

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\WX041720\
 Data File : VX015738.D
 Acq On : 17 Apr 2020 15:16
 Operator : JC/SP
 Sample : L2312-01
 Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40693-40720-40531

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\82X032720W.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	1.064	23	29	38	rBV	2159064	2684905	11.64%	2.861%
2	5.478	742	753	760	rBV2	454637	1385361	6.01%	1.476%
3	5.563	760	767	772	rVV	537220	1578072	6.84%	1.681%
4	5.630	772	778	799	rVB	893992	3062905	13.28%	3.263%
5	5.886	808	820	835	rBV	1138460	3249411	14.09%	3.462%
6	6.039	835	845	858	rVB	526306	1424619	6.18%	1.518%
7	6.246	866	879	886	rBV4	166944	570483	2.47%	0.608%
8	6.667	937	948	961	rBV	1968121	4753401	20.61%	5.065%
9	6.831	965	975	988	rVB	1321418	3216996	13.95%	3.428%
10	7.435	1064	1074	1085	rVB2	294817	711786	3.09%	0.758%
11	7.709	1112	1119	1127	rVB2	146548	277527	1.20%	0.296%
12	8.697	1275	1281	1287	rBV	2722283	4445504	19.27%	4.737%
13	8.770	1287	1293	1310	rVB	14102740	23066353	100.00%	24.577%
14	10.099	1506	1511	1524	rVB	2678202	4079206	17.68%	4.346%
15	10.343	1540	1551	1557	rVV2	241916	464097	2.01%	0.494%
16	10.398	1557	1560	1569	rVB2	173012	239808	1.04%	0.256%
17	11.129	1674	1680	1690	rVB	2643779	3644037	15.80%	3.883%
18	11.422	1724	1728	1734	rBV	236641	439893	1.91%	0.469%
19	11.513	1738	1743	1749	rVB2	196448	401089	1.74%	0.427%
20	11.660	1762	1767	1773	rVB3	173879	276952	1.20%	0.295%
21	11.794	1785	1789	1798	rVB	404044	558711	2.42%	0.595%
22	12.068	1828	1834	1839	rBV	3759934	4770606	20.68%	5.083%
23	12.355	1877	1881	1889	rVV3	319671	632451	2.74%	0.674%
24	12.464	1890	1899	1903	rVV	228259	364473	1.58%	0.388%
25	12.861	1958	1964	1967	rBV3	253504	321288	1.39%	0.342%
26	13.086	1995	2001	2003	rBV3	187129	303096	1.31%	0.323%
27	13.208	2014	2021	2026	rBV5	283373	556009	2.41%	0.592%
28	13.306	2031	2037	2039	rVV4	214711	375188	1.63%	0.400%
29	13.336	2039	2042	2047	rVB2	658505	847566	3.67%	0.903%
30	13.464	2058	2063	2071	rVB	562843	939003	4.07%	1.000%
31	13.543	2072	2076	2079	rBV2	166640	233939	1.01%	0.249%
32	13.629	2086	2090	2094	rBV3	274706	436705	1.89%	0.465%
33	13.708	2100	2103	2108	rVB3	207869	302282	1.31%	0.322%
34	13.897	2127	2134	2139	rVB3	546491	888096	3.85%	0.946%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

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\82X032720W.M
Title : SW846 8260

35	13.970	2139	2146	2151	rBV5	507408	1070971	4.64%	1.141%
36	14.074	2161	2163	2166	rVB2	232026	235536	1.02%	0.251%
37	14.117	2166	2170	2174	rBV2	447580	555351	2.41%	0.592%
38	14.269	2188	2195	2201	rBV2	1463683	2412661	10.46%	2.571%
39	14.360	2207	2210	2216	rBV4	266745	403476	1.75%	0.430%
40	14.415	2216	2219	2224	rVV	537600	678769	2.94%	0.723%
41	14.458	2224	2226	2232	rVV4	132266	237405	1.03%	0.253%
42	14.525	2232	2237	2245	rVV2	887378	1292506	5.60%	1.377%
43	14.659	2255	2259	2265	rBV2	1112375	1978588	8.58%	2.108%
44	14.714	2265	2268	2273	rVB2	537459	722260	3.13%	0.770%
45	14.769	2273	2277	2280	rBV2	277784	375884	1.63%	0.400%
46	14.824	2283	2286	2289	rVV2	179226	251933	1.09%	0.268%
47	14.860	2289	2292	2295	rVV2	288516	404359	1.75%	0.431%
48	14.891	2295	2297	2302	rVV4	292931	321821	1.40%	0.343%
49	14.946	2302	2306	2317	rVB2	304863	540207	2.34%	0.576%
50	15.092	2324	2330	2335	rBV4	178403	345804	1.50%	0.368%
51	15.238	2348	2354	2361	rBV	5947205	8261617	35.82%	8.803%
52	15.427	2380	2385	2389	rBV4	190348	298355	1.29%	0.318%
53	15.531	2398	2402	2407	rBV3	252759	369445	1.60%	0.394%
54	15.665	2419	2424	2428	rBV2	213072	364569	1.58%	0.388%
55	15.714	2428	2432	2439	rVB4	153137	326534	1.42%	0.348%
56	16.031	2477	2484	2490	rBV	468974	904245	3.92%	0.963%

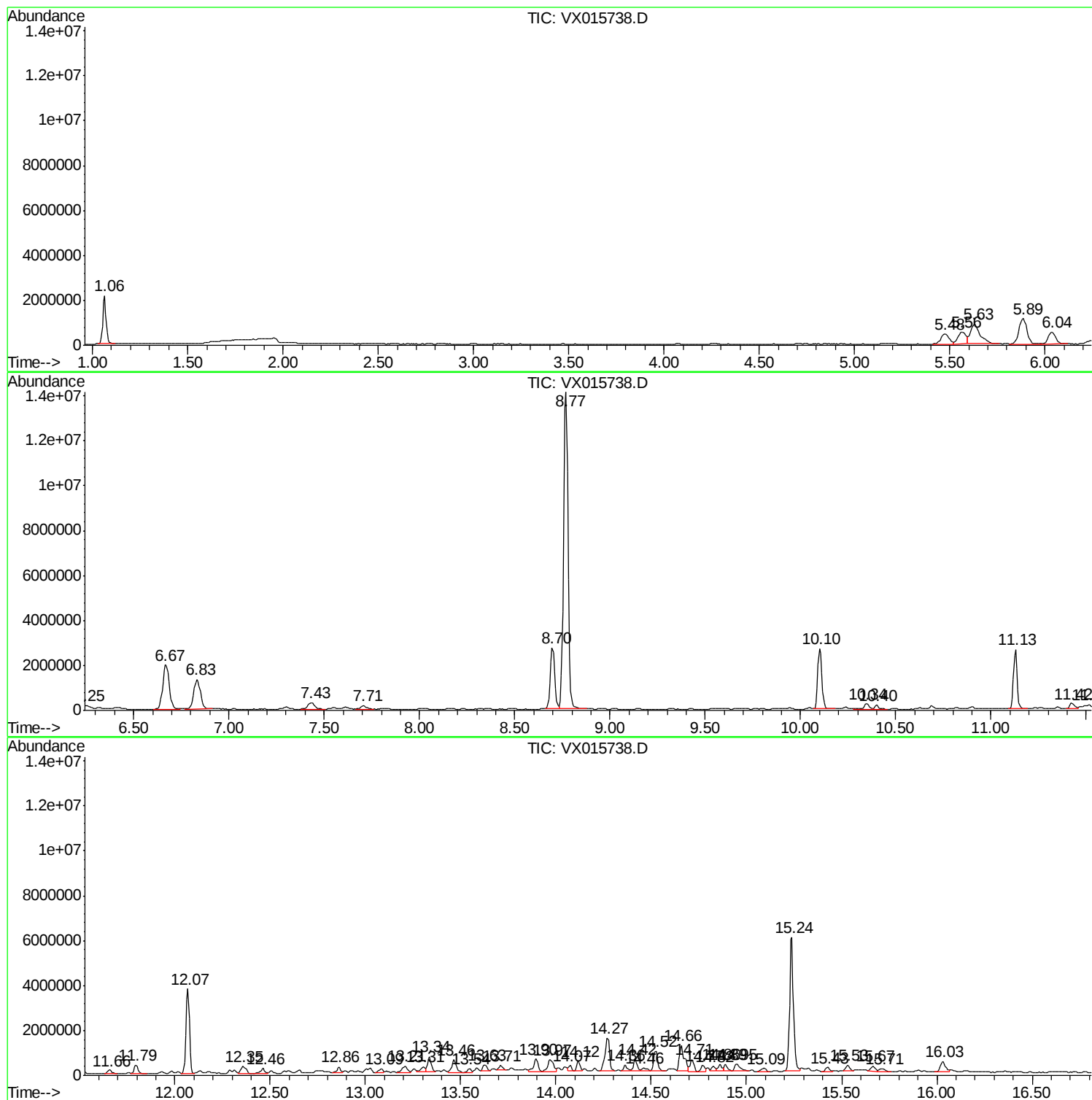
Sum of corrected areas: 93854114

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µL/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

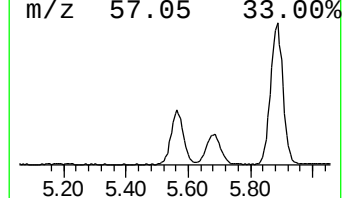
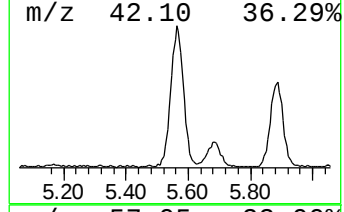
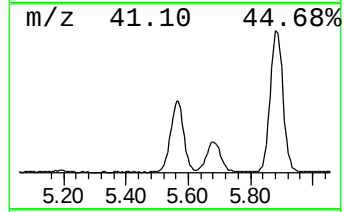
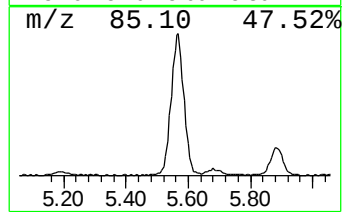
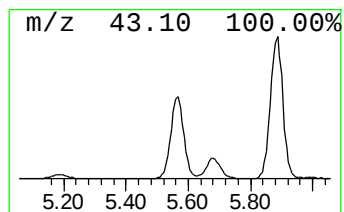
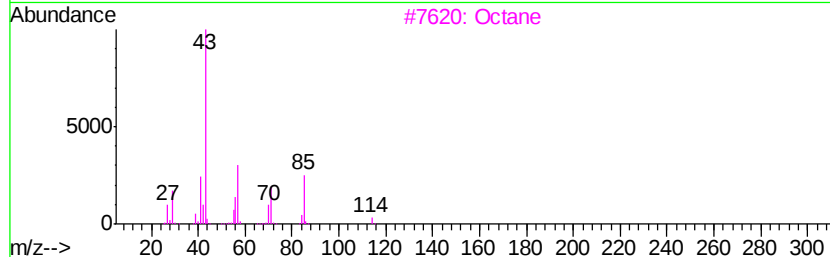
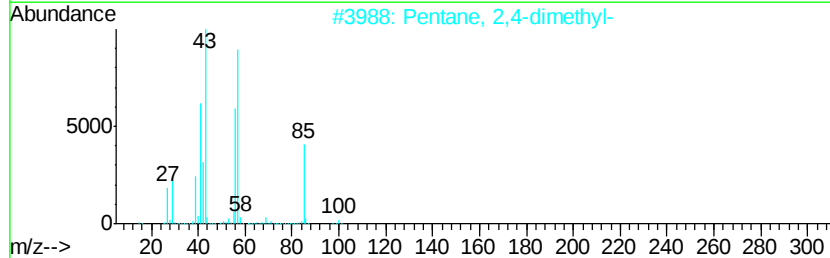
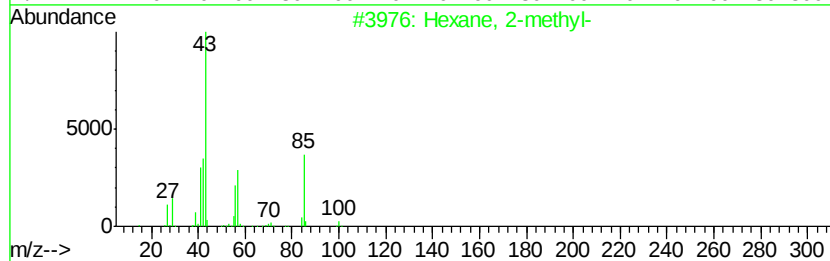
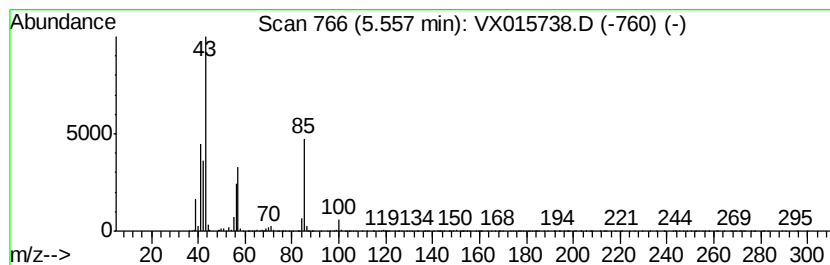
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	25.76 ug/l	1578070	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2-methyl-	100	C7H16	000591-76-4	91
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	59
3		Octane	114	C8H18	000111-65-9	50
4		Furan, tetrahydro-2,4-dimethyl-,...	100	C6H12O	039168-02-0	47
5		Oxetane, 2-ethyl-3-methyl-	100	C6H12O	053778-62-4	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µL/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

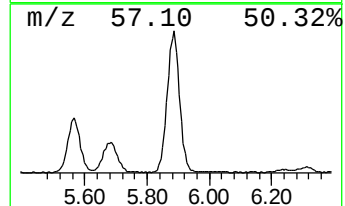
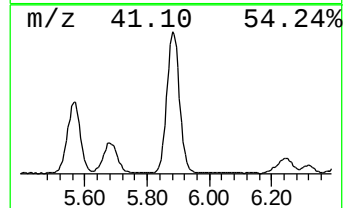
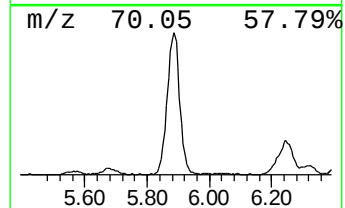
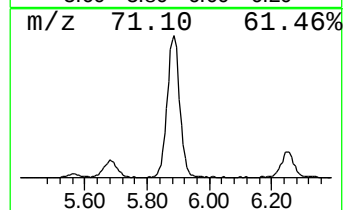
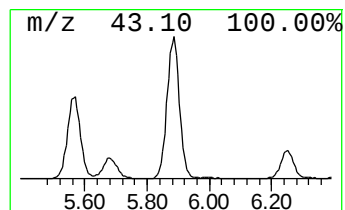
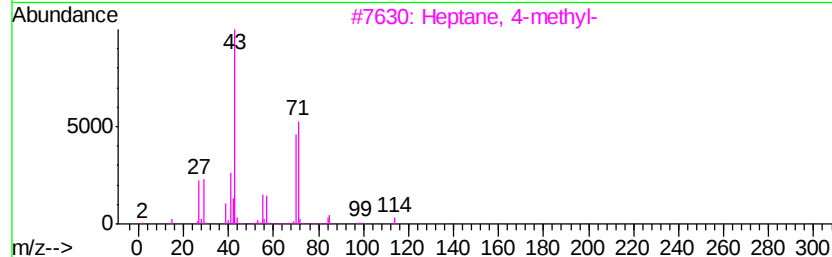
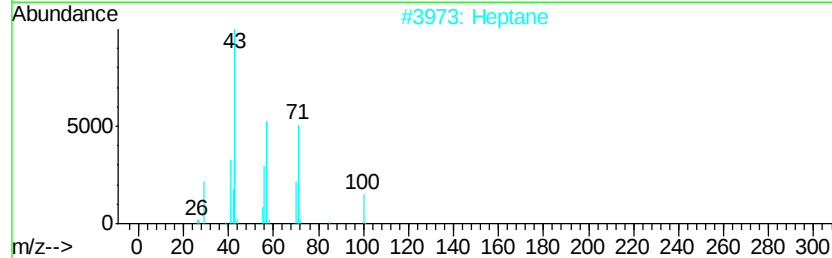
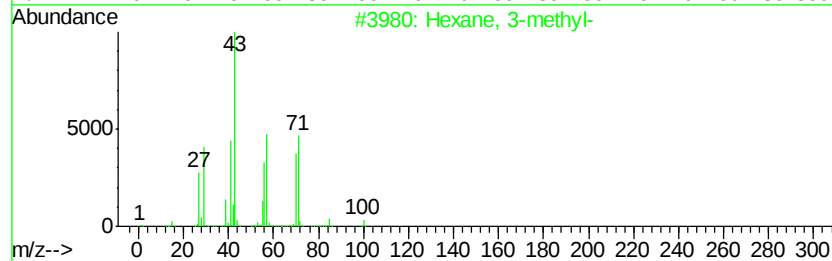
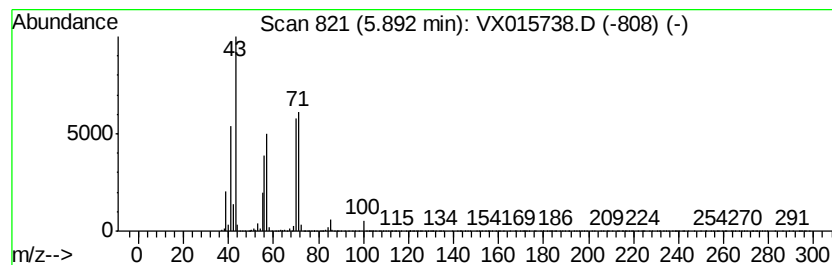
Instrument :
MSVOA_X
ClientSampleID :
40693-40720-40531

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 3 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.89	53.04 ug/l	3249410	Pentafluorobenzene	5.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-		100	C7H16	000589-34-4	94
2	Heptane		100	C7H16	000142-82-5	72
3	Heptane, 4-methyl-		114	C8H18	000589-53-7	64
4	Hexane, 3,3,4-trimethyl-		128	C9H20	016747-31-2	53
5	Heptane, 3,4-dimethyl-		128	C9H20	000922-28-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

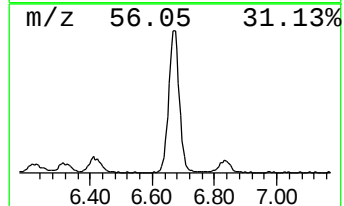
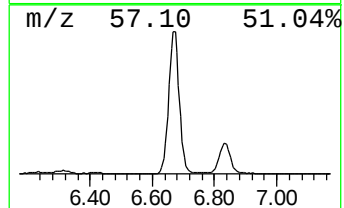
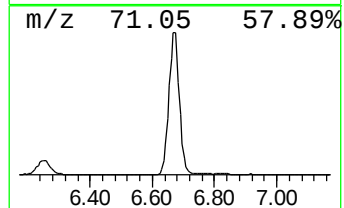
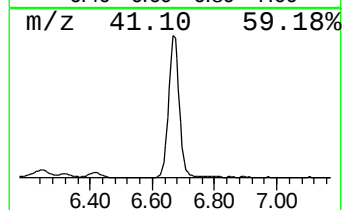
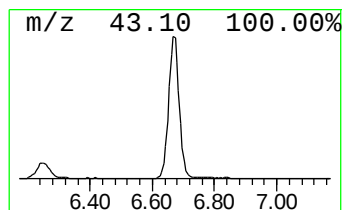
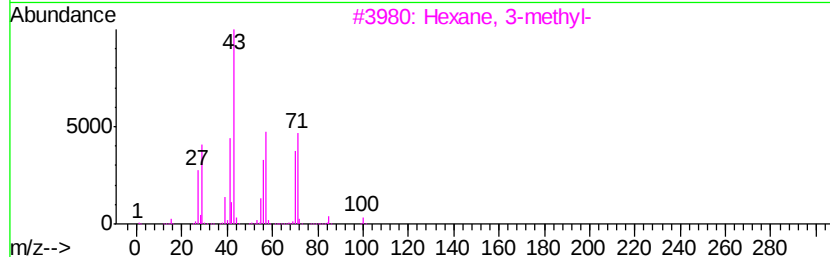
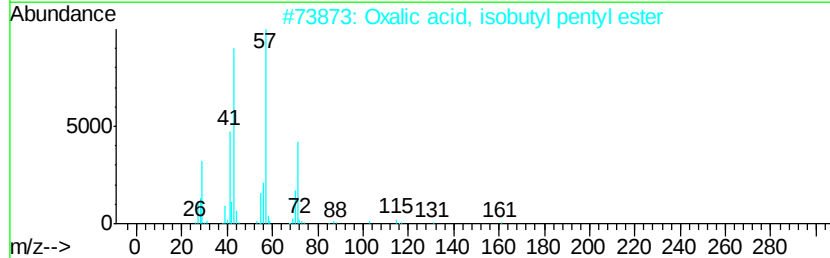
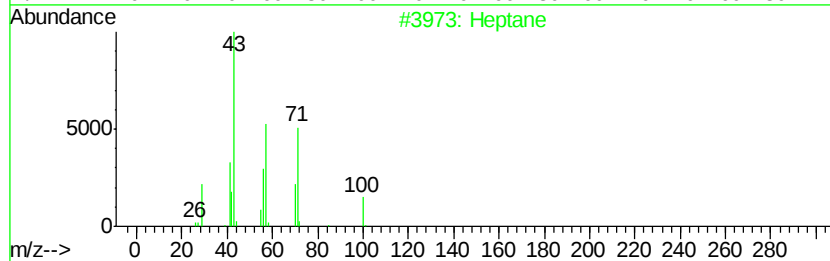
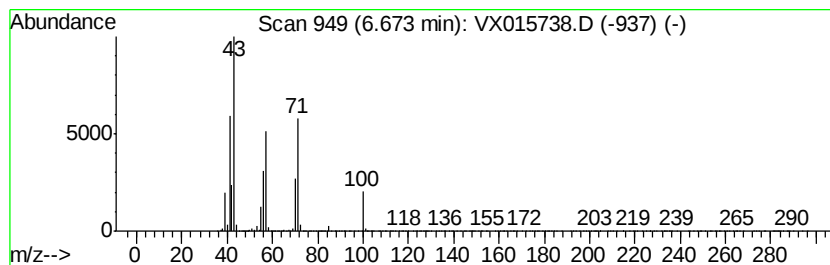
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 4 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	73.88 ug/l	4753400	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	38
4		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37
5		3-Hexanone	100	C6H12O	000589-38-8	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µL/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

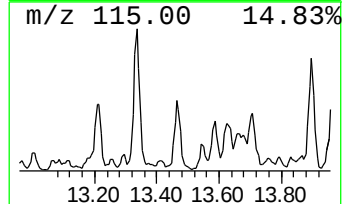
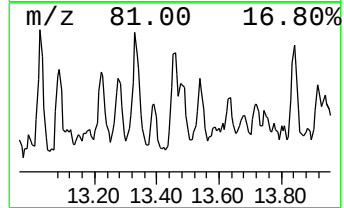
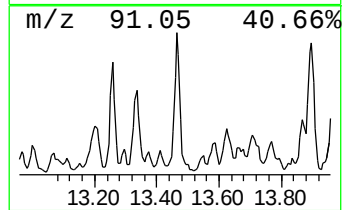
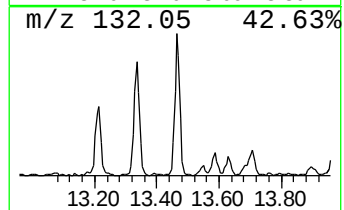
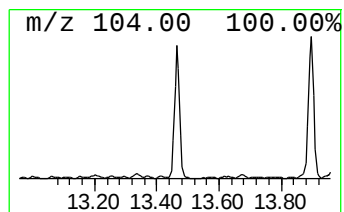
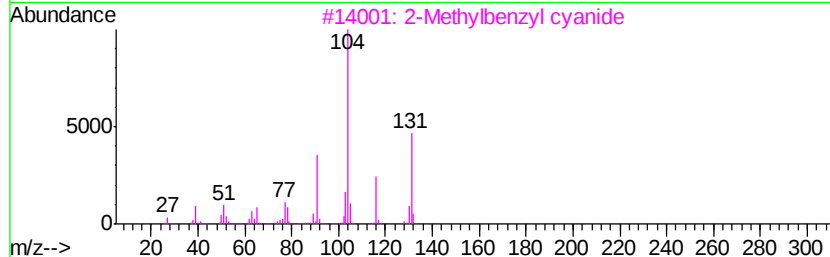
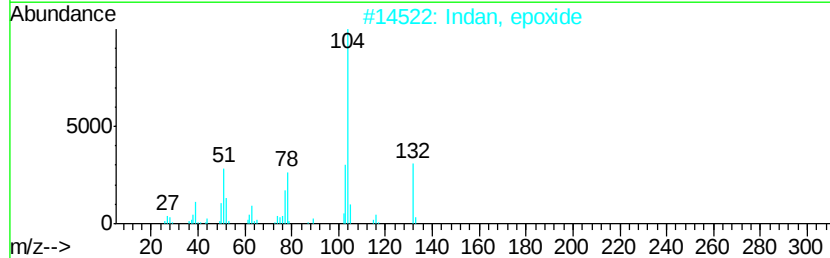
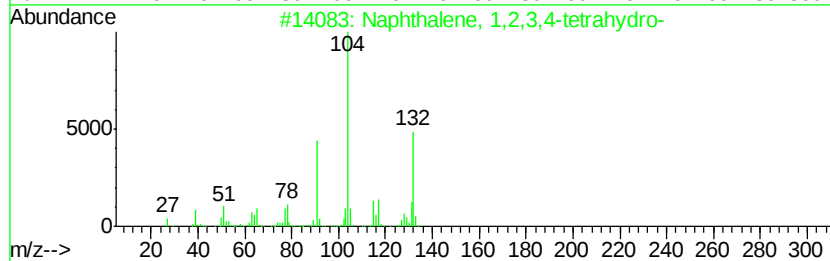
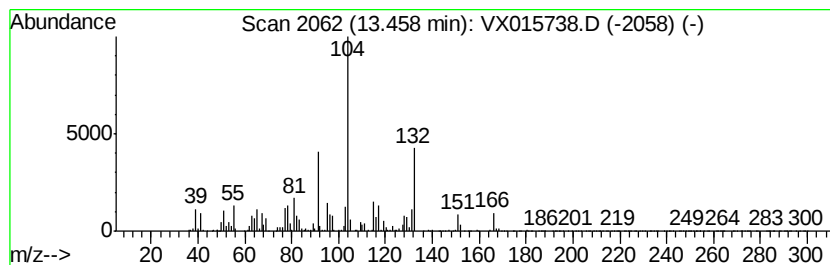
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	9.84 ug/l	939003	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2		Indan, epoxide	132	C9H8O	000768-22-9	64
3		2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	60
4		Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	43
5		Phensuximide	189	C11H11NO2	000086-34-0	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µl/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

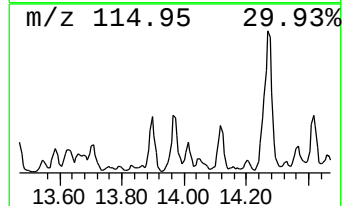
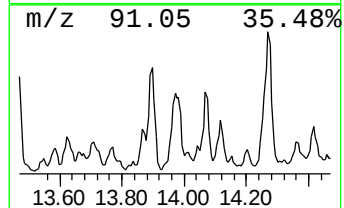
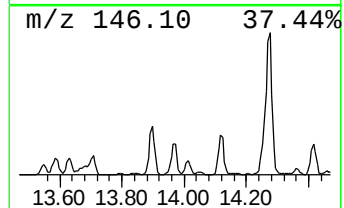
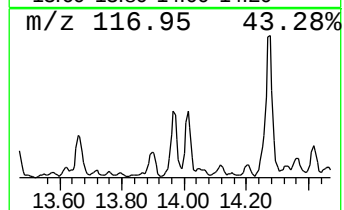
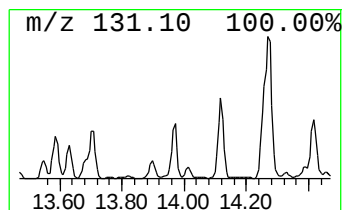
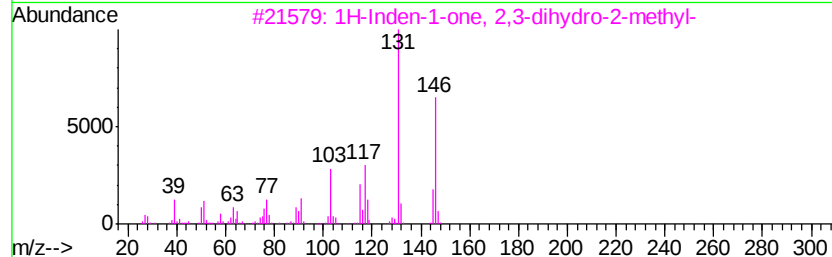
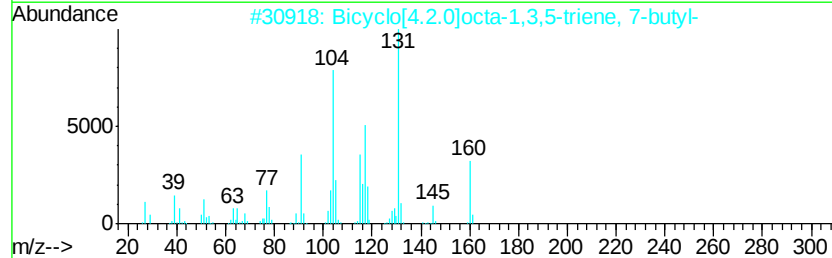
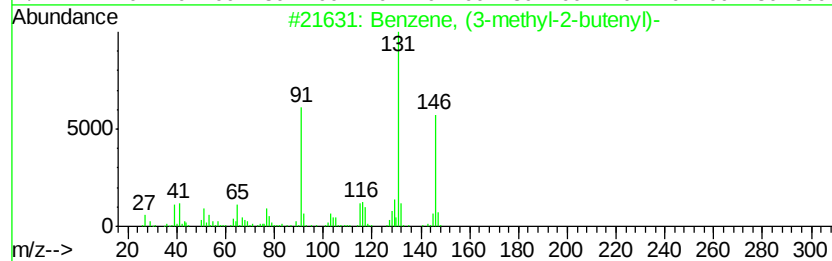
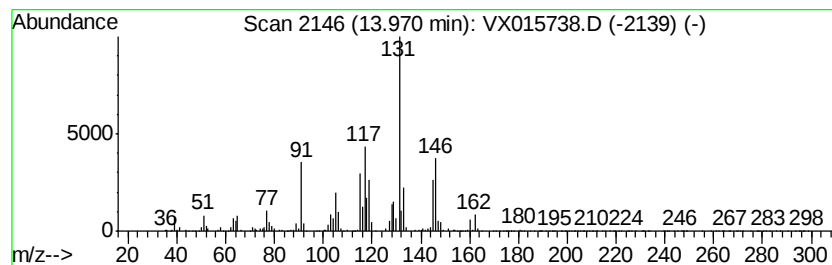
Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	11.22 ug/l	1070970	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, (3-methyl-2-butenyl)-	146 C11H14	004489-84-3 90
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	160 C12H16	078920-29-3 64
3		1H-Inden-1-one, 2,3-dihydro-2-methyl-	146 C10H10O	017496-14-9 62
4		Naphthalene, 1,2,3,4-tetrahydro-	146 C11H14	001680-51-9 60
5		1H-Indene, 2,3-dihydro-4,7-dimethyl-	146 C11H14	006682-71-9 60



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µl/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

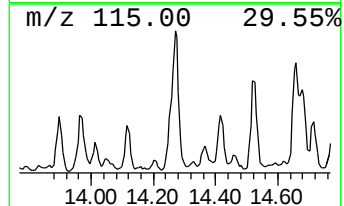
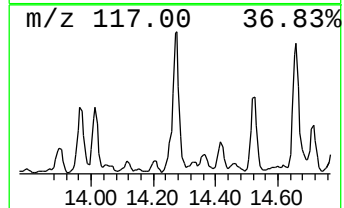
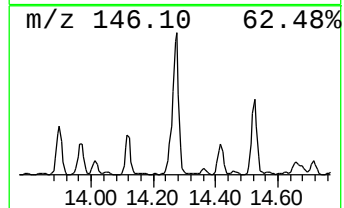
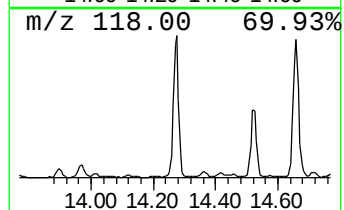
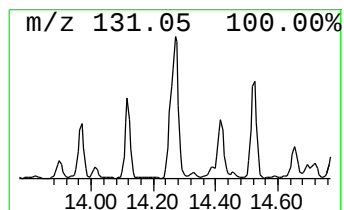
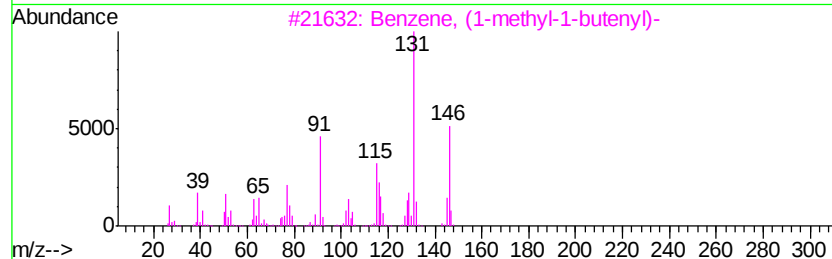
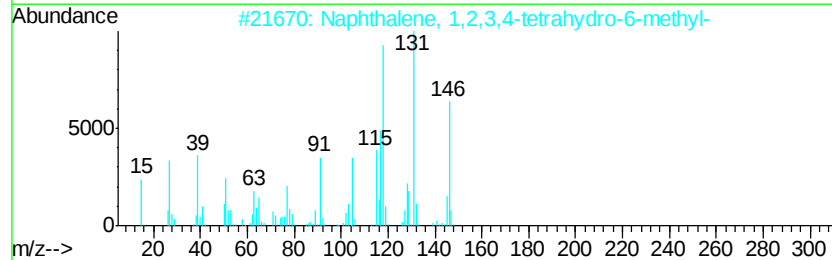
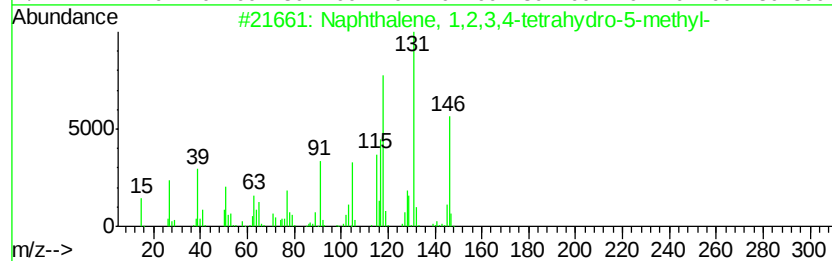
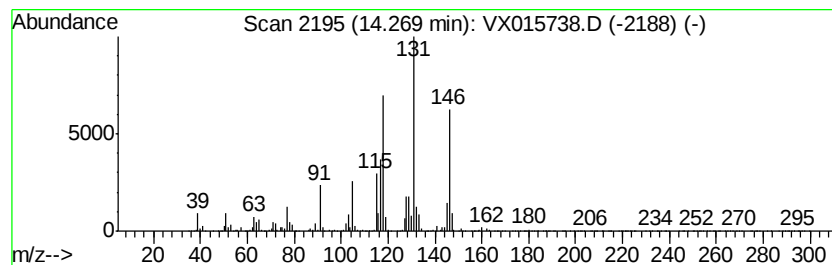
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	25.29 ug/l	2412660	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	97
3		Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	89
4		Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	86
5		1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

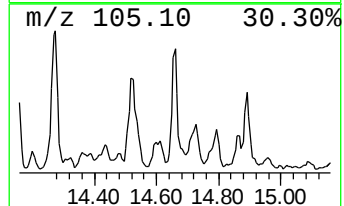
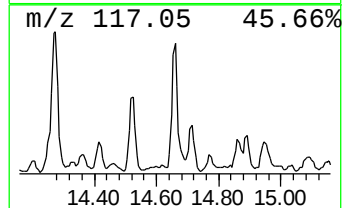
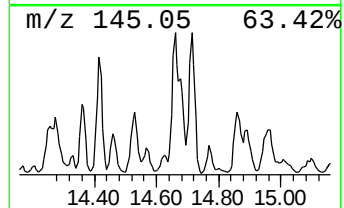
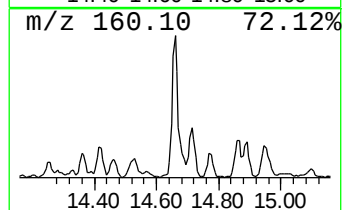
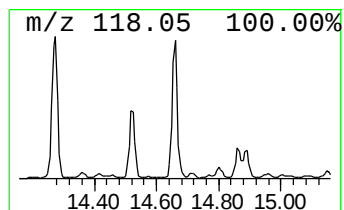
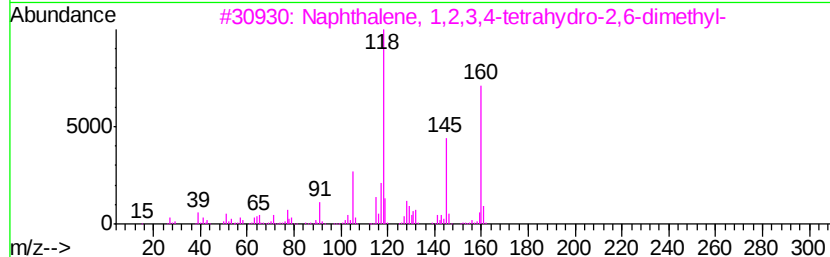
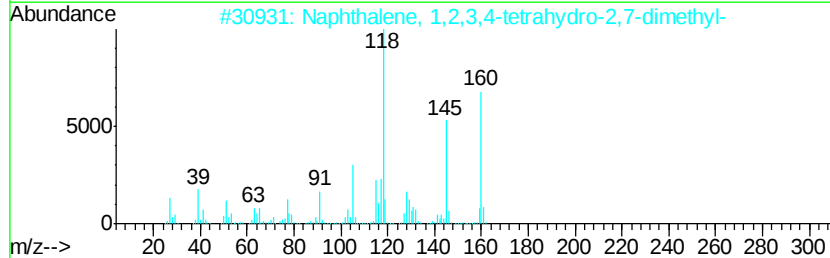
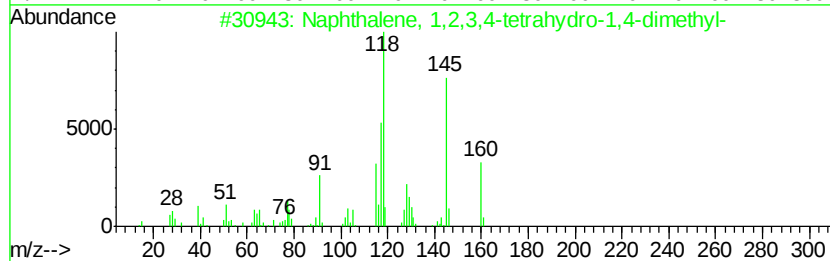
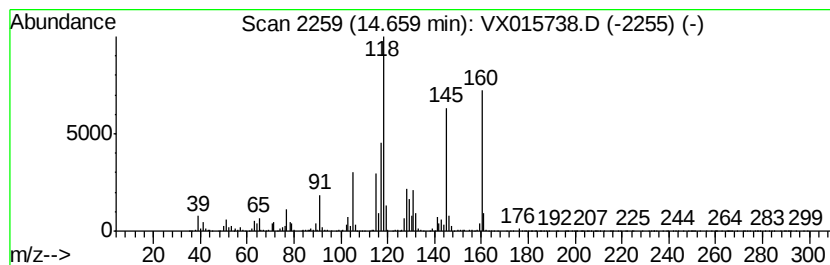
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	20.74 ug/l	1978590	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	93
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	76
4		Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	68
5		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05µL/10mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

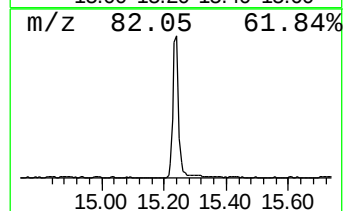
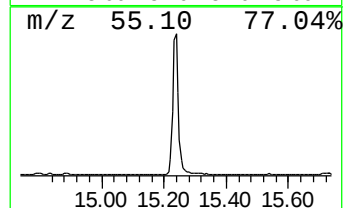
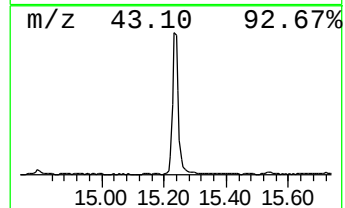
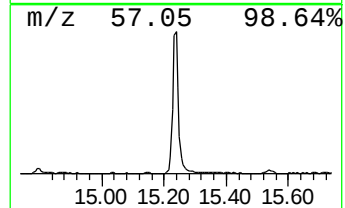
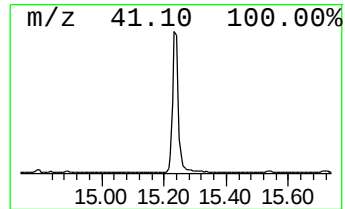
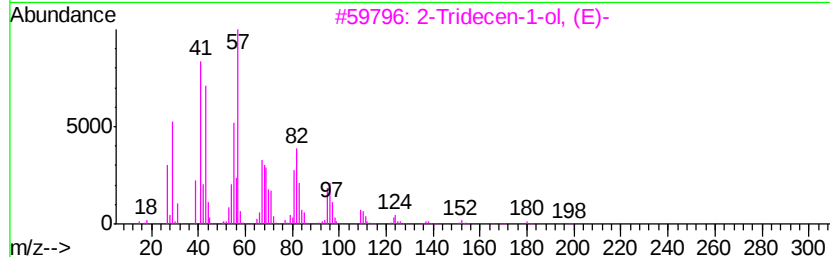
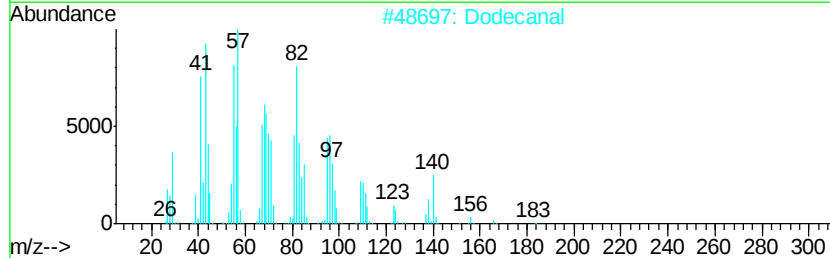
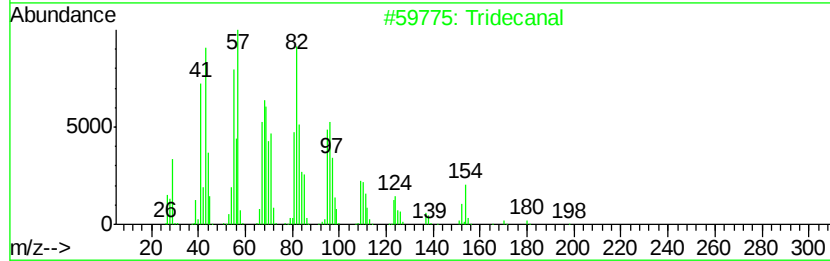
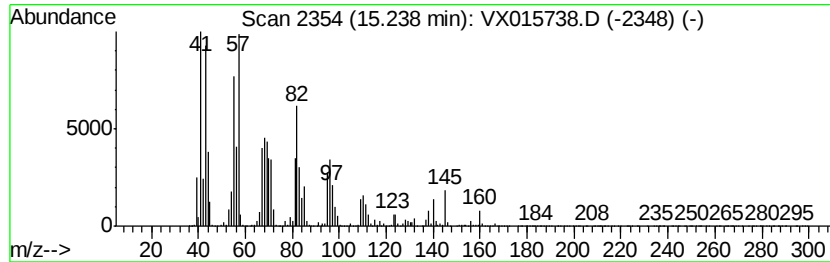
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 10 Tridecanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	86.59 ug/l	8261620	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanal	198	C13H26O	010486-19-8	94
2		Dodecanal	184	C12H24O	000112-54-9	94
3		2-Tridecen-1-ol, (E)-	198	C13H26O	074962-98-4	93
4		1,1-Dodecanediol, diacetate	286	C16H30O4	056438-07-4	91
5		9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041720\
Data File : VX015738.D
Acq On : 17 Apr 2020 15:16
Operator : JC/SP
Sample : L2312-01
Misc : 1.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40693-40720-40531

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.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
Hexane, 2-methyl-	5.56	25.8	ug/l	1578070	1	5.63	3062910	50.0
Hexane, 3-methyl-	5.89	53.0	ug/l	3249410	1	5.63	3062910	50.0
Heptane	6.67	73.9	ug/l	4753400	2	6.83	3217000	50.0
Naphthalene, 1,2,...	13.46	9.8	ug/l	939003	4	12.07	4770610	50.0
Benzene, (3-methy...	13.97	11.2	ug/l	1070970	4	12.07	4770610	50.0
Naphthalene, 1,2,...	14.27	25.3	ug/l	2412660	4	12.07	4770610	50.0
Naphthalene, 1,2,...	14.66	20.7	ug/l	1978590	4	12.07	4770610	50.0
Tridecanal	15.24	86.6	ug/l	8261620	4	12.07	4770610	50.0