

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062618\
 Data File : VX002918.D
 Acq On : 27 Jun 2018 02:22
 Operator : JC/MD
 Sample : J3707-12 50X
 Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WP021SB480-21-23-180622

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	527826	735081	43.05%	4.323%
2	1.264	108	111	119	rBV2	12931	20590	1.21%	0.121%
3	4.599	647	658	673	rBV	228583	635164	37.20%	3.735%
4	5.507	795	807	820	rBV	178139	504209	29.53%	2.965%
5	5.666	823	833	852	rVB	267725	760017	44.51%	4.470%
6	6.074	888	900	917	rBV	187090	497749	29.15%	2.927%
7	6.348	936	945	953	rVB2	8335	24714	1.45%	0.145%
8	6.708	996	1004	1011	rBV3	10026	25099	1.47%	0.148%
9	6.867	1019	1030	1049	rBV	383385	891659	52.22%	5.244%
10	7.464	1118	1128	1136	rBV2	18960	43807	2.57%	0.258%
11	8.720	1327	1334	1342	rVB	913128	1407348	82.42%	8.277%
12	8.976	1371	1376	1383	rVB	12961	18428	1.08%	0.108%
13	9.964	1533	1538	1544	rVB	26691	38184	2.24%	0.225%
14	10.067	1549	1555	1558	rBV	21572	30257	1.77%	0.178%
15	10.116	1558	1563	1573	rVB	825030	1066356	62.45%	6.271%
16	10.415	1608	1612	1623	rVB	162086	214121	12.54%	1.259%
17	10.646	1643	1650	1657	rBV4	40751	71627	4.19%	0.421%
18	10.726	1657	1663	1667	rVV4	30830	48907	2.86%	0.288%
19	10.768	1667	1670	1674	rVB	13983	17492	1.02%	0.103%
20	10.835	1674	1681	1686	rVB2	73662	116781	6.84%	0.687%
21	10.884	1686	1689	1690	rBV	17991	19341	1.13%	0.114%
22	10.915	1690	1694	1697	rVV	74188	102128	5.98%	0.601%
23	10.951	1697	1700	1705	rVB	27398	38019	2.23%	0.224%
24	11.018	1705	1711	1714	rVB4	15460	23916	1.40%	0.141%
25	11.085	1714	1722	1725	rBV3	65576	117187	6.86%	0.689%
26	11.140	1725	1731	1741	rVB2	987200	1462743	85.67%	8.602%
27	11.244	1741	1748	1752	rBV	153776	227053	13.30%	1.335%
28	11.281	1752	1754	1757	rVV2	27664	29186	1.71%	0.172%
29	11.360	1763	1767	1770	rBV	20239	27680	1.62%	0.163%
30	11.396	1770	1773	1778	rVB2	18064	24433	1.43%	0.144%
31	11.451	1778	1782	1785	rBV3	37446	58508	3.43%	0.344%
32	11.488	1785	1788	1791	rVV	54527	66279	3.88%	0.390%
33	11.530	1791	1795	1801	rVB	1453996	1707465	100.00%	10.042%
34	11.689	1813	1821	1825	rBV5	78219	136882	8.02%	0.805%

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Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON
Sampling : 1
Start Thrs: 0.2
Stop Thrs : 0
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Max Peaks: 100
Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	11.738	1825	1829	1831	rVV	93968	126230	7.39%	0.742%
36	11.774	1831	1835	1838	rVV	259224	334252	19.58%	1.966%
37	11.835	1838	1845	1851	rVB7	81623	216798	12.70%	1.275%
38	11.896	1851	1855	1857	rBV	77240	107681	6.31%	0.633%
39	11.921	1857	1859	1861	rVV	83189	106482	6.24%	0.626%
40	11.945	1861	1863	1868	rVV2	99987	142562	8.35%	0.838%
41	12.000	1868	1872	1875	rVV	112500	151510	8.87%	0.891%
42	12.079	1879	1885	1891	rVV	1025090	1537215	90.03%	9.040%
43	12.128	1891	1893	1895	rVV	132096	140434	8.22%	0.826%
44	12.158	1895	1898	1902	rVV	198107	230441	13.50%	1.355%
45	12.232	1906	1910	1917	rVB2	166393	229179	13.42%	1.348%
46	12.305	1917	1922	1928	rBV2	46225	78591	4.60%	0.462%
47	12.372	1928	1933	1941	rBV4	144789	277907	16.28%	1.634%
48	12.482	1946	1951	1955	rBV	918178	1050519	61.53%	6.178%
49	12.524	1955	1958	1964	rVB2	58361	87030	5.10%	0.512%
50	12.591	1964	1969	1972	rBV	60945	97170	5.69%	0.571%
51	12.640	1974	1977	1979	rVV3	35017	46449	2.72%	0.273%
52	12.671	1979	1982	1985	rVB	94724	102942	6.03%	0.605%
53	12.780	1995	2000	2005	rVB3	80273	144824	8.48%	0.852%
54	12.853	2007	2012	2014	rBV2	35417	59204	3.47%	0.348%
55	12.957	2024	2029	2031	rBV3	44146	83052	4.86%	0.488%
56	12.981	2031	2033	2037	rVV2	57413	75343	4.41%	0.443%
57	13.024	2037	2040	2046	rVB2	74552	107033	6.27%	0.629%
58	13.091	2046	2051	2055	rBV3	25052	43423	2.54%	0.255%
59	13.152	2059	2061	2066	rVB	14917	19323	1.13%	0.114%
60	13.219	2066	2072	2076	rVB4	19104	28991	1.70%	0.170%
61	13.323	2083	2089	2092	rBV2	83904	103530	6.06%	0.609%
62	13.353	2092	2094	2099	rVB4	20743	24132	1.41%	0.142%
63	13.481	2111	2115	2124	rVB7	20985	43332	2.54%	0.255%

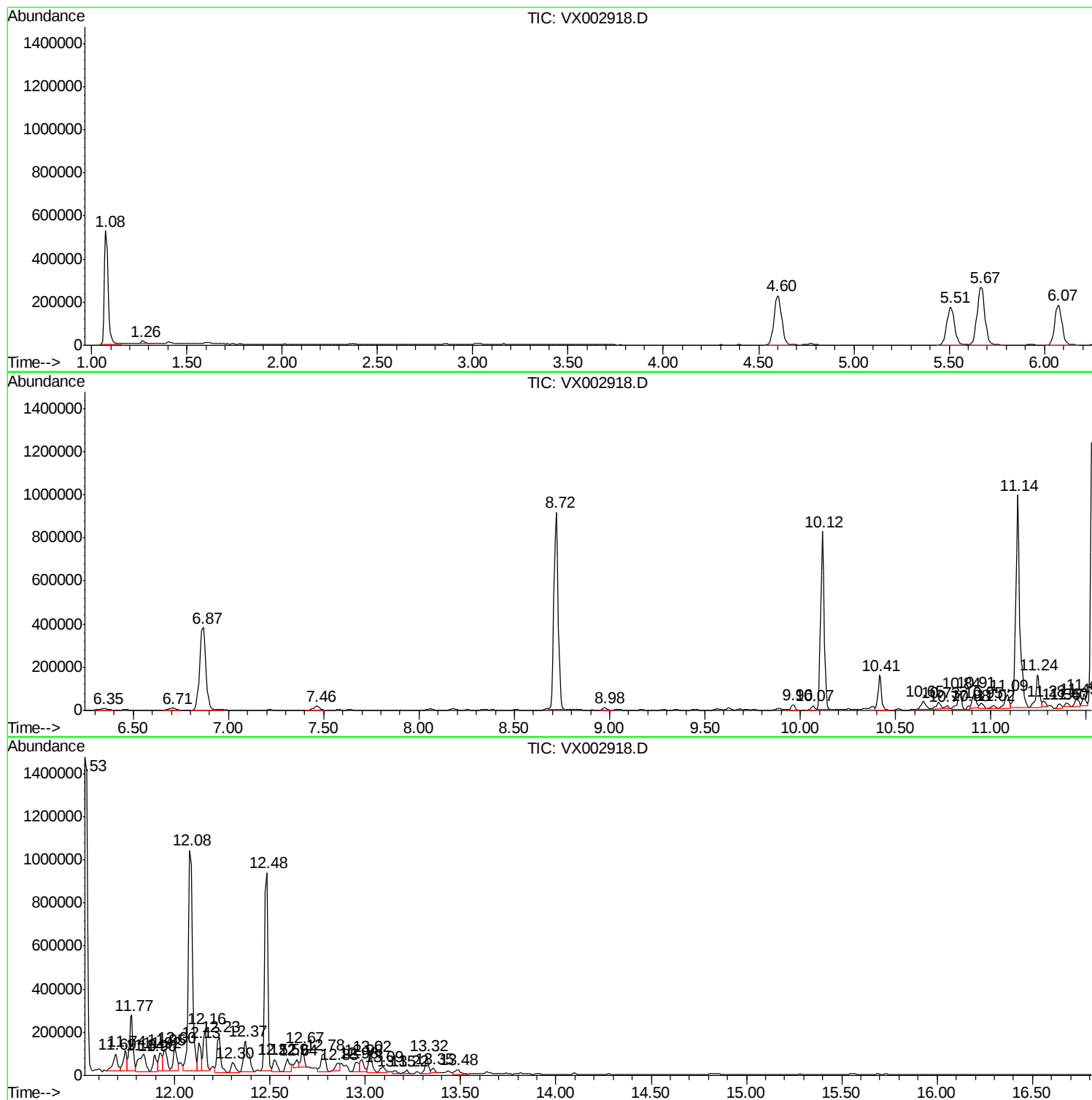
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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



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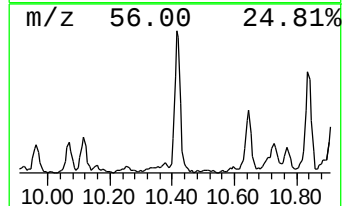
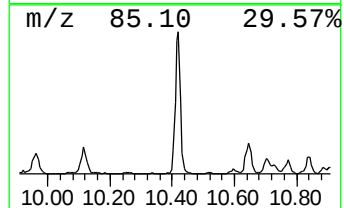
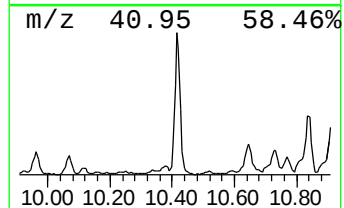
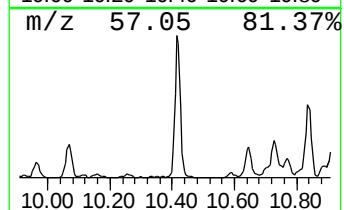
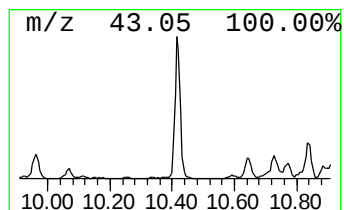
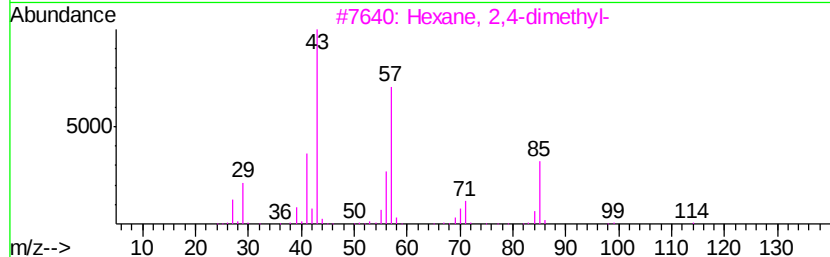
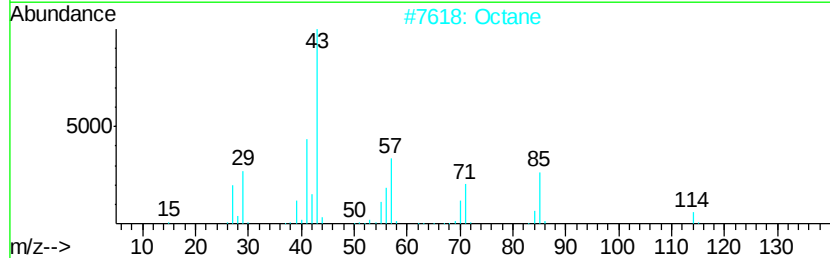
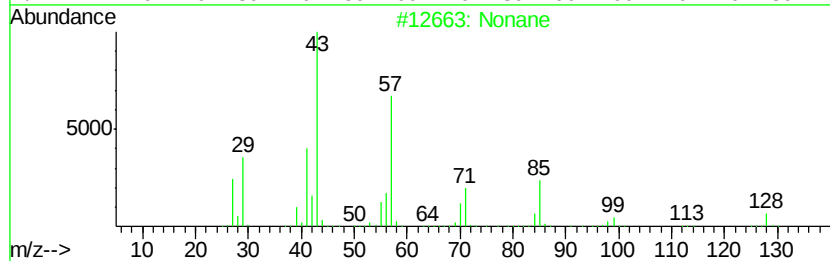
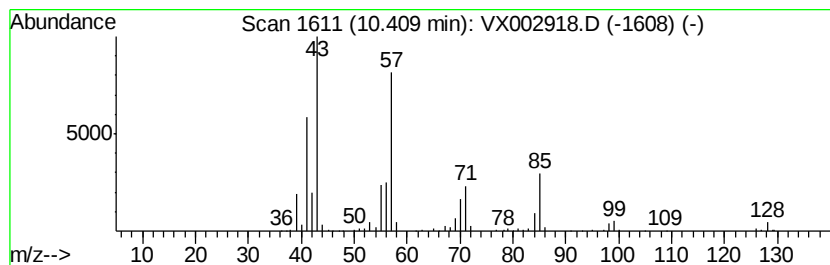
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Nonane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	10.04 ug/l	214121	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane		128	C9H20	000111-84-2	94
2	Octane		114	C8H18	000111-65-9	59
3	Hexane, 2,4-dimethyl-		114	C8H18	000589-43-5	50
4	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	47
5	1-Pentanol, 2-methyl-		102	C6H14O	000105-30-6	43



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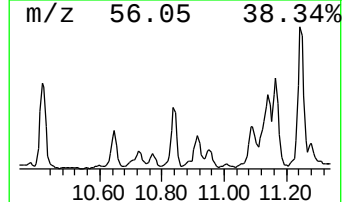
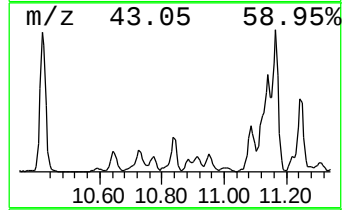
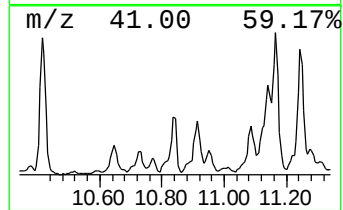
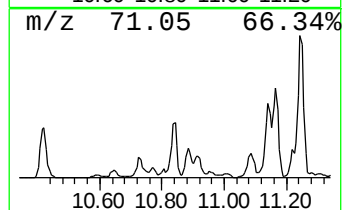
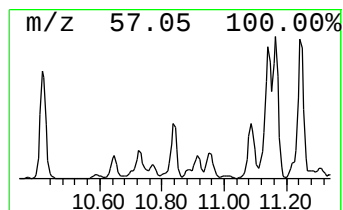
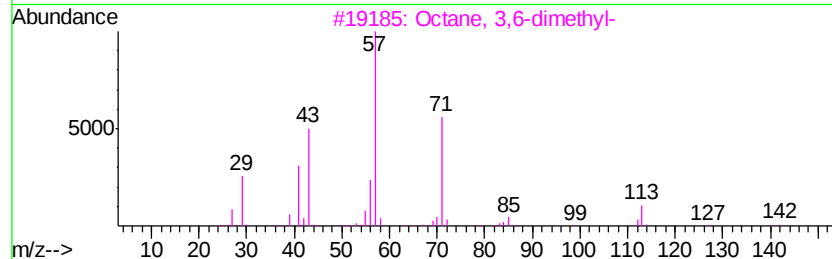
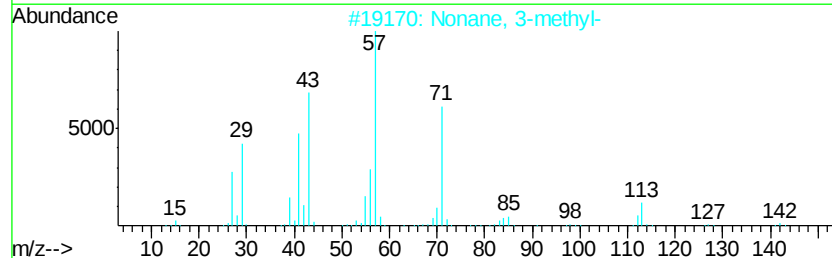
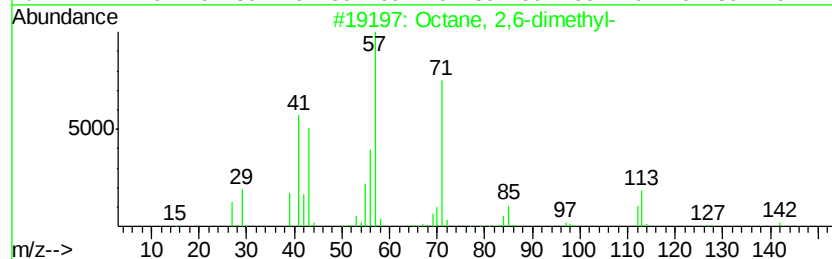
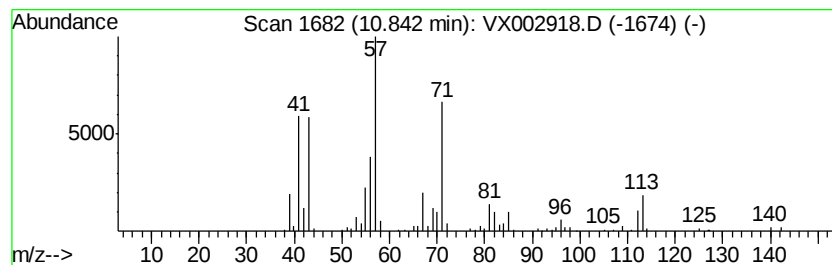
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	5.48 ug/l	116781	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	70
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	58
4		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	53
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
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Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

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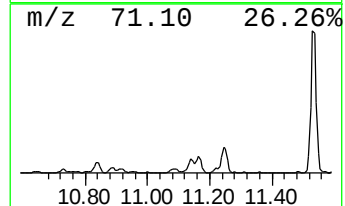
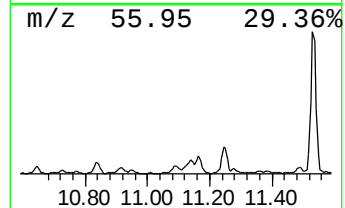
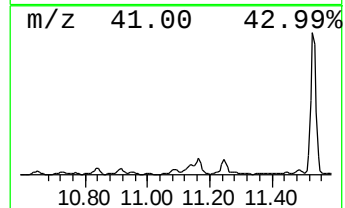
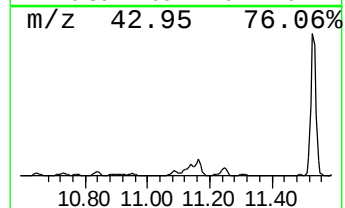
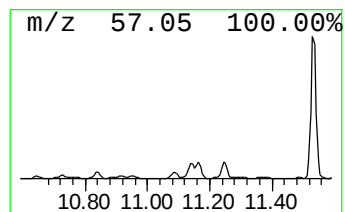
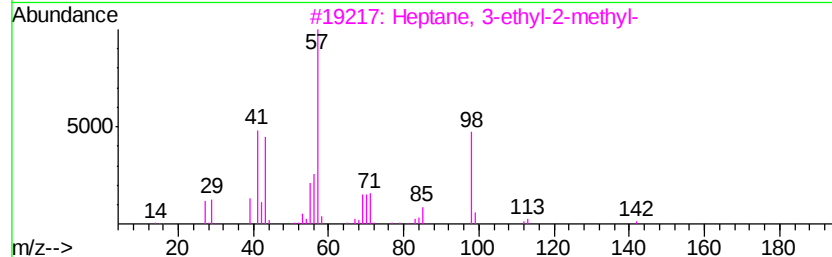
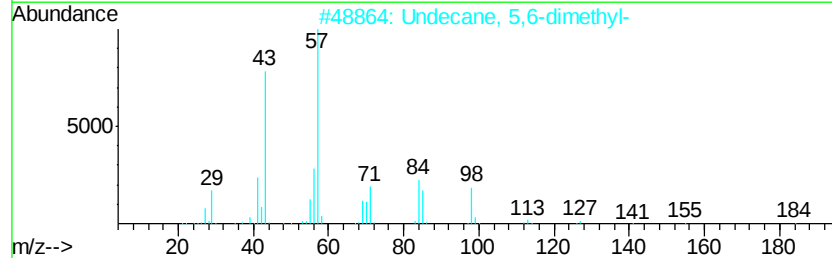
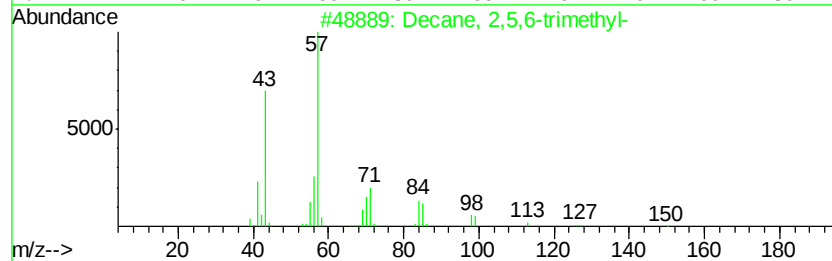
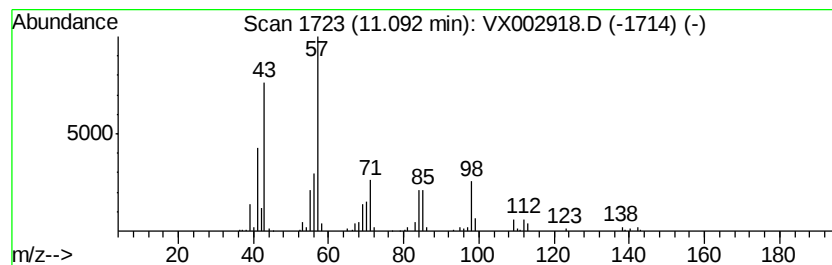
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 4 Decane, 2,5,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	5.49 ug/l	117187	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	64
2		Undecane, 5,6-dimethyl-	184	C13H28	017615-91-7	53
3		Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	53
4		Decane	142	C10H22	000124-18-5	47
5		1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	43



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ALS Vial : 31 Sample Multiplier: 1

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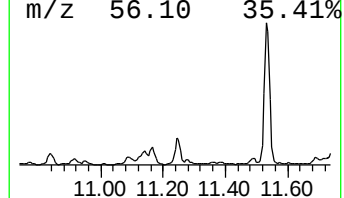
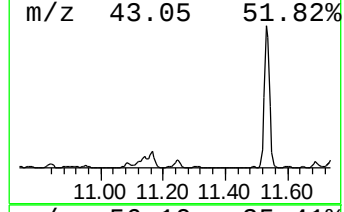
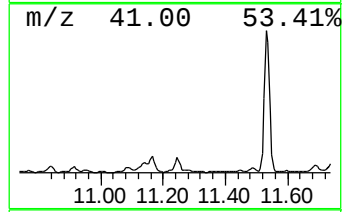
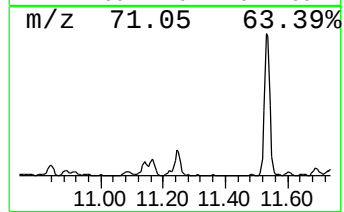
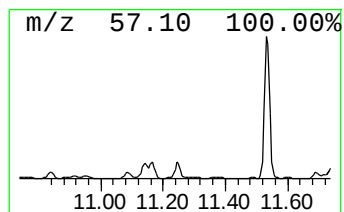
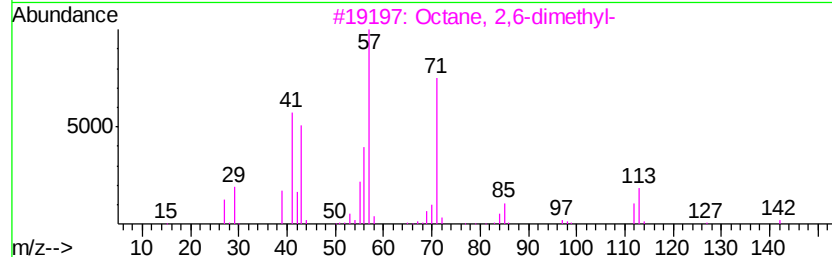
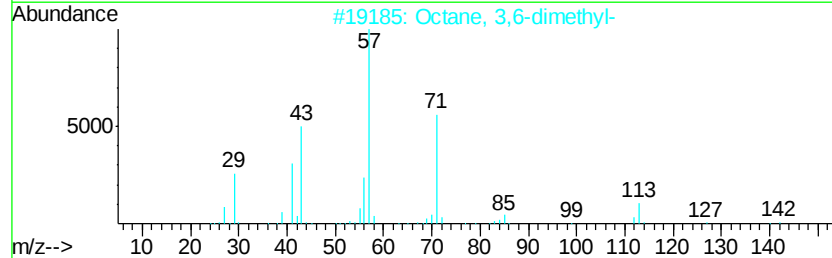
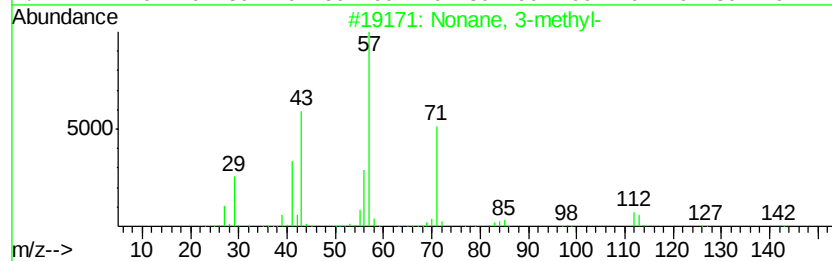
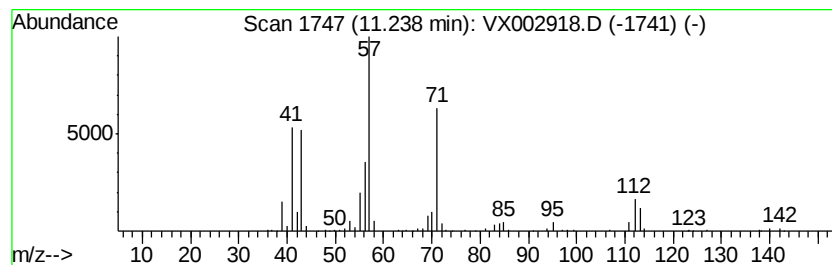
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Quant Title : SW846 8260

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Peak Number 5 Nonane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	7.39 ug/l	227053	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 3-methyl-	142	C10H22	005911-04-6	90
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
3		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4		Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	59
5		Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
Data File : VX002918.D
Acq On : 27 Jun 2018 02:22
Operator : JC/MD
Sample : J3707-12 50X
Misc : 5.91µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

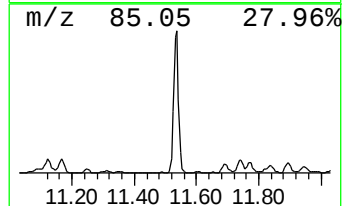
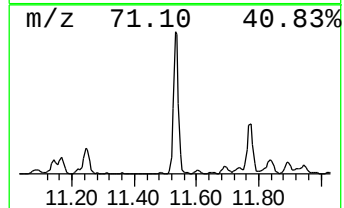
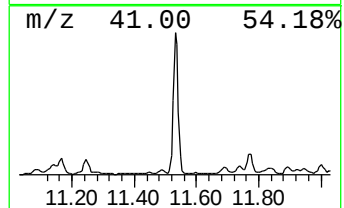
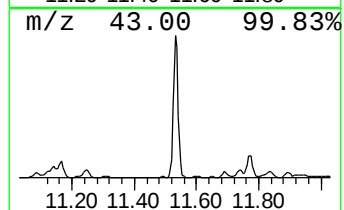
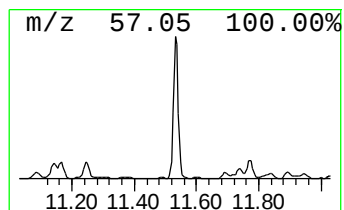
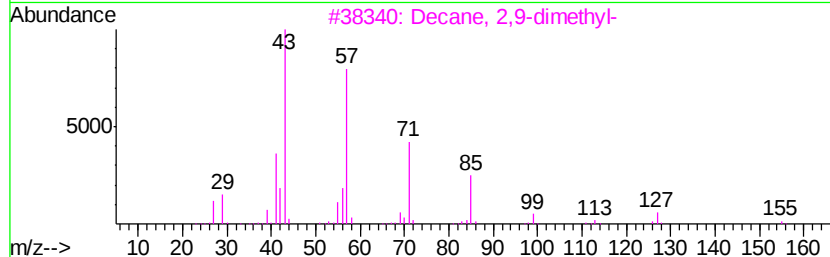
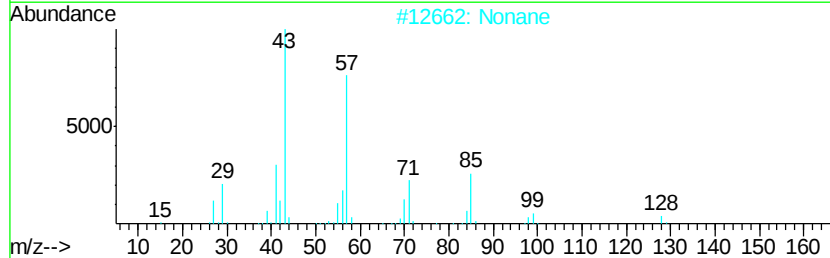
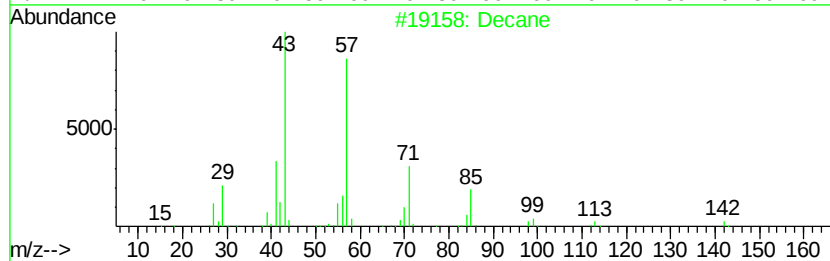
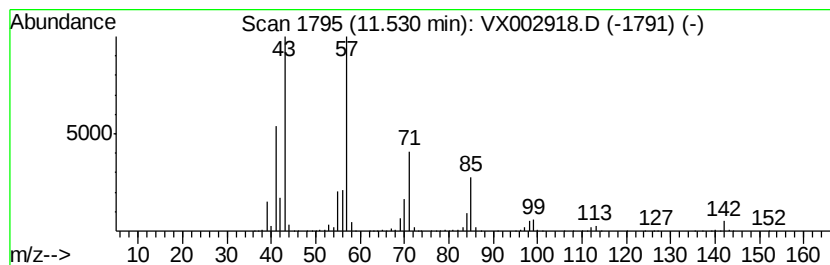
Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

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 Decane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.53	55.54 ug/l	1707470	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	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
4	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	59
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
Data File : VX002918.D
Acq On : 27 Jun 2018 02:22
Operator : JC/MD
Sample : J3707-12 50X
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

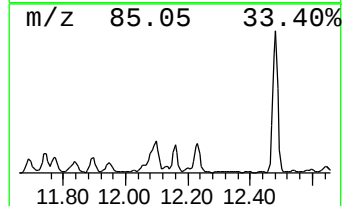
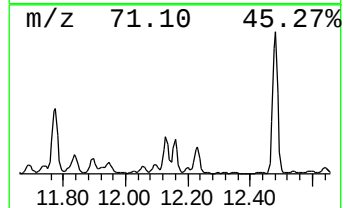
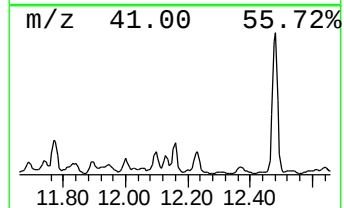
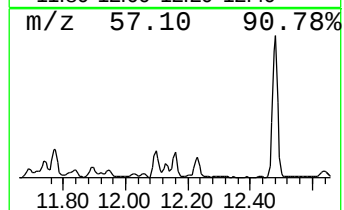
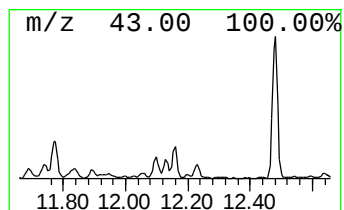
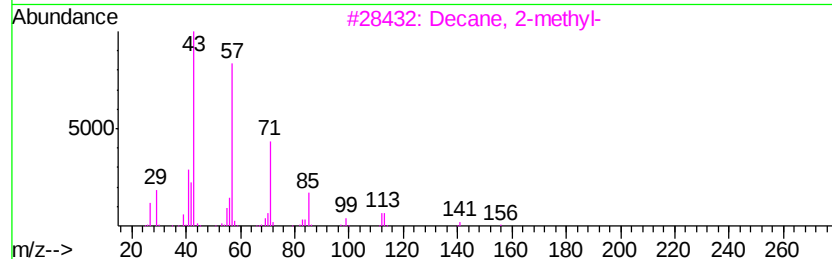
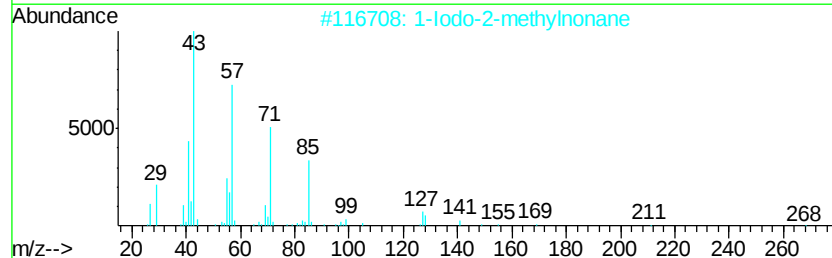
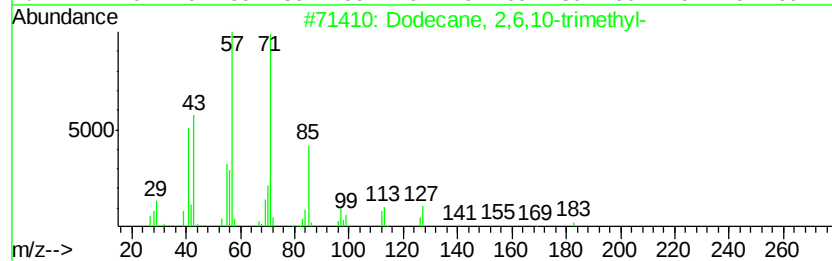
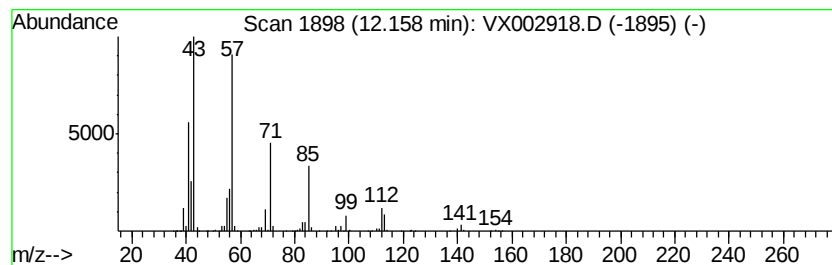
Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

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 Dodecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.16	7.50 ug/l	230441	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
2	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	64
3	Decane, 2-methyl-	156	C11H24	006975-98-0	64
4	Octane, 2-methyl-	128	C9H20	003221-61-2	59
5	Tridecane, 7-methyl-	198	C14H30	026730-14-3	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
Data File : VX002918.D
Acq On : 27 Jun 2018 02:22
Operator : JC/MD
Sample : J3707-12 50X
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

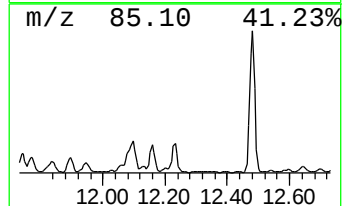
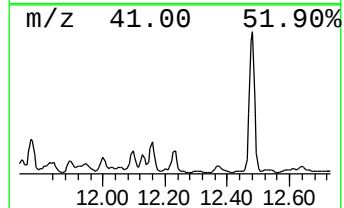
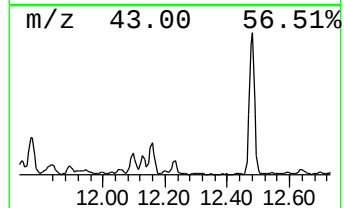
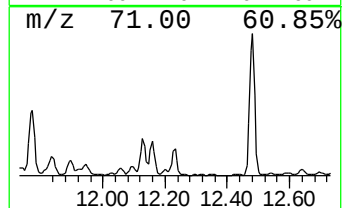
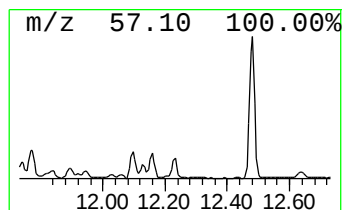
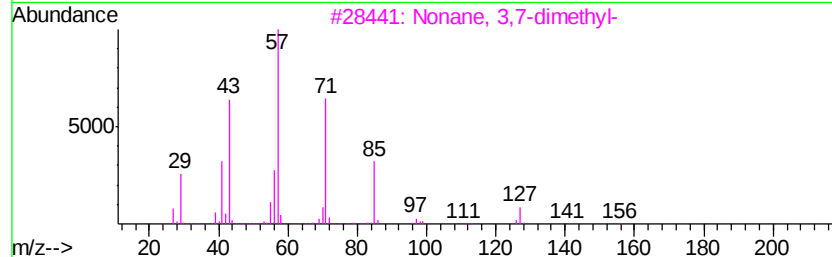
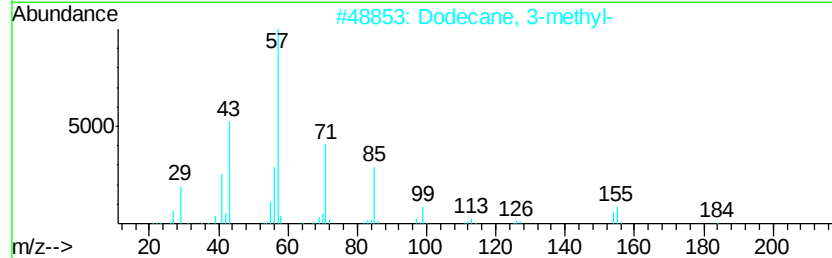
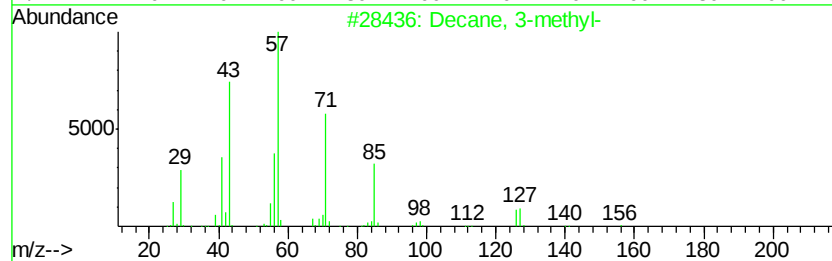
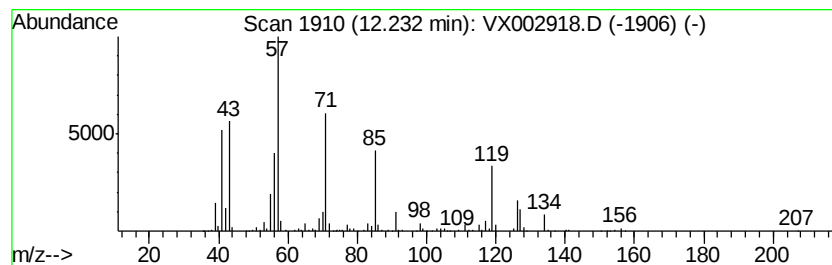
Instrument :
MSVOA_X
ClientSampleID :
WP021SB480-21-23-180622

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 8 Decane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	7.45 ug/l	229179	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane, 3-methyl-	156 C11H24	013151-34-3	64
2	Dodecane, 3-methyl-	184 C13H28	017312-57-1	59
3	Nonane, 3,7-dimethyl-	156 C11H24	017302-32-8	50
4	Undecane, 3,4-dimethyl-	184 C13H28	017312-78-6	50
5	Nonane, 5-(2-methylpropyl)-	184 C13H28	062185-53-9	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX062618\
Data File : VX002918.D
Acq On : 27 Jun 2018 02:22
Operator : JC/MD
Sample : J3707-12 50X
Misc : 5.91µ/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

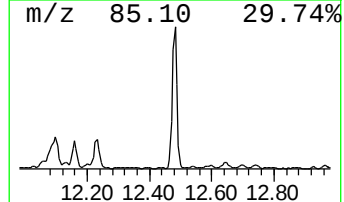
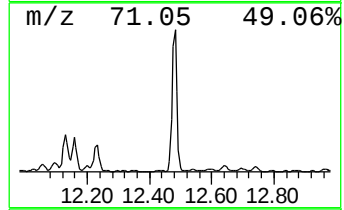
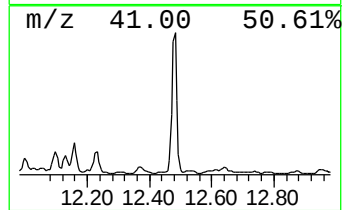
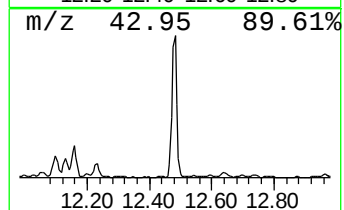
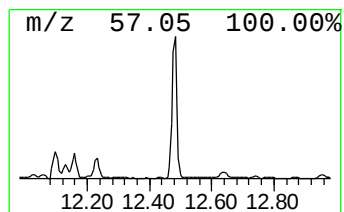
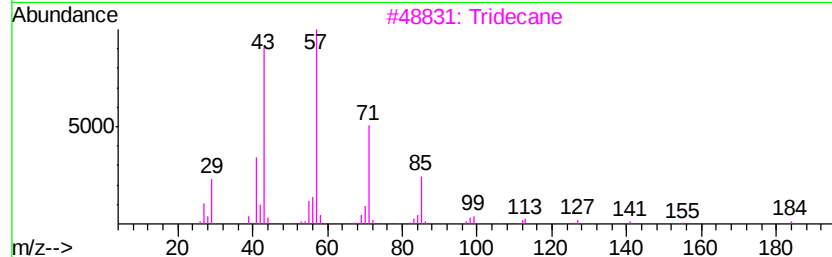
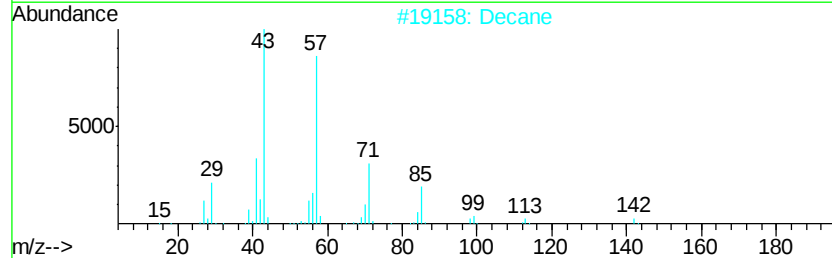
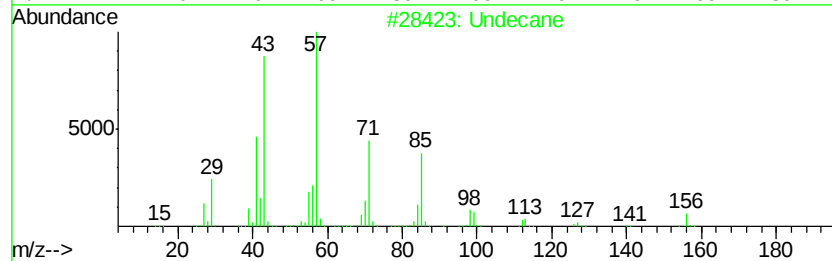
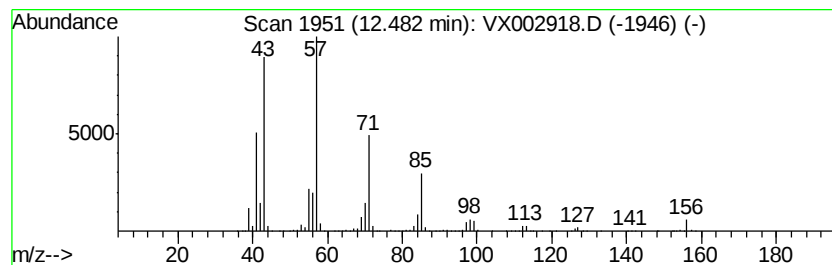
Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

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 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	34.17 ug/l	1050520	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	94
2	Decane	142 C10H22	000124-18-5	86
3	Tridecane	184 C13H28	000629-50-5	80
4	Tetradecane	198 C14H30	000629-59-4	64
5	Hexadecane	226 C16H34	000544-76-3	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX062618\
Data File : VX002918.D
Acq On : 27 Jun 2018 02:22
Operator : JC/MD
Sample : J3707-12 50X
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WP021SB480-21-23-180622

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Nonane	10.41	10.0	ug/l	214121	3	10.12	1066360	50.0
Octane, 2,6-dimet...	10.84	5.5	ug/l	116781	3	10.12	1066360	50.0
Decane, 2,5,6-tri...	11.09	5.5	ug/l	117187	3	10.12	1066360	50.0
Nonane, 3-methyl-	11.24	7.4	ug/l	227053	4	12.08	1537220	50.0
Decane	11.53	55.5	ug/l	1707470	4	12.08	1537220	50.0
Dodecane, 2,6,10-...	12.16	7.5	ug/l	230441	4	12.08	1537220	50.0
Decane, 3-methyl-	12.23	7.5	ug/l	229179	4	12.08	1537220	50.0
Undecane	12.48	34.2	ug/l	1050520	4	12.08	1537220	50.0