

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062718\
 Data File : VX002944.D
 Acq On : 27 Jun 2018 18:43
 Operator : JC/MD
 Sample : J3707-11 20X
 Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WP021SB480-19-21-180622

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	1.075	76	80	93	rBV	523249	738757	42.22%	4.251%
2	1.264	108	111	120	rVB	12909	19820	1.13%	0.114%
3	4.599	646	658	673	rBV	268576	751448	42.95%	4.324%
4	4.769	679	686	696	rVB2	5802	18041	1.03%	0.104%
5	5.507	795	807	820	rBV	175208	502052	28.69%	2.889%
6	5.666	822	833	851	rVB2	268952	762392	43.57%	4.387%
7	6.074	887	900	916	rBV	192505	501276	28.65%	2.885%
8	6.348	936	945	955	rVB3	6855	21739	1.24%	0.125%
9	6.708	996	1004	1012	rVB3	10968	25583	1.46%	0.147%
10	6.867	1019	1030	1048	rBV	381150	904897	51.72%	5.208%
11	7.464	1118	1128	1137	rVB2	17927	41505	2.37%	0.239%
12	8.720	1327	1334	1343	rVB	936933	1422811	81.32%	8.188%
13	8.976	1370	1376	1382	rBV	14188	20817	1.19%	0.120%
14	9.964	1534	1538	1544	rVB	28258	39907	2.28%	0.230%
15	10.067	1549	1555	1558	rBV	21541	31303	1.79%	0.180%
16	10.116	1558	1563	1572	rVB	813500	1080936	61.78%	6.221%
17	10.415	1608	1612	1622	rVB	166851	225110	12.87%	1.295%
18	10.646	1643	1650	1657	rBV3	41402	73585	4.21%	0.423%
19	10.726	1657	1663	1668	rVV3	30564	51652	2.95%	0.297%
20	10.841	1674	1682	1686	rVB2	72385	115904	6.62%	0.667%
21	10.884	1686	1689	1690	rBV	18423	19178	1.10%	0.110%
22	10.915	1690	1694	1698	rVV2	74615	109034	6.23%	0.627%
23	10.951	1698	1700	1705	rVB	27372	31872	1.82%	0.183%
24	11.018	1705	1711	1714	rVB2	15443	22706	1.30%	0.131%
25	11.085	1714	1722	1725	rBV2	66453	116302	6.65%	0.669%
26	11.140	1725	1731	1741	rVB2	994574	1473458	84.21%	8.480%
27	11.244	1741	1748	1752	rBV	151212	223155	12.75%	1.284%
28	11.280	1752	1754	1757	rVV3	27595	30019	1.72%	0.173%
29	11.360	1763	1767	1770	rBV2	15521	21269	1.22%	0.122%
30	11.396	1770	1773	1777	rBV4	17883	24788	1.42%	0.143%
31	11.451	1777	1782	1785	rBV4	34126	55387	3.17%	0.319%
32	11.488	1785	1788	1791	rVV	55353	68595	3.92%	0.395%
33	11.536	1791	1796	1801	rVB	1436451	1749715	100.00%	10.069%
34	11.689	1813	1821	1825	rBV5	78682	129973	7.43%	0.748%

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 ALS Vial : 18 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE
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 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

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35	11.738	1825	1829	1832	rVV	93652	145368	8.31%	0.837%
36	11.774	1832	1835	1838	rVV	258486	317115	18.12%	1.825%
37	11.835	1838	1845	1851	rVB5	83276	213492	12.20%	1.229%
38	11.896	1851	1855	1857	rBV	81617	114920	6.57%	0.661%
39	11.927	1857	1860	1861	rVV	88301	111428	6.37%	0.641%
40	11.945	1861	1863	1868	rVV	104464	147187	8.41%	0.847%
41	12.000	1868	1872	1875	rVV	117421	155490	8.89%	0.895%
42	12.079	1879	1885	1891	rVV	1043582	1546813	88.40%	8.902%
43	12.128	1891	1893	1895	rVV	130962	138721	7.93%	0.798%
44	12.158	1895	1898	1902	rVV	200940	235150	13.44%	1.353%
45	12.231	1906	1910	1917	rVB2	170570	229862	13.14%	1.323%
46	12.305	1917	1922	1928	rBV3	34636	55701	3.18%	0.321%
47	12.372	1928	1933	1940	rBV4	150315	287373	16.42%	1.654%
48	12.481	1946	1951	1955	rBV	953177	1079687	61.71%	6.213%
49	12.524	1955	1958	1964	rVB2	60589	92707	5.30%	0.534%
50	12.591	1964	1969	1974	rBV3	55929	109623	6.27%	0.631%
51	12.640	1974	1977	1979	rVV2	41068	53261	3.04%	0.307%
52	12.670	1979	1982	1985	rVB	90712	100229	5.73%	0.577%
53	12.780	1995	2000	2005	rVB3	83206	152169	8.70%	0.876%
54	12.853	2005	2012	2014	rVV2	42605	80247	4.59%	0.462%
55	12.896	2018	2019	2023	rVV2	32412	32168	1.84%	0.185%
56	12.957	2023	2029	2031	rVV4	51187	95463	5.46%	0.549%
57	12.981	2031	2033	2037	rVV2	60792	81908	4.68%	0.471%
58	13.024	2037	2040	2046	rVV2	58895	96374	5.51%	0.555%
59	13.097	2046	2052	2055	rVV3	29777	58679	3.35%	0.338%
60	13.152	2059	2061	2066	rVV	15824	19946	1.14%	0.115%
61	13.219	2066	2072	2076	rVB4	18872	29091	1.66%	0.167%
62	13.323	2083	2089	2092	rBV2	83459	106857	6.11%	0.615%
63	13.353	2092	2094	2099	rVB4	18166	23010	1.32%	0.132%
64	13.487	2110	2116	2124	rVB7	15438	41558	2.38%	0.239%

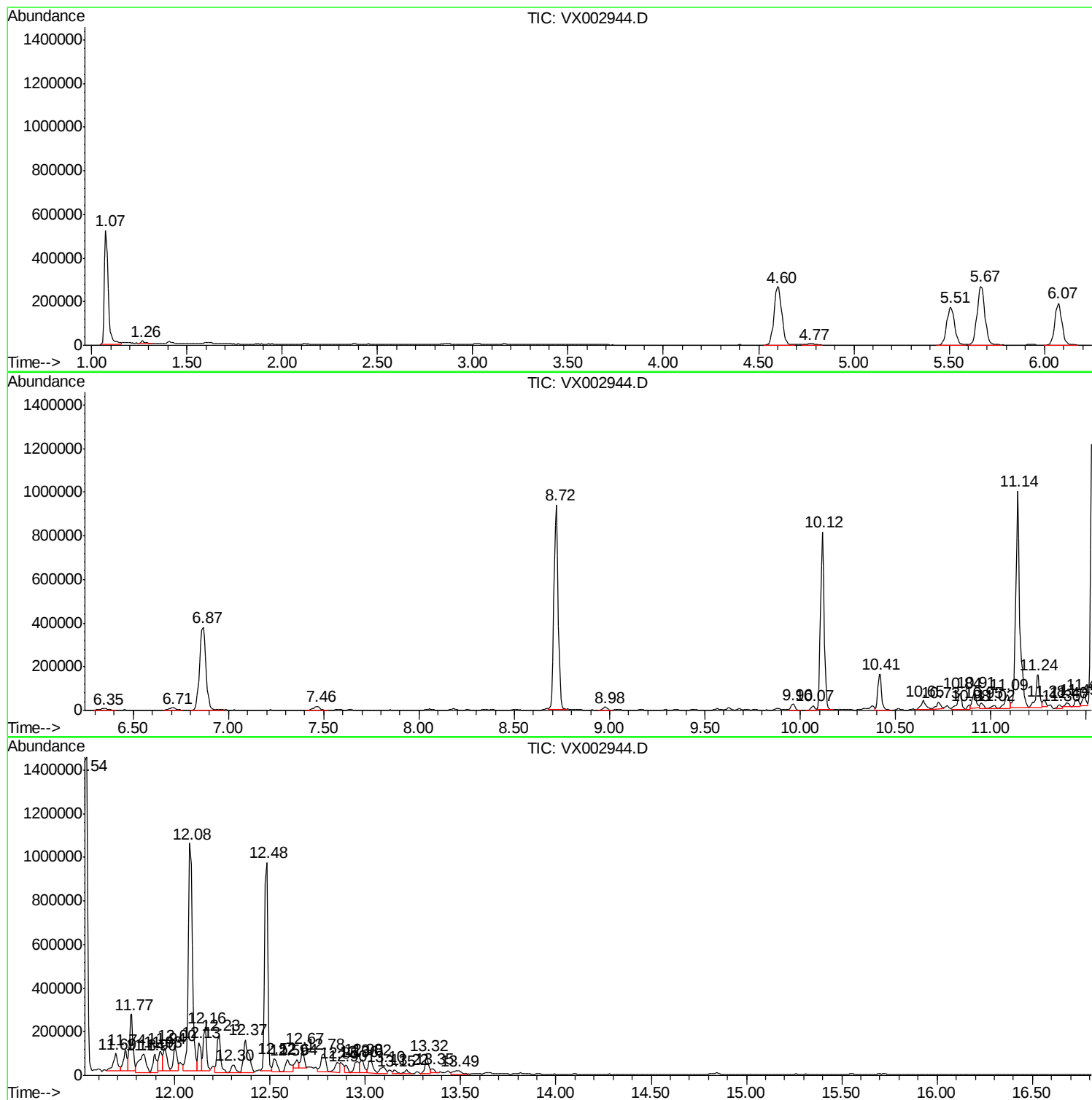
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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



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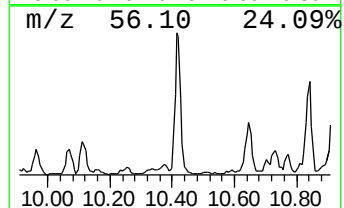
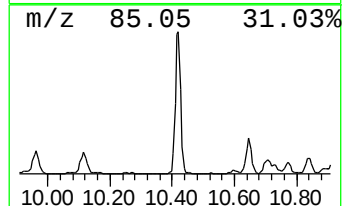
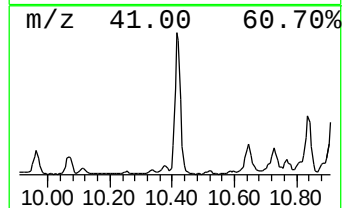
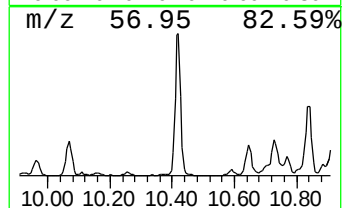
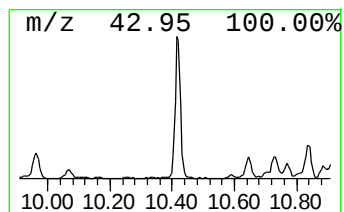
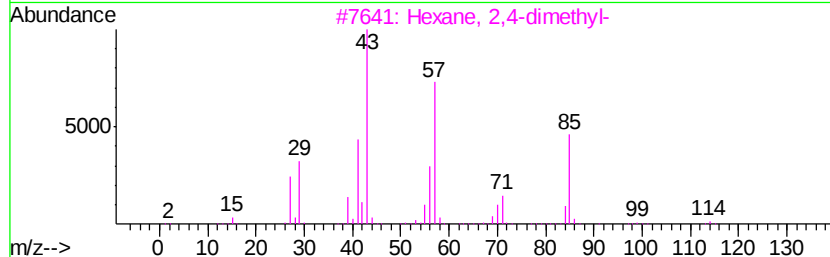
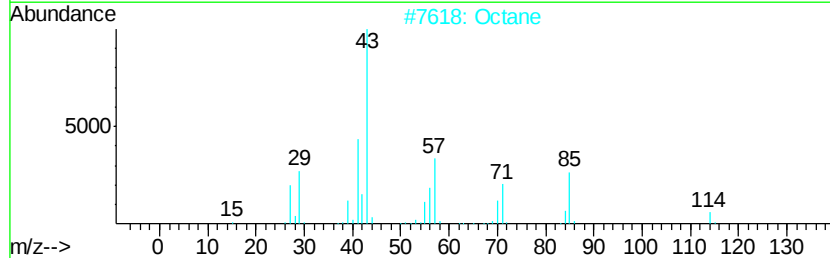
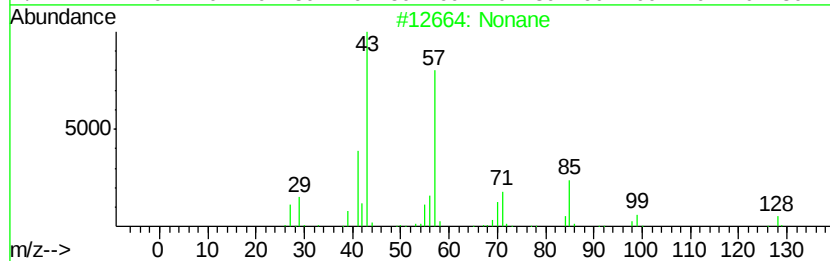
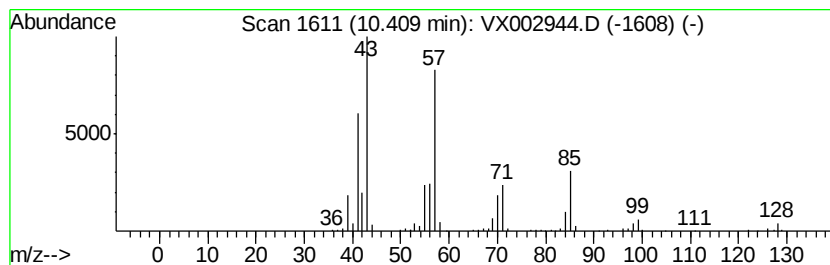
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Nonane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	10.41 ug/l	225110	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane		128	C9H20	000111-84-2	91
2	Octane		114	C8H18	000111-65-9	53
3	Hexane, 2,4-dimethyl-		114	C8H18	000589-43-5	53
4	Oxalic acid, isobutyl nonyl ester		272	C15H28O4	1000309-37-4	50
5	Hexane, 2,2,3,3-tetramethyl-		142	C10H22	013475-81-5	47



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ClientSampleId :
WP021SB480-19-21-180622

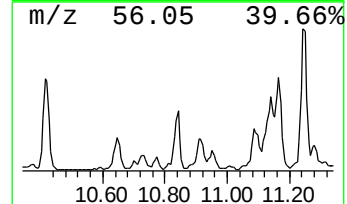
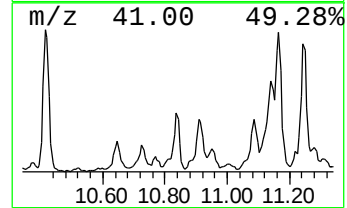
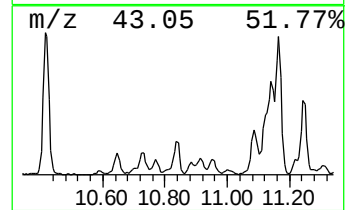
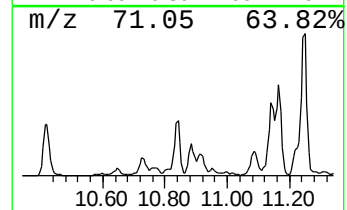
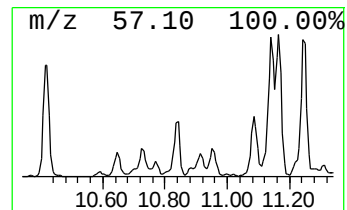
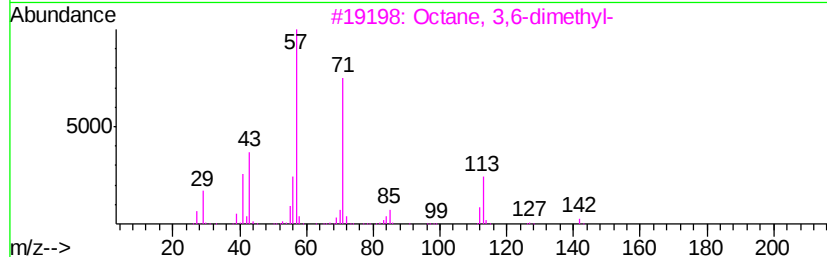
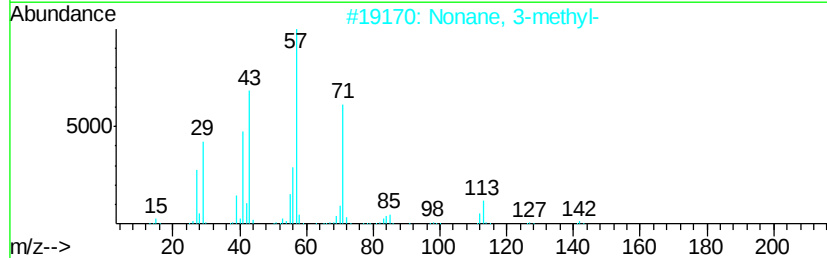
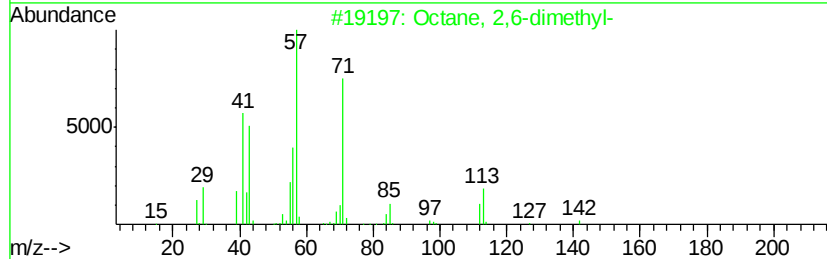
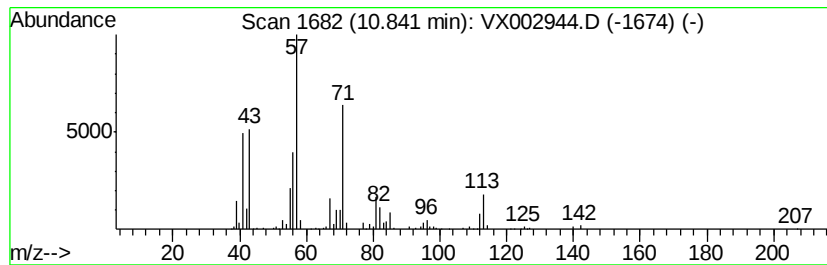
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	5.36 ug/l	115904	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2		Nonane, 3-methyl-	142	C10H22	005911-04-6	90
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	70
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
5		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	50



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Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-19-21-180622

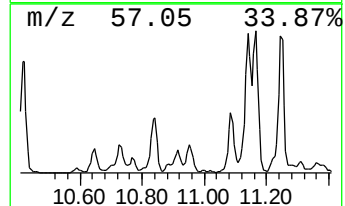
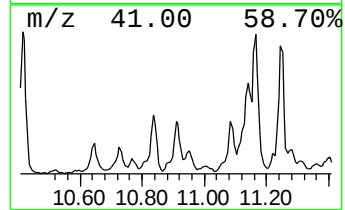
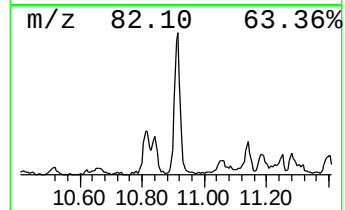
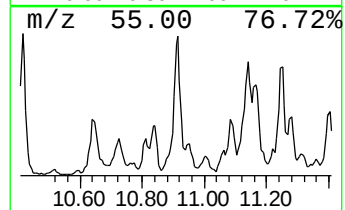
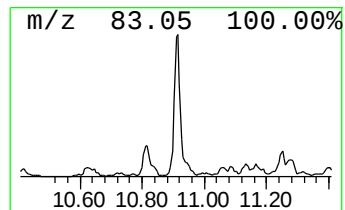
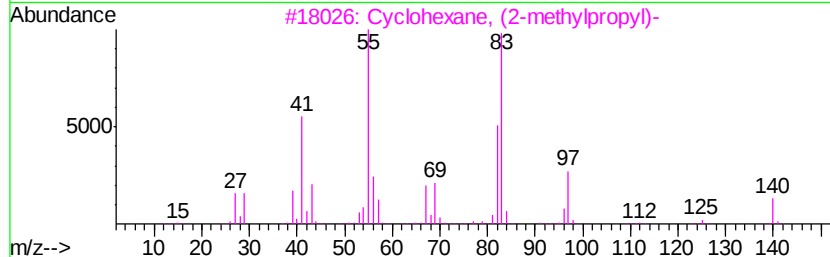
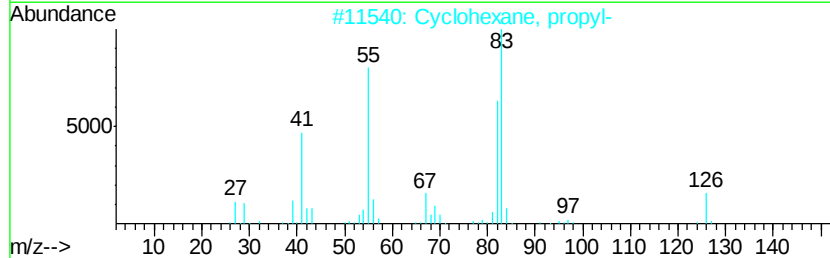
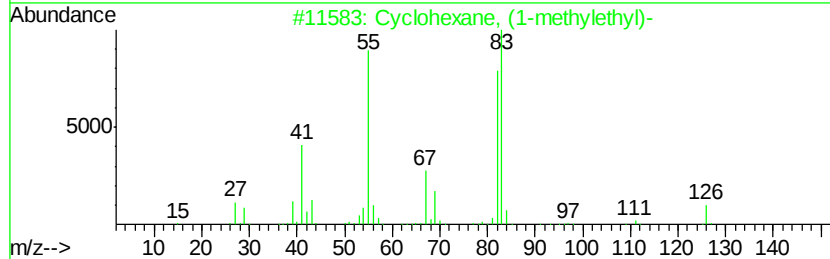
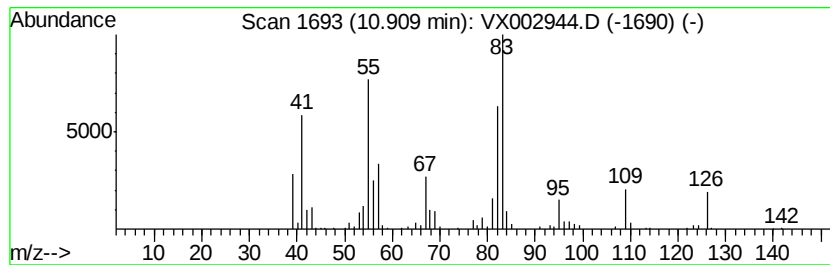
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, (1-methylethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	5.04 ug/l	109034	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	76
2		Cyclohexane, propyl-	126	C9H18	001678-92-8	64
3		Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	59
4		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	58
5		Cyclohexane, 1,1'-(1,4-butanedi...	222	C16H30	006165-44-2	53



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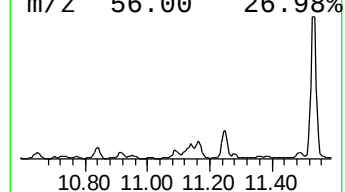
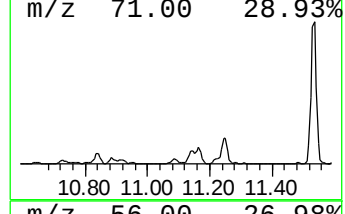
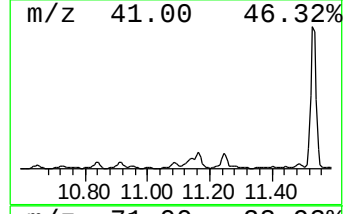
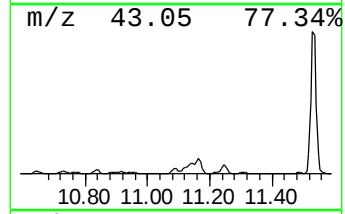
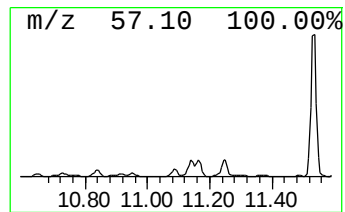
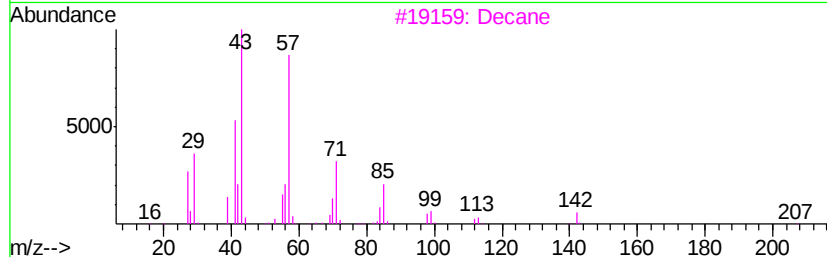
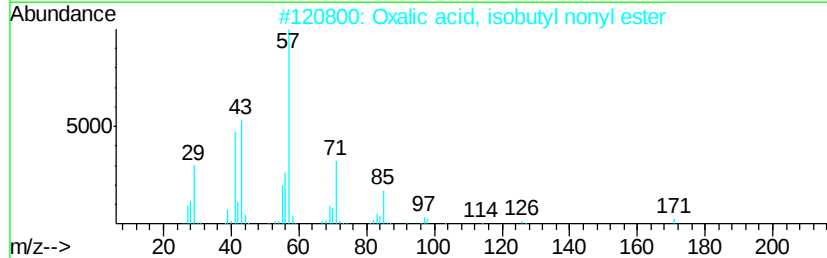
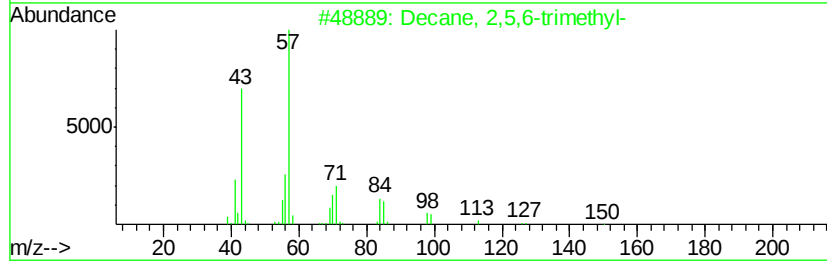
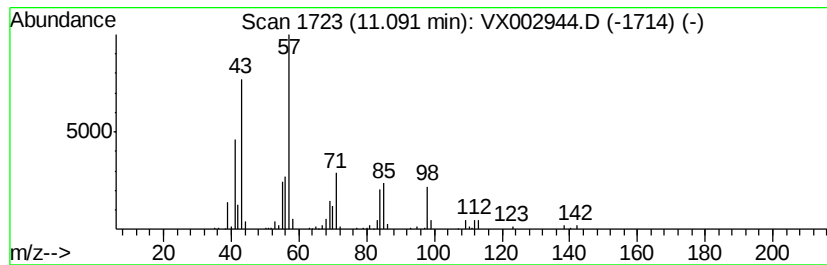
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Peak Number 5 Decane, 2,5,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	5.38 ug/l	116302	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	58	
2	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	50	
3	Decane	142	C10H22	000124-18-5	50	
4	Octane	114	C8H18	000111-65-9	43	
5	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	43	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

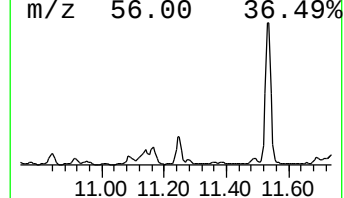
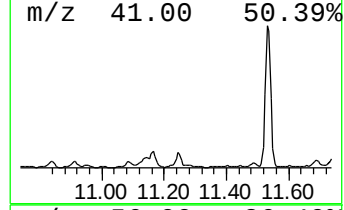
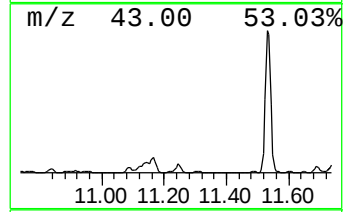
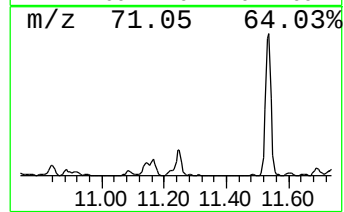
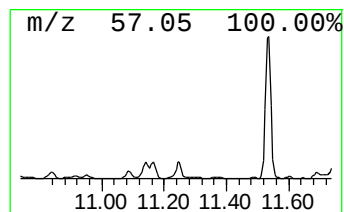
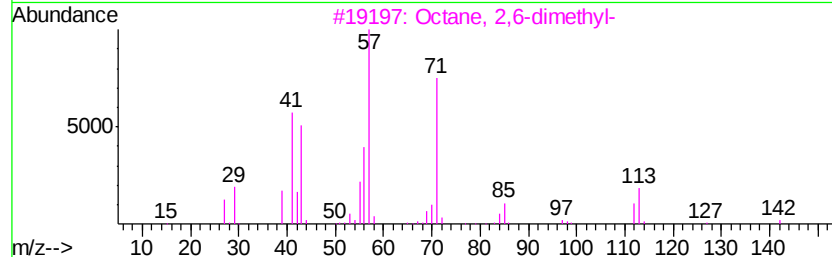
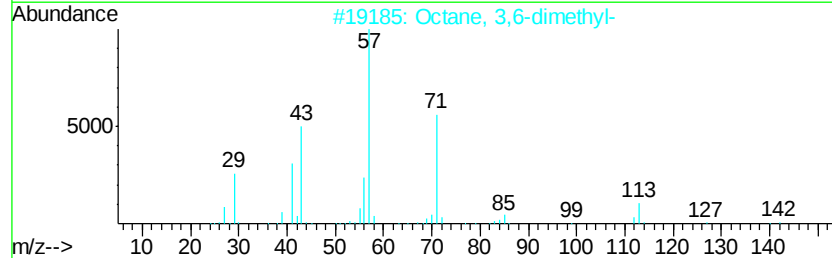
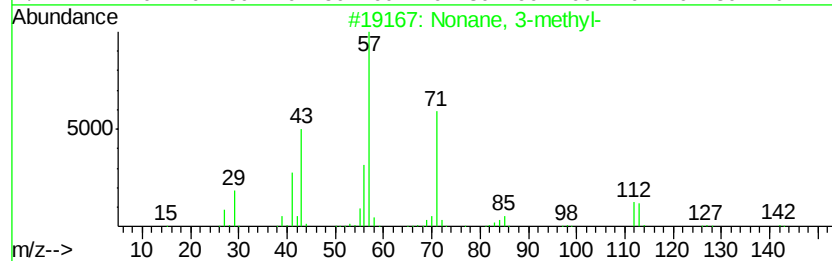
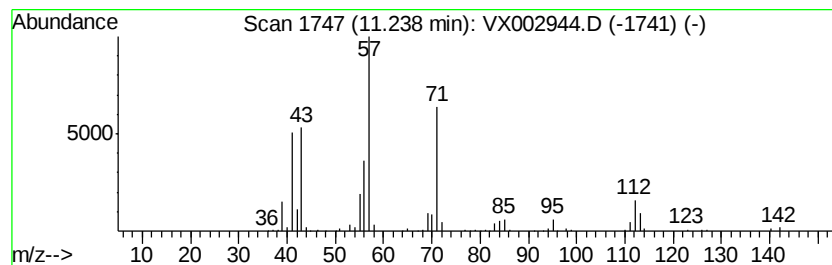
Instrument :
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ClientSampleId :
WP021SB480-19-21-180622

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 Nonane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	7.21 ug/l	223155	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonane, 3-methyl-	142 C10H22	005911-04-6	90
2	Octane, 3,6-dimethyl-	142 C10H22	015869-94-0	80
3	Octane, 2,6-dimethyl-	142 C10H22	002051-30-1	72
4	Tridecane, 7-methyl-	198 C14H30	026730-14-3	64
5	Octane, 3-ethyl-	142 C10H22	005881-17-4	62



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

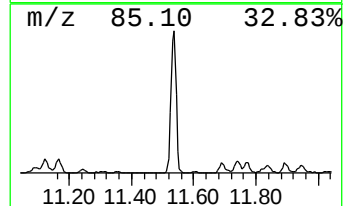
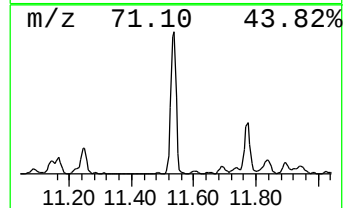
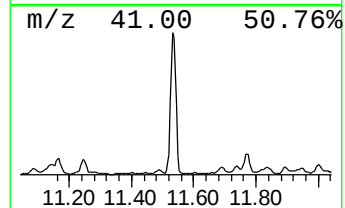
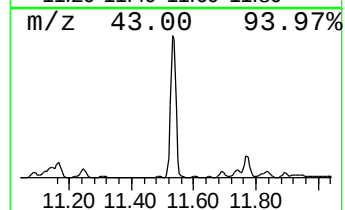
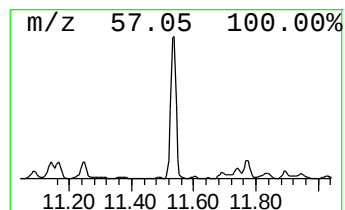
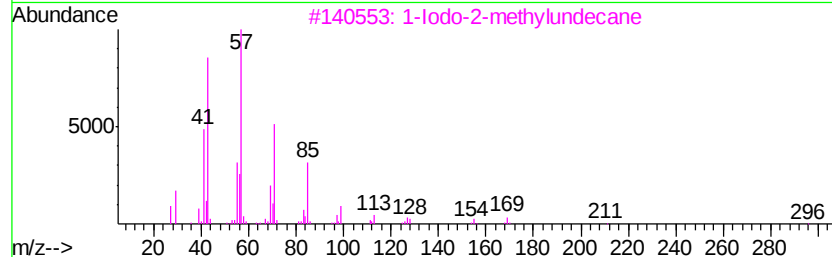
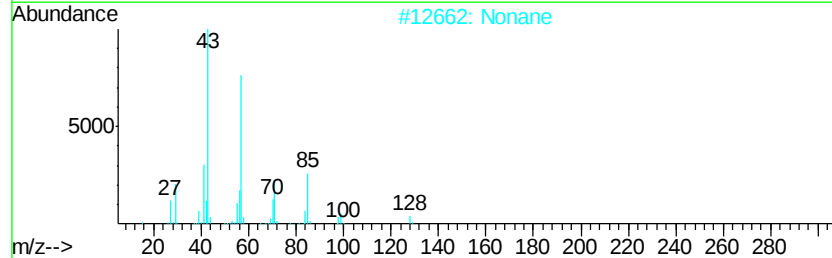
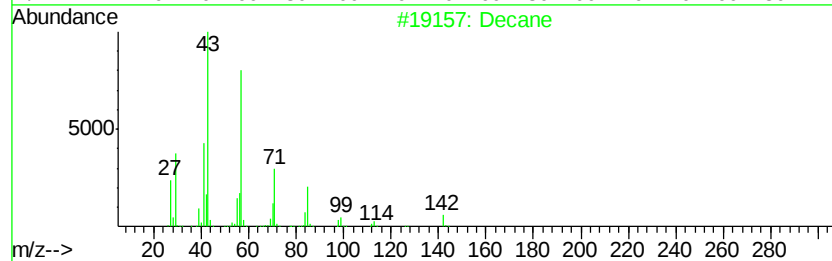
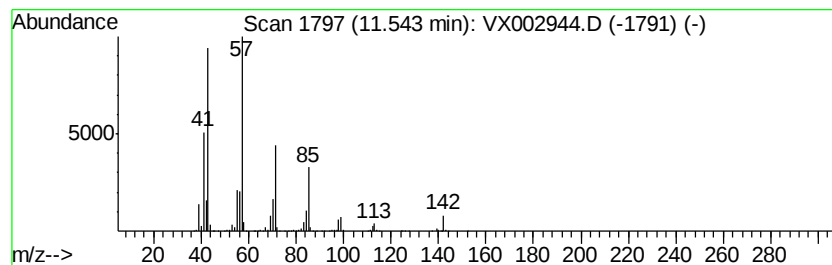
Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-19-21-180622

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 7 Decane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	56.56 ug/l	1749720	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane		142 C10H22	000124-18-5 94
2	Nonane		128 C9H20	000111-84-2 72
3	1-Iodo-2-methylundecane		296 C12H25I	073105-67-6 72
4	Decane, 2,9-dimethyl-		170 C12H26	001002-17-1 64
5	Hexadecane		226 C16H34	000544-76-3 64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-19-21-180622

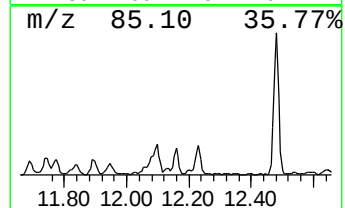
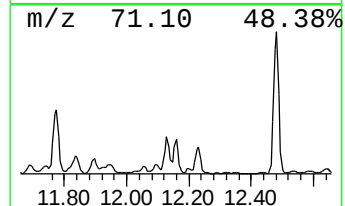
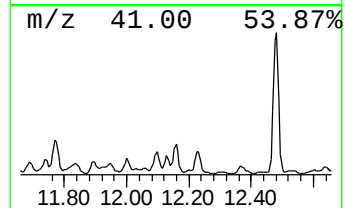
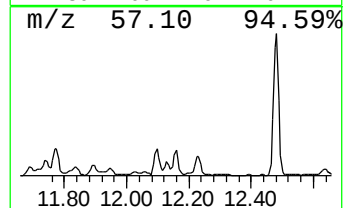
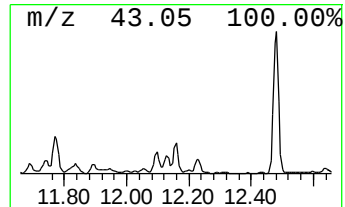
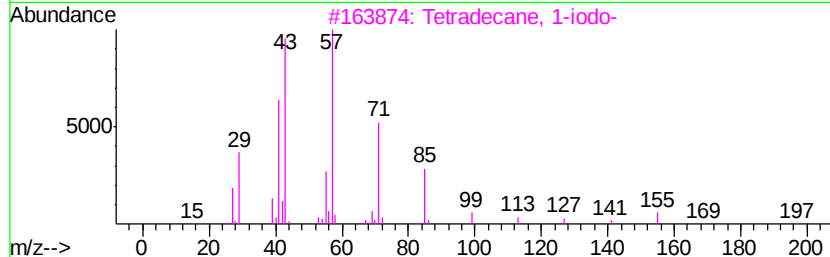
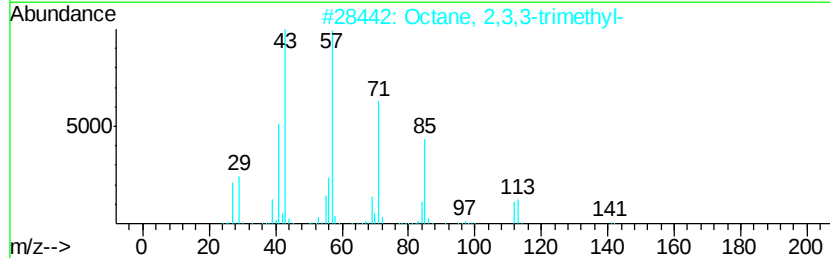
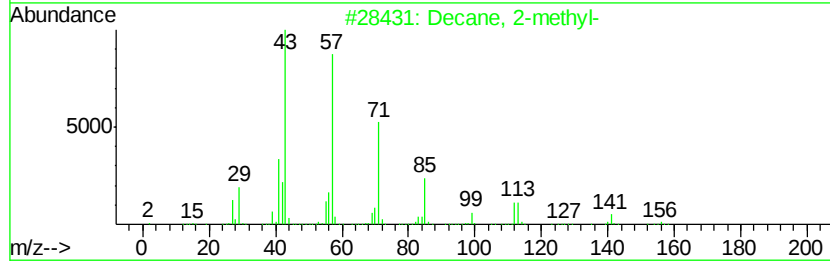
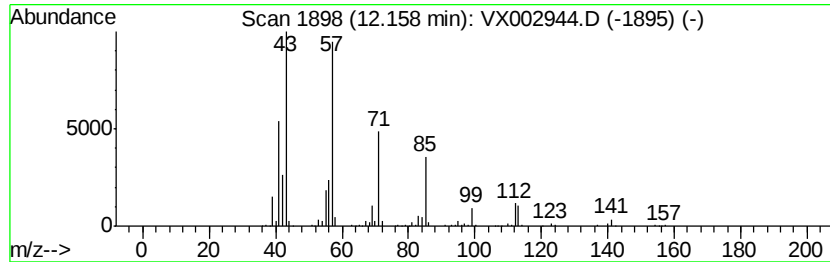
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	7.60 ug/l	235150	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 2-methyl-	156	C11H24	006975-98-0	83
2		Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	59
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	58
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	53
5		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

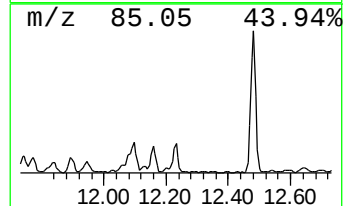
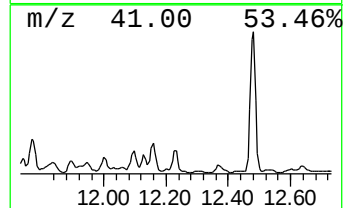
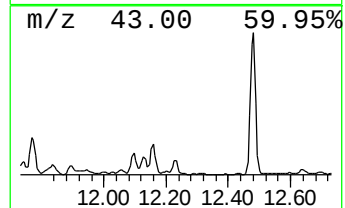
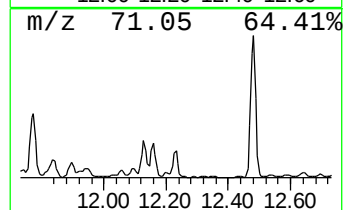
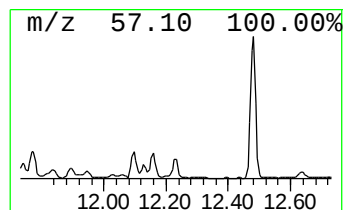
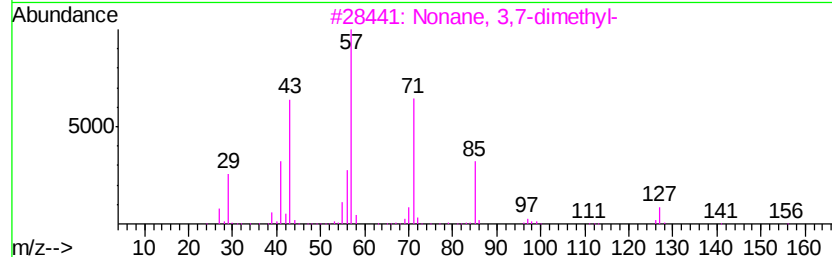
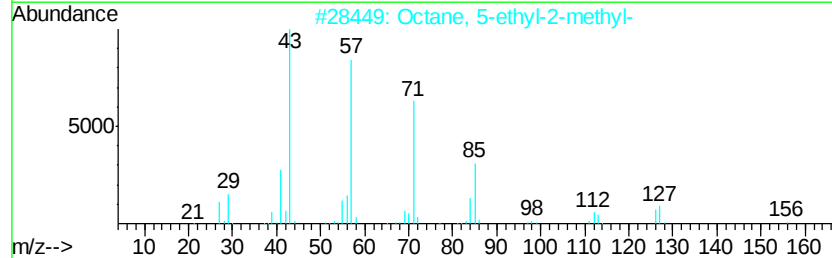
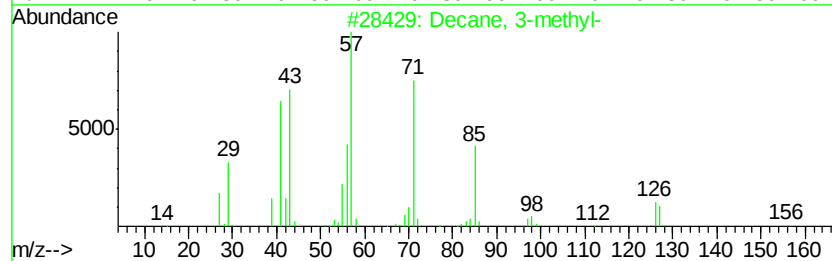
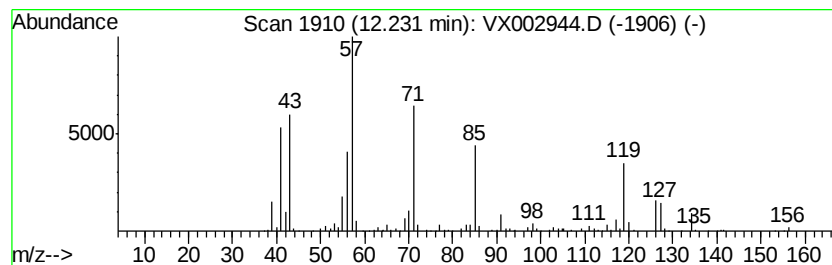
Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-19-21-180622

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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	7.43 ug/l	229862	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane, 3-methyl-	156 C11H24	013151-34-3	70
2	Octane, 5-ethyl-2-methyl-	156 C11H24	062016-18-6	50
3	Nonane, 3,7-dimethyl-	156 C11H24	017302-32-8	50
4	Nonane, 5-(2-methylpropyl)-	184 C13H28	062185-53-9	49
5	Decane, 2,9-dimethyl-	170 C12H26	001002-17-1	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

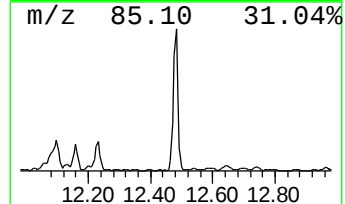
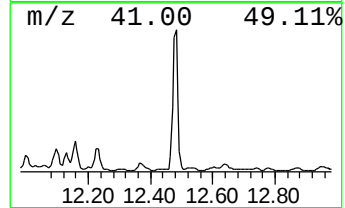
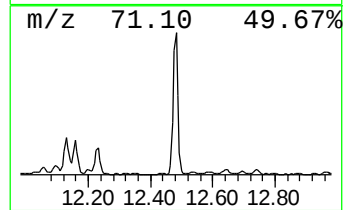
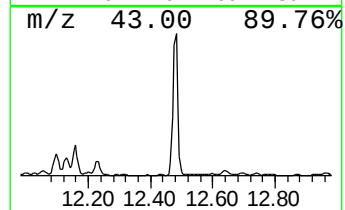
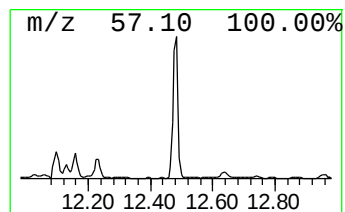
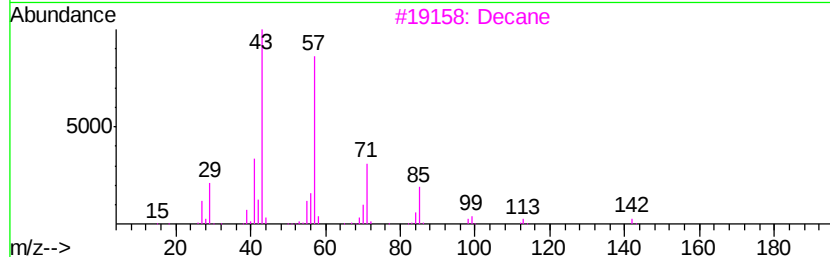
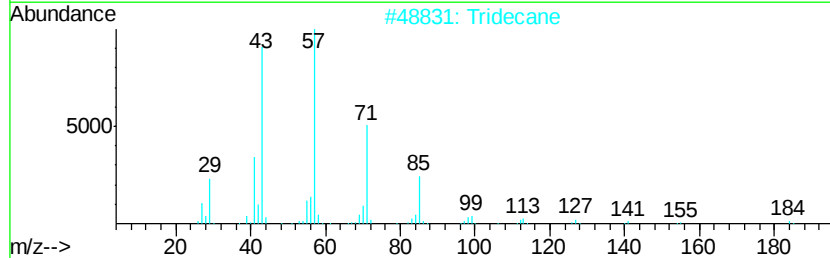
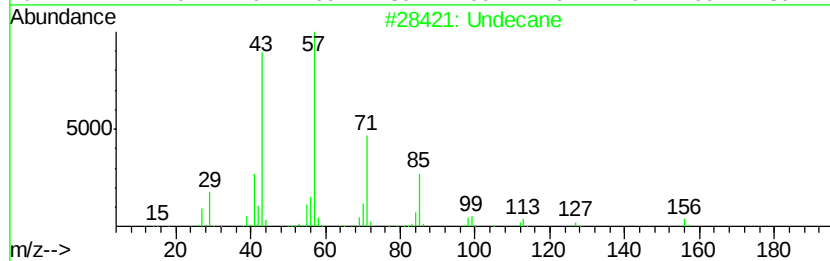
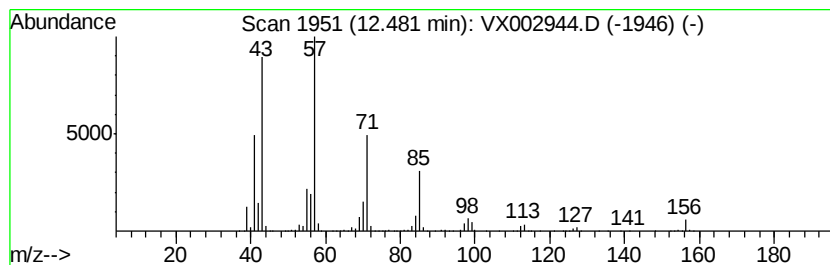
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ClientSampleId :
WP021SB480-19-21-180622

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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	34.90 ug/l	1079690	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	94
2	Tridecane	184 C13H28	000629-50-5	80
3	Decane	142 C10H22	000124-18-5	78
4	Hexadecane	226 C16H34	000544-76-3	64
5	Nonane	128 C9H20	000111-84-2	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062718\
Data File : VX002944.D
Acq On : 27 Jun 2018 18:43
Operator : JC/MD
Sample : J3707-11 20X
Misc : 7.12g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-19-21-180622

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
Nonane	10.41	10.4	ug/l	225110	3	10.12	1080940	50.0
Octane, 2,6-dimet...	10.84	5.4	ug/l	115904	3	10.12	1080940	50.0
Cyclohexane, (1-m...	10.91	5.0	ug/l	109034	3	10.12	1080940	50.0
Decane, 2,5,6-tri...	11.09	5.4	ug/l	116302	3	10.12	1080940	50.0
Nonane, 3-methyl-	11.24	7.2	ug/l	223155	4	12.08	1546810	50.0
Decane	11.54	56.6	ug/l	1749720	4	12.08	1546810	50.0
Decane, 2-methyl-	12.16	7.6	ug/l	235150	4	12.08	1546810	50.0
Decane, 3-methyl-	12.23	7.4	ug/l	229862	4	12.08	1546810	50.0
Undecane	12.48	34.9	ug/l	1079690	4	12.08	1546810	50.0