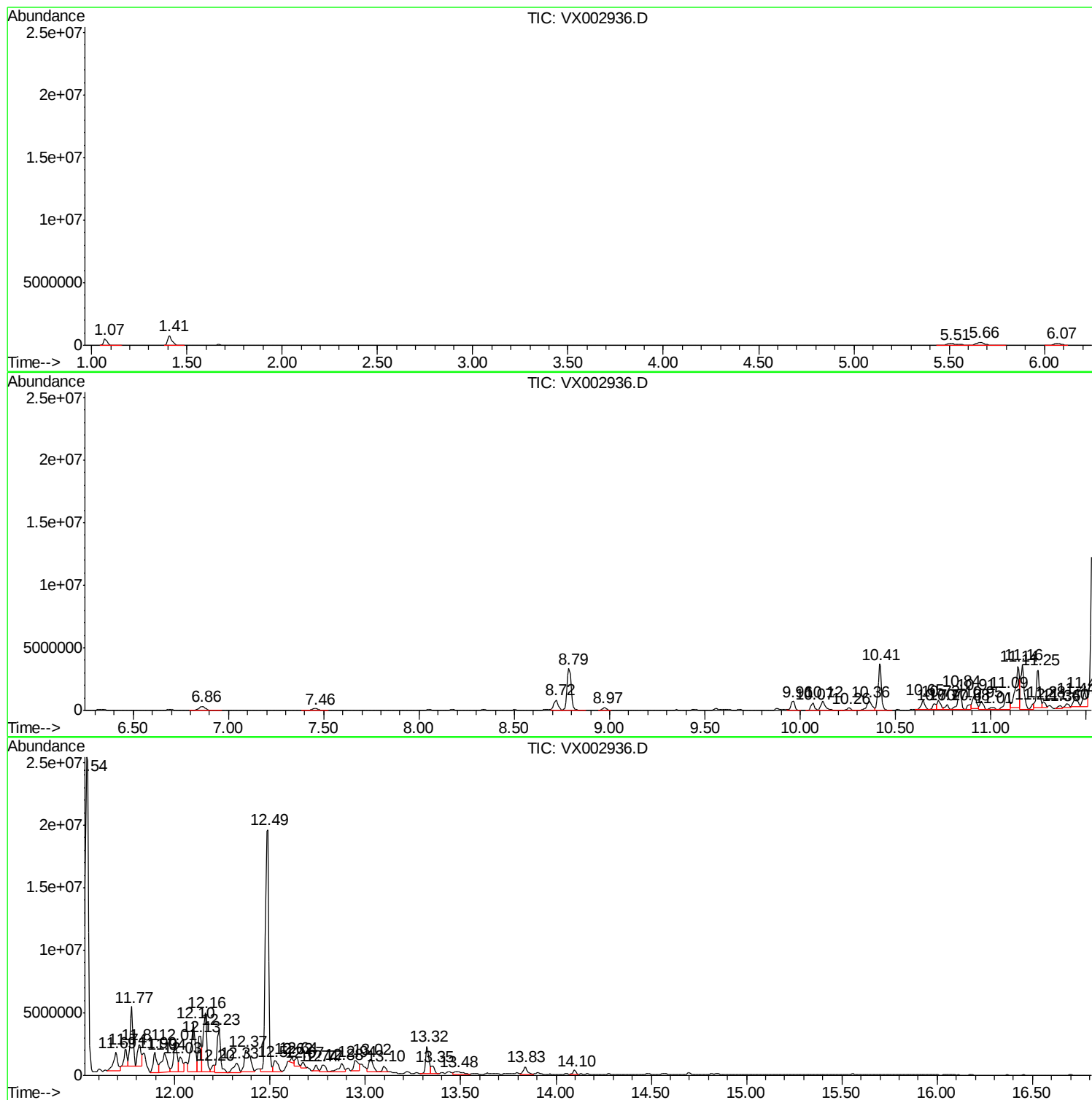
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Instrument :
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ClientSampleId :
WP021SB488-23-25-180622

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-23-25-180622

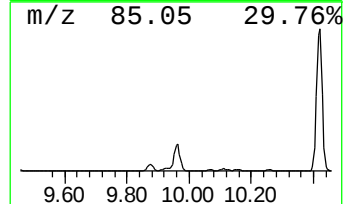
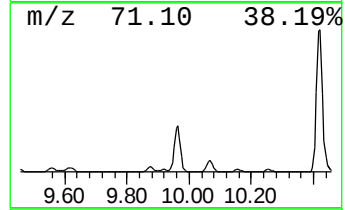
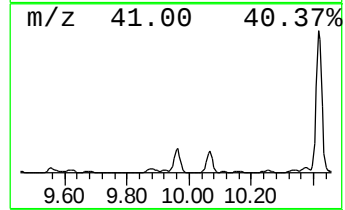
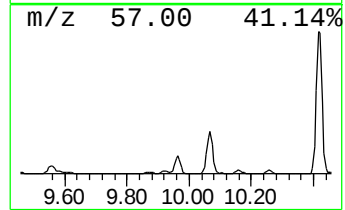
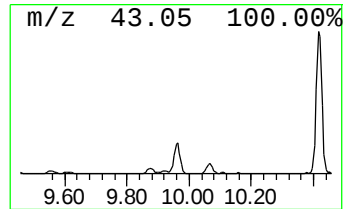
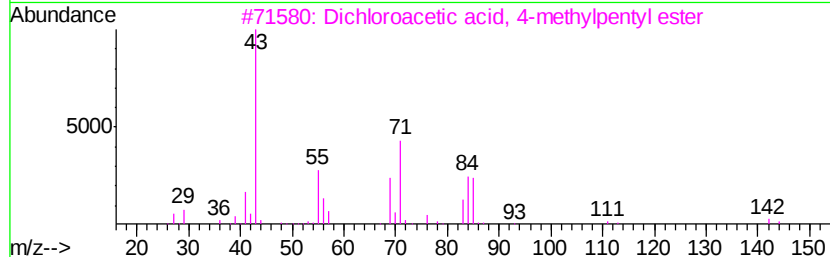
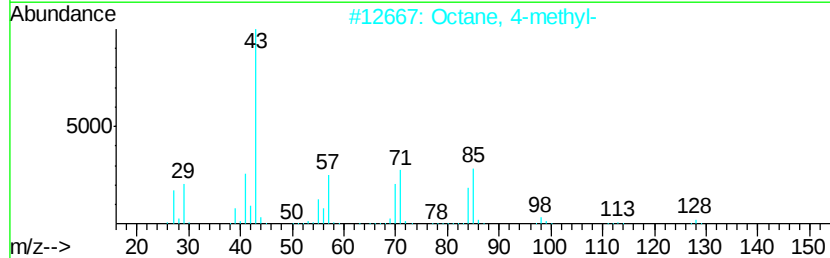
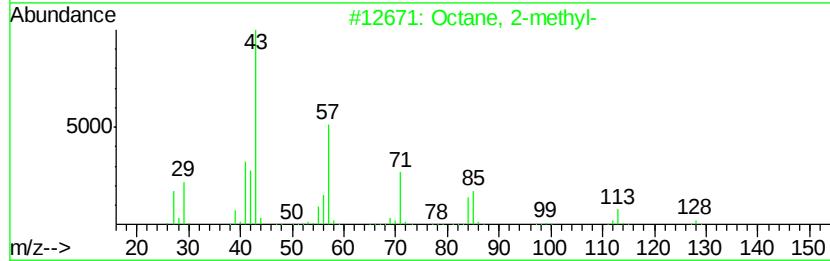
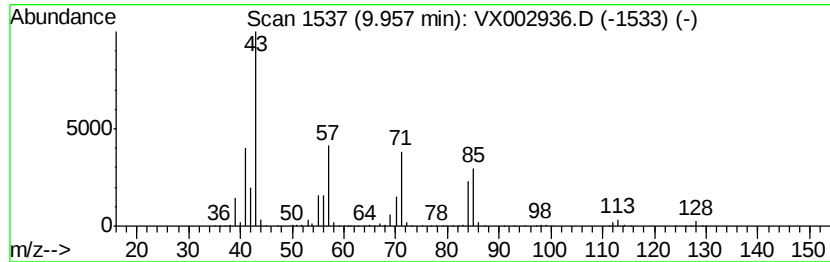
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Octane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.96	40.67 ug/l	1037250	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2-methyl-	128	C9H20	003221-61-2	87
2		Octane, 4-methyl-	128	C9H20	002216-34-4	72
3		Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	64
4		Dodecane, 5-methyl-	184	C13H28	017453-93-9	59
5		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	53



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ALS Vial : 10 Sample Multiplier: 1

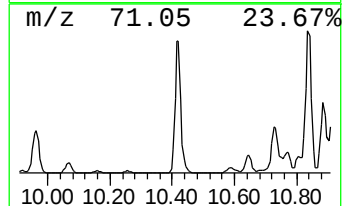
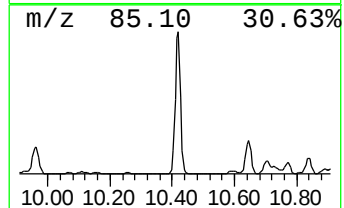
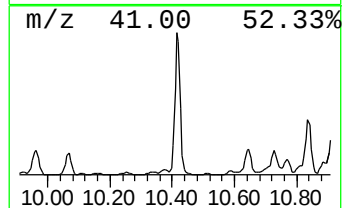
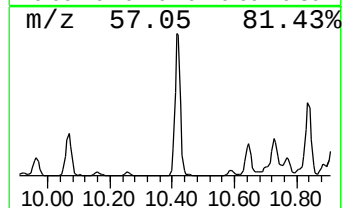
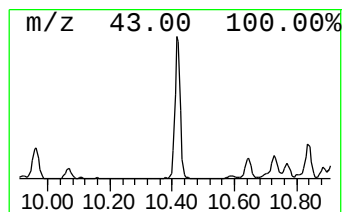
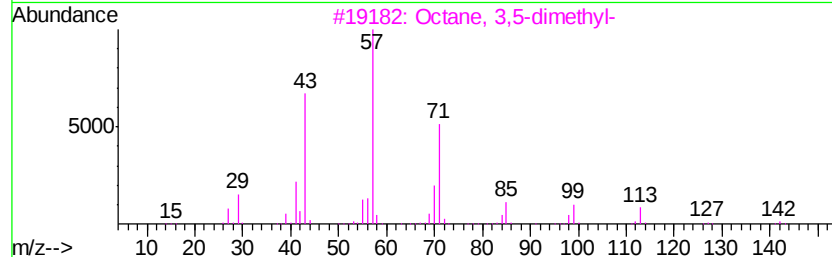
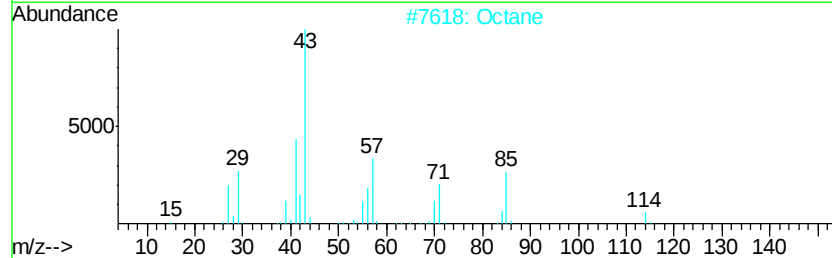
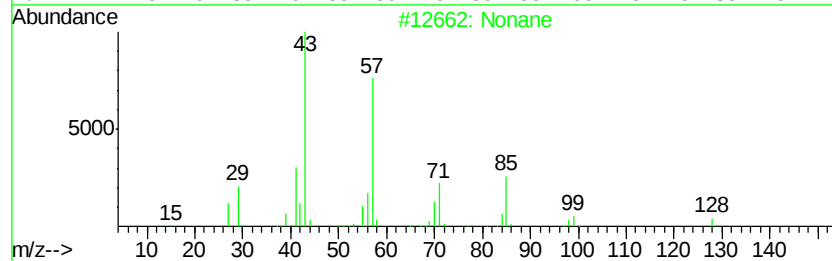
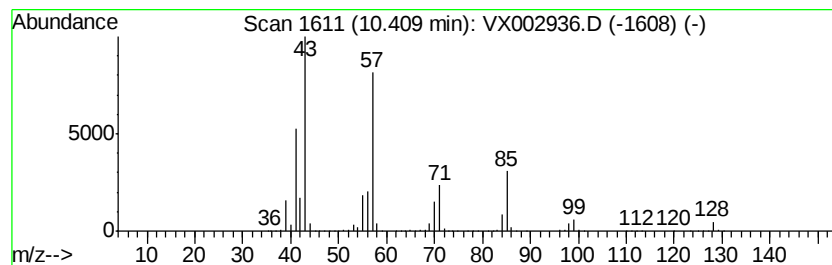
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 3 Nonane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	189.87 ug/l	4842880	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonane		128 C9H20	000111-84-2 97
2	Octane		114 C8H18	000111-65-9 74
3	Octane, 3,5-dimethyl-		142 C10H22	015869-93-9 53
4	Hexane, 2,4-dimethyl-		114 C8H18	000589-43-5 53
5	Butanoic acid, 3-oxo-, 1,1-dimet...		158 C8H14O3	001694-31-1 50



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ALS Vial : 10 Sample Multiplier: 1

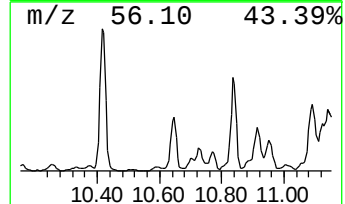
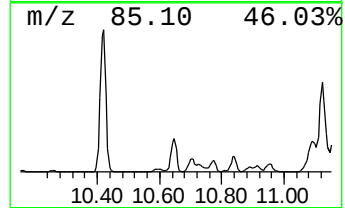
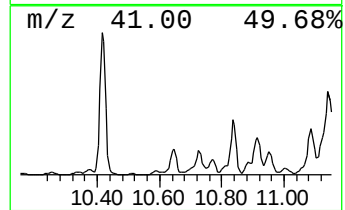
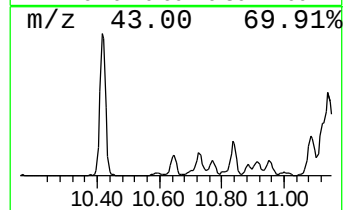
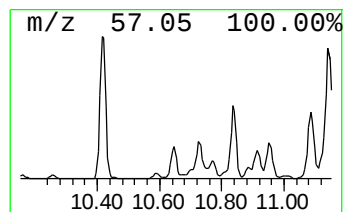
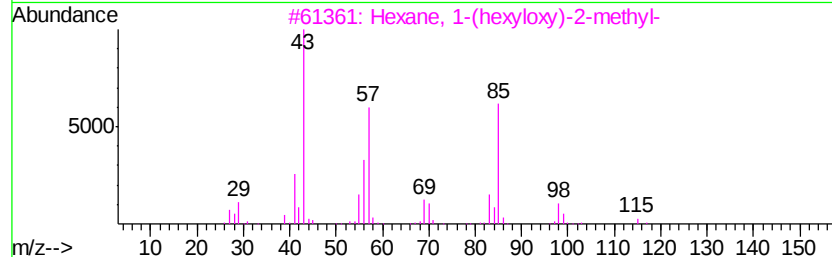
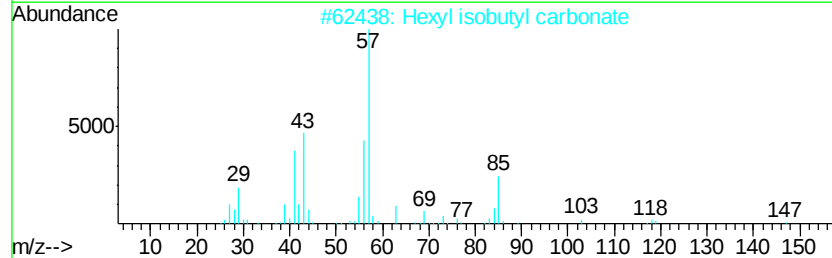
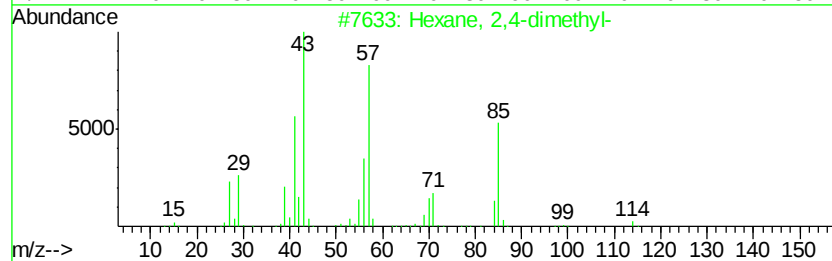
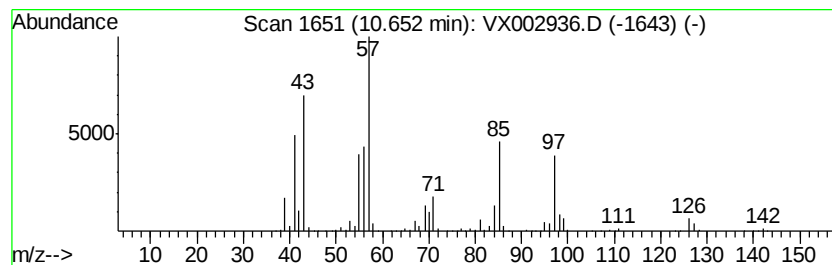
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	42.59 ug/l	1086350	Chlorobenzene-d5	10.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexane, 2,4-dimethyl-	114 C8H18	000589-43-5	59
2	Hexyl isobutyl carbonate	202 C11H22O3	959067-98-2	53
3	Hexane, 1-(hexyloxy)-2-methyl-	200 C13H28O	074421-17-3	47
4	Pentane, 2,2-dimethyl-	100 C7H16	000590-35-2	47
5	Hexane, 2,2,3,3-tetramethyl-	142 C10H22	013475-81-5	47



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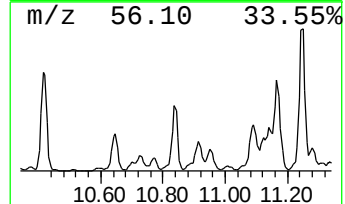
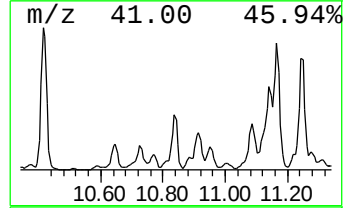
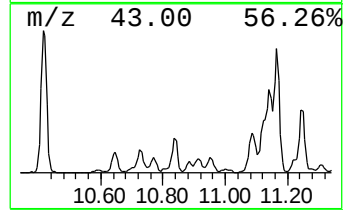
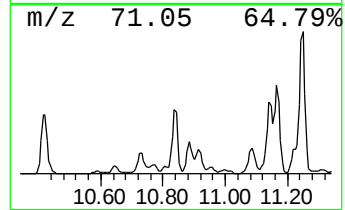
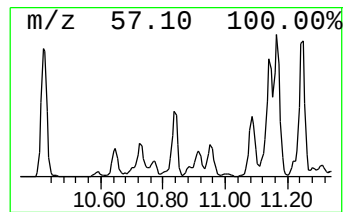
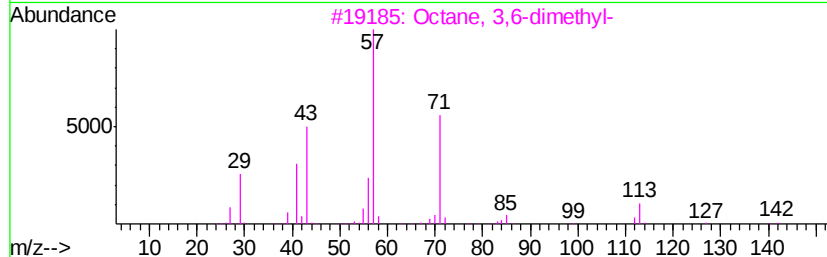
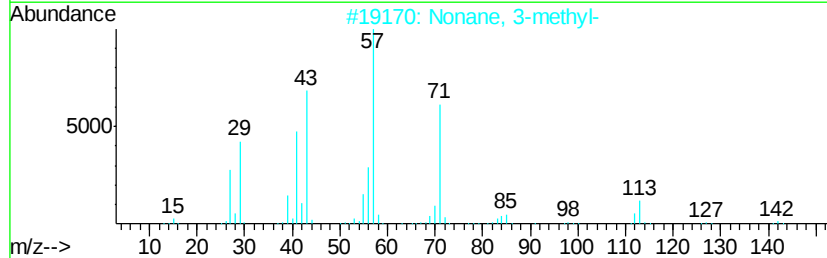
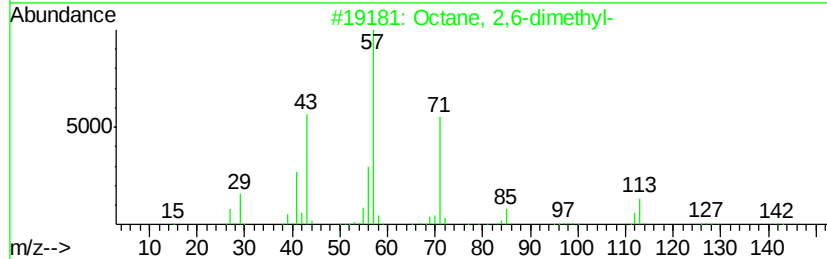
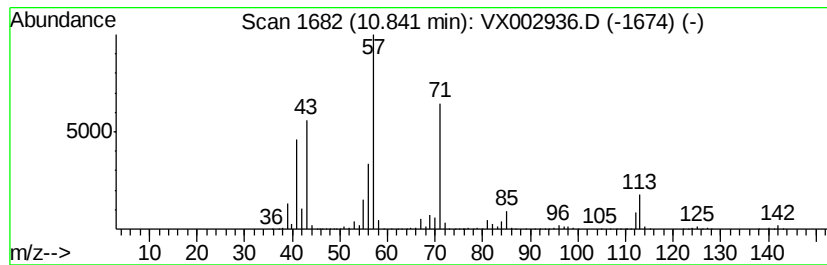
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	84.39 ug/l	2152510	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2		Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
4		3-Bromooctane	192	C8H17Br	000999-64-4	64
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97µL/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

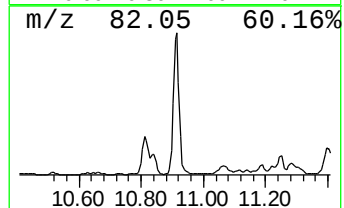
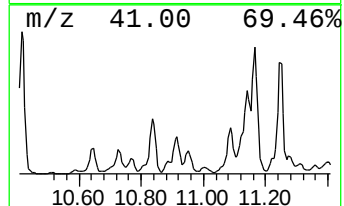
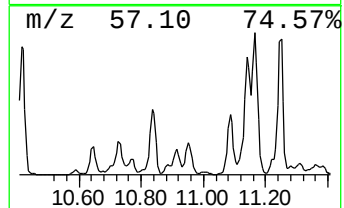
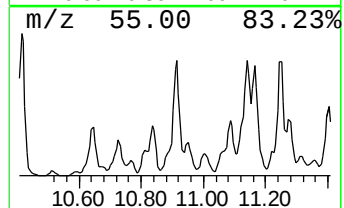
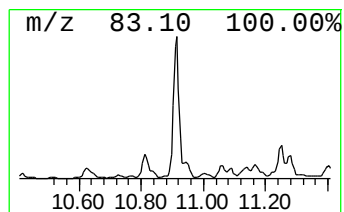
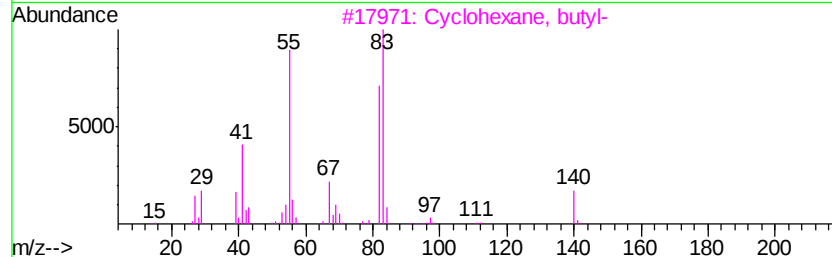
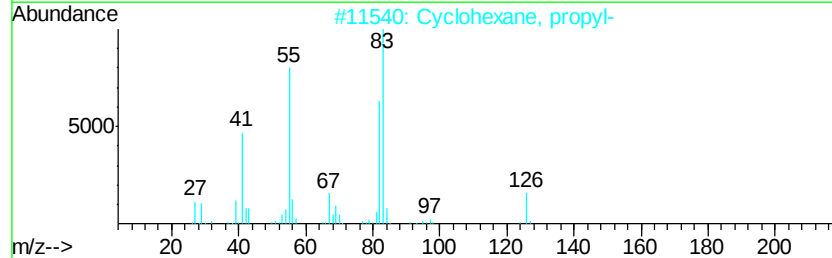
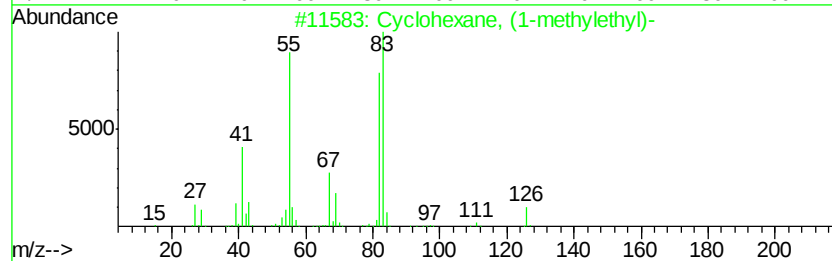
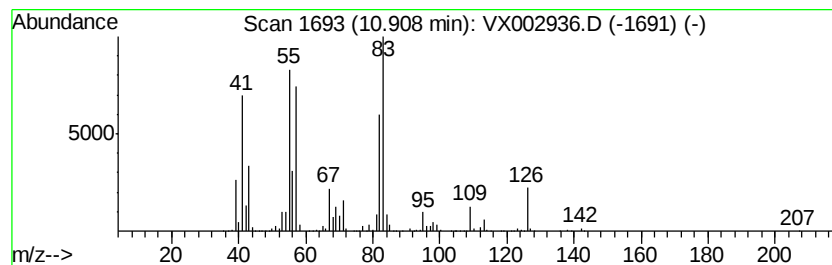
Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-23-25-180622

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, (1-methylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.91	58.24 ug/l	1485580	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, (1-methvlethvl)-	126	C9H18	000696-29-7	58
2		Cvclohexane, propyl-	126	C9H18	001678-92-8	52
3		Cvclohexane, butvl-	140	C10H20	001678-93-9	47
4		Cvclohexane, undecvl-	238	C17H34	054105-66-7	47
5		Cvclohexane, 1,1'-(1,4-butanedi...	222	C16H30	006165-44-2	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
WP021SB488-23-25-180622

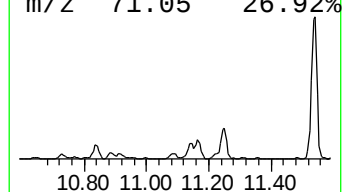
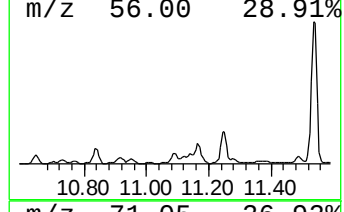
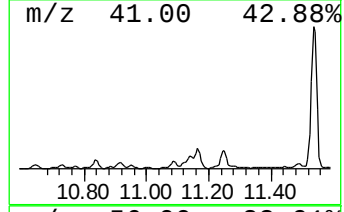
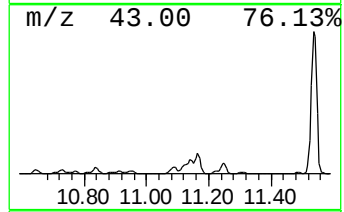
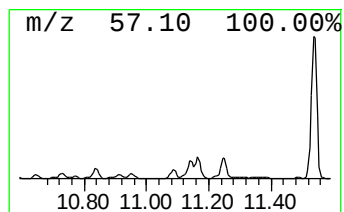
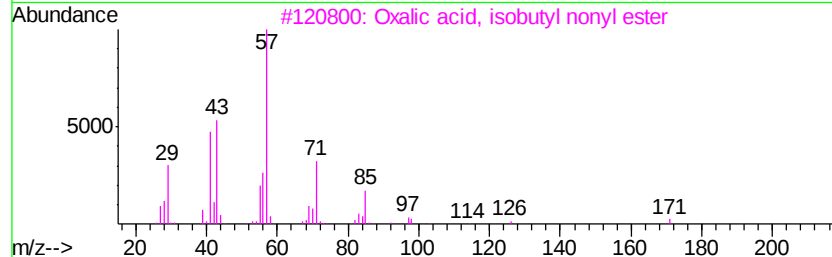
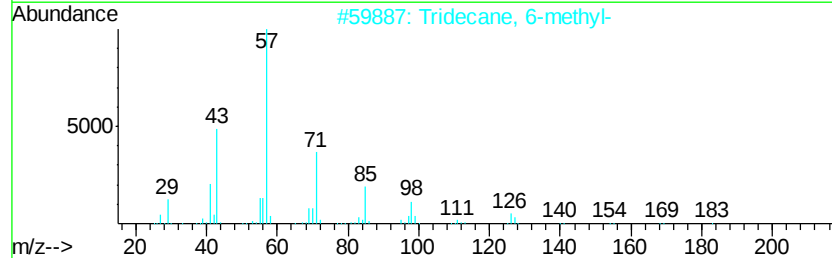
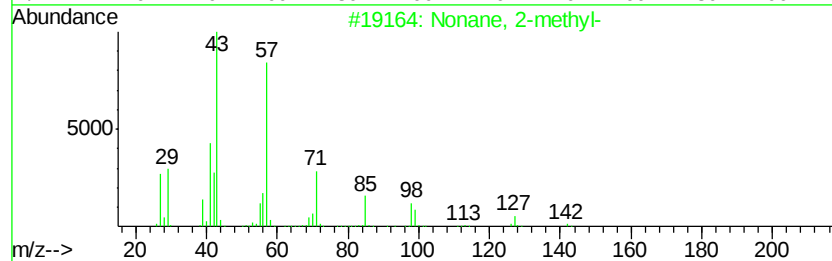
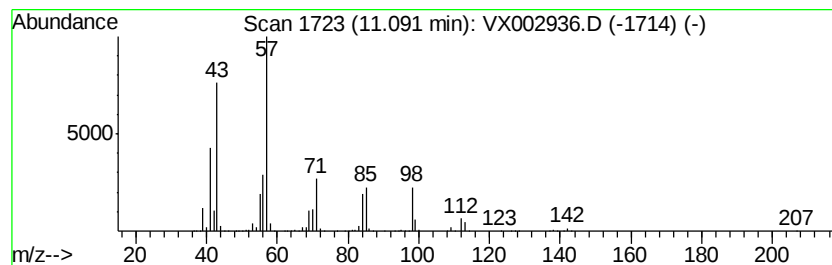
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Quant Title : SW846 8260

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

Peak Number 7 Nonane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	92.26 ug/l	2353260	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 2-methyl-	142	C10H22	000871-83-0	58
2		Tridecane, 6-methyl-	198	C14H30	013287-21-3	50
3		Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	50
4		Decane	142	C10H22	000124-18-5	50
5		Heptane, 4-propyl-	142	C10H22	003178-29-8	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-23-25-180622

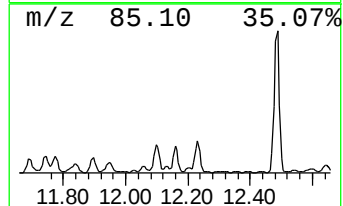
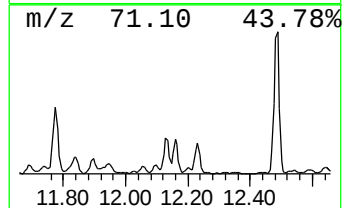
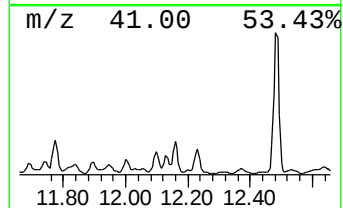
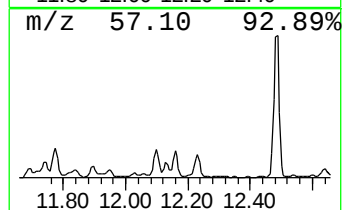
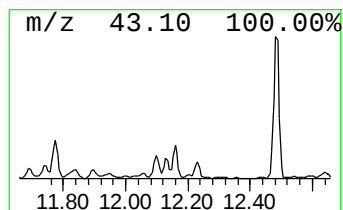
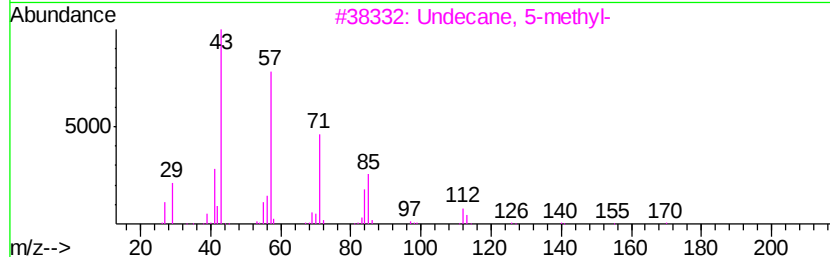
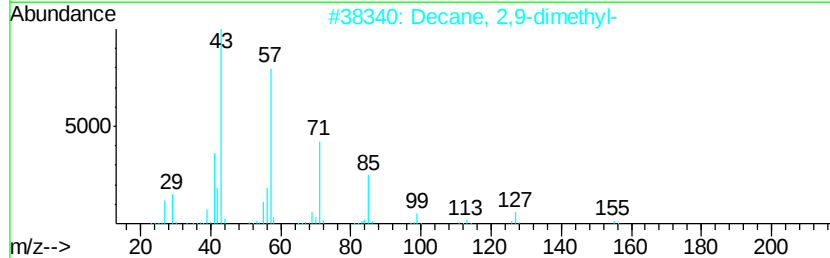
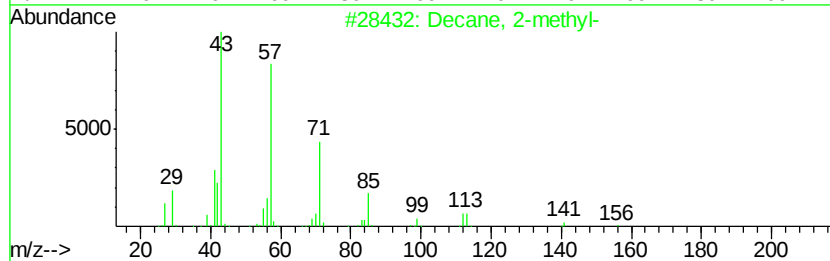
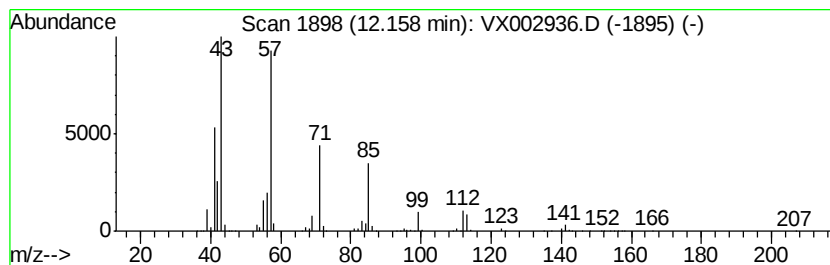
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Quant Title : SW846 8260

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

Peak Number 8 Decane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	47.41 ug/l	5808250	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2-methyl-	156	C11H24	006975-98-0	83
2		Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	78
3		Undecane, 5-methyl-	170	C12H26	001632-70-8	72
4		Tetradecane	198	C14H30	000629-59-4	64
5		Nonane, 3-methyl-	142	C10H22	005911-04-6	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

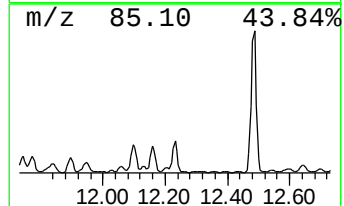
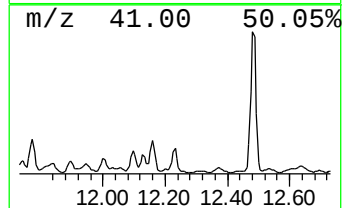
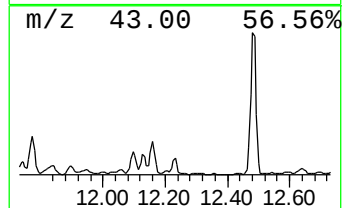
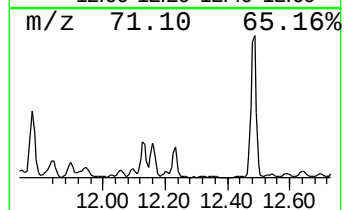
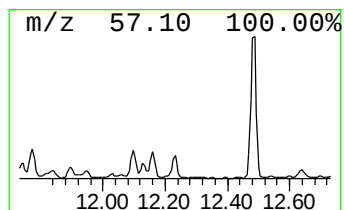
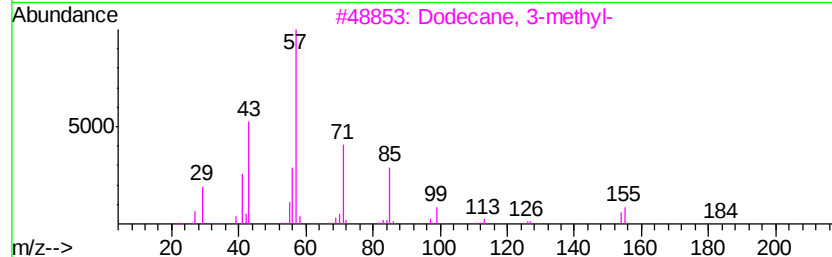
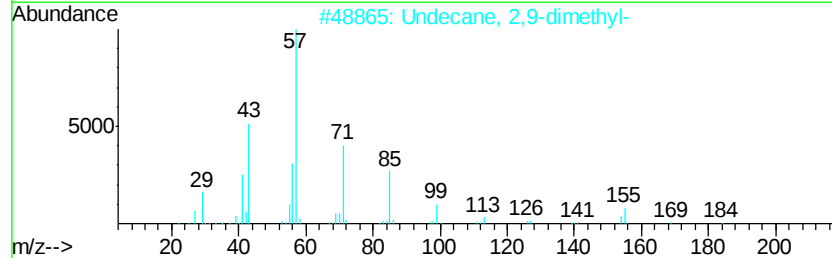
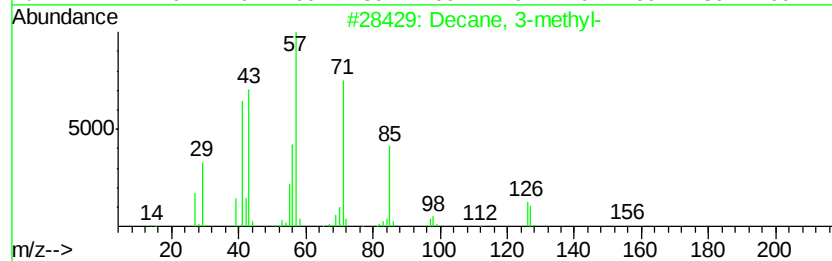
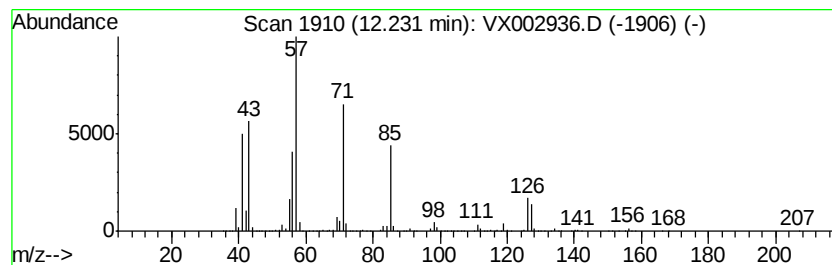
Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-23-25-180622

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 9 Decane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	36.09 ug/l	4421280	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane, 3-methyl-	156 C11H24	013151-34-3	86
2	Undecane, 2,9-dimethyl-	184 C13H28	017301-26-7	72
3	Dodecane, 3-methyl-	184 C13H28	017312-57-1	53
4	Tetradecane	198 C14H30	000629-59-4	50
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

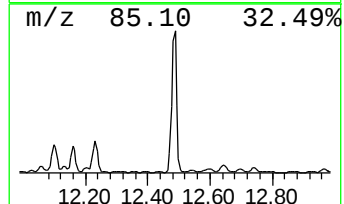
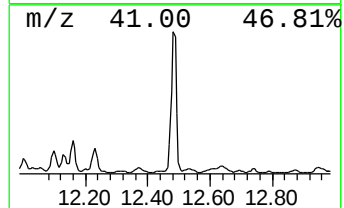
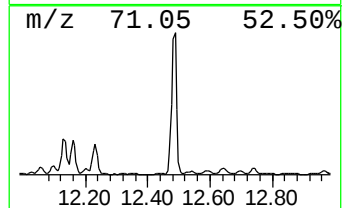
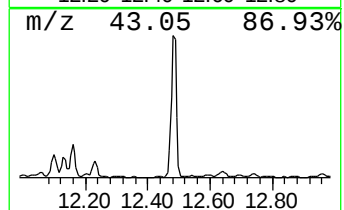
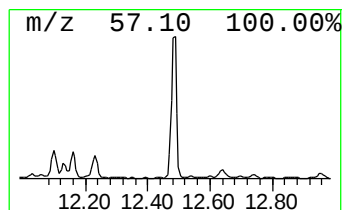
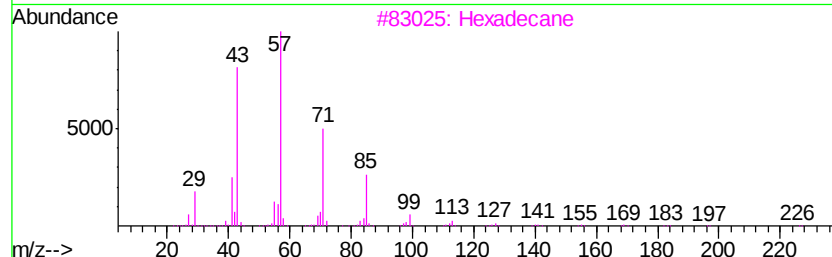
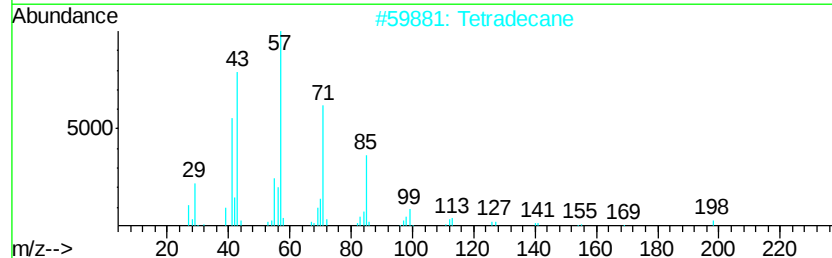
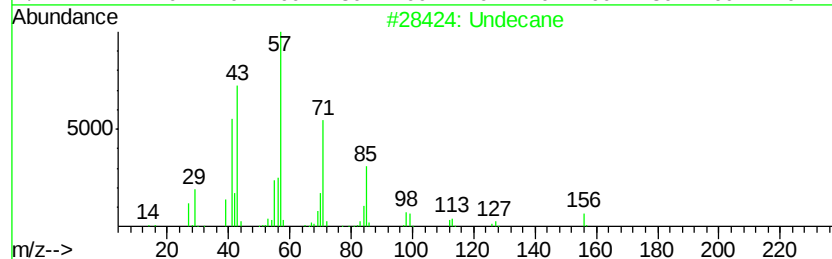
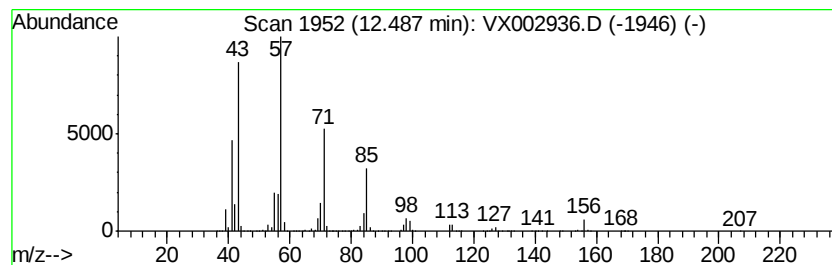
Instrument :
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ClientSampleId :
WP021SB488-23-25-180622

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 10 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	194.44 ug/l	23821200	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	96
2	Tetradecane	198 C14H30	000629-59-4	90
3	Hexadecane	226 C16H34	000544-76-3	80
4	Tridecane	184 C13H28	000629-50-5	80
5	Decane	142 C10H22	000124-18-5	74



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002936.D
Acq On : 27 Jun 2018 15:11
Operator : JC/MD
Sample : J3707-02
Misc : 5.97g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB488-23-25-180622

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.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
Octane, 2-methyl-	9.96	40.7	ug/l	1037250	3	10.12	1275310	50.0
Nonane	10.41	189.9	ug/l	4842880	3	10.12	1275310	50.0
Hexane, 2,4-dimet...	10.65	42.6	ug/l	1086350	3	10.12	1275310	50.0
Octane, 2,6-dimet...	10.84	84.4	ug/l	2152510	3	10.12	1275310	50.0
Cyclohexane, (1-m...	10.91	58.2	ug/l	1485580	3	10.12	1275310	50.0
Nonane, 2-methyl-	11.09	92.3	ug/l	2353260	3	10.12	1275310	50.0
Decane, 2-methyl-	12.16	47.4	ug/l	5808250	4	12.09	6125520	50.0
Decane, 3-methyl-	12.23	36.1	ug/l	4421280	4	12.09	6125520	50.0
Undecane	12.49	194.4	ug/l	23821200	4	12.09	6125520	50.0