

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX011020\
 Data File : VX014545.D
 Acq On : 10 Jan 2020 18:18
 Operator : JC/SP
 Sample : L1080-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-1R

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\82X010720W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	44	rBV	1999959	2331436	92.81%	7.396%
2	1.271	59	63	70	rBV	29391	46719	1.86%	0.148%
3	1.594	109	116	119	rVB6	25930	45947	1.83%	0.146%
4	1.783	143	147	154	rVB	188973	264667	10.54%	0.840%
5	2.387	239	246	257	rVB	80080	164670	6.56%	0.522%
6	2.588	272	279	286	rBV	60458	110647	4.40%	0.351%
7	2.838	312	320	332	rBV	399892	899572	35.81%	2.854%
8	3.173	366	375	387	rBV2	399611	995448	39.63%	3.158%
9	4.130	526	532	544	rVB4	20533	55983	2.23%	0.178%
10	4.307	546	561	572	rBV2	81586	251705	10.02%	0.798%
11	4.545	591	600	614	rVB3	23001	89197	3.55%	0.283%
12	5.240	703	714	725	rBV3	35042	128006	5.10%	0.406%
13	5.490	742	755	766	rBV2	264630	750919	29.89%	2.382%
14	5.654	771	782	787	rVV	472525	1308655	52.10%	4.152%
15	5.722	787	793	811	rVB	483992	1462088	58.21%	4.638%
16	5.935	821	828	838	rVB3	30767	95657	3.81%	0.303%
17	6.057	838	848	857	rBV	283967	741013	29.50%	2.351%
18	6.258	870	881	886	rBV2	125289	389047	15.49%	1.234%
19	6.343	886	895	907	rVV2	815356	2511961	100.00%	7.969%
20	6.453	907	913	923	rVB4	23392	58967	2.35%	0.187%
21	6.849	970	978	989	rBV	709256	1671071	66.52%	5.301%
22	7.441	1065	1075	1083	rBV3	68777	161867	6.44%	0.513%
23	7.569	1091	1096	1101	rBV3	38928	79465	3.16%	0.252%
24	7.636	1101	1107	1110	rVV2	80733	167488	6.67%	0.531%
25	7.678	1110	1114	1122	rVB	67985	137593	5.48%	0.436%
26	7.843	1134	1141	1148	rVB2	85781	183257	7.30%	0.581%
27	8.050	1165	1175	1183	rVB	517970	1082053	43.08%	3.433%
28	8.172	1186	1195	1203	rBV	781611	1534090	61.07%	4.867%
29	8.252	1203	1208	1213	rBV	74056	125842	5.01%	0.399%
30	8.386	1223	1230	1235	rBV6	33530	72540	2.89%	0.230%
31	8.447	1235	1240	1244	rVV	36602	73543	2.93%	0.233%
32	8.483	1244	1246	1250	rVV3	25659	41494	1.65%	0.132%
33	8.532	1250	1254	1257	rVV2	33549	62815	2.50%	0.199%
34	8.581	1258	1262	1269	rVB	47686	78590	3.13%	0.249%

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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\82X010720W.M
 Title : SW846 8260

35	8.672	1269	1277	1278	rBV2	134417	208150	8.29%	0.660%
36	8.709	1278	1283	1292	rVB	1503054	2379198	94.71%	7.548%
37	8.831	1299	1303	1307	rBV	33065	52255	2.08%	0.166%
38	8.880	1307	1311	1313	rVV4	18563	28998	1.15%	0.092%
39	9.038	1331	1337	1342	rVB3	47064	86744	3.45%	0.275%
40	9.160	1350	1357	1362	rVB2	91791	158468	6.31%	0.503%
41	9.215	1362	1366	1370	rBV	45605	67705	2.70%	0.215%
42	9.434	1397	1402	1407	rBV2	21723	37639	1.50%	0.119%
43	9.514	1407	1415	1420	rVV	355404	547157	21.78%	1.736%
44	9.568	1420	1424	1429	rVB3	45703	75206	2.99%	0.239%
45	9.672	1437	1441	1444	rBV2	17096	27367	1.09%	0.087%
46	9.818	1460	1465	1469	rBV5	20077	33488	1.33%	0.106%
47	9.995	1488	1494	1498	rBV2	24396	38307	1.52%	0.122%
48	10.111	1507	1513	1519	rVV	1396299	1975776	78.65%	6.268%
49	10.178	1522	1524	1532	rVB3	18800	35988	1.43%	0.114%
50	10.635	1592	1599	1602	rBV5	20156	33343	1.33%	0.106%
51	10.910	1639	1644	1648	rBV8	12982	25151	1.00%	0.080%
52	11.062	1664	1669	1675	rBV	45780	71014	2.83%	0.225%
53	11.135	1675	1681	1686	rBV	1136870	1523169	60.64%	4.832%
54	11.629	1758	1762	1765	rBV	37425	52817	2.10%	0.168%
55	11.666	1765	1768	1775	rVB2	21377	29599	1.18%	0.094%
56	11.763	1777	1784	1787	rBV3	25976	41255	1.64%	0.131%
57	11.940	1806	1813	1818	rVB2	22566	38294	1.52%	0.121%
58	12.074	1830	1835	1841	rVB	1477494	1815964	72.29%	5.761%
59	12.202	1846	1856	1857	rBV	20228	32944	1.31%	0.105%
60	12.226	1857	1860	1866	rVV	47602	64950	2.59%	0.206%
61	12.294	1866	1871	1878	rVV	1688233	2079152	82.77%	6.596%
62	12.361	1878	1882	1891	rVB	166621	213314	8.49%	0.677%
63	12.525	1903	1909	1914	rVB	103365	130856	5.21%	0.415%
64	12.659	1924	1931	1933	rBV3	17951	29398	1.17%	0.093%
65	12.696	1933	1937	1942	rVB	109989	136919	5.45%	0.434%
66	12.751	1942	1946	1948	rBV	70235	93911	3.74%	0.298%
67	12.812	1953	1956	1959	rVV	24612	29131	1.16%	0.092%
68	12.891	1961	1969	1975	rBV2	56286	84903	3.38%	0.269%
69	13.080	1995	2000	2009	rVB3	74410	123498	4.92%	0.392%
70	13.165	2009	2014	2015	rBV2	23221	27471	1.09%	0.087%
71	13.184	2015	2017	2020	rVV2	29926	37954	1.51%	0.120%

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Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
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72	13.220	2020	2023	2025	rVV	27921	36986	1.47%	0.117%
73	13.245	2025	2027	2031	rVB	40469	41770	1.66%	0.133%
74	13.342	2039	2043	2048	rBV	213014	267366	10.64%	0.848%
75	13.476	2062	2065	2069	rVB4	21914	28260	1.13%	0.090%
76	13.635	2088	2091	2094	rBV	28684	35741	1.42%	0.113%
77	13.714	2094	2104	2108	rVB2	152127	290562	11.57%	0.922%
78	13.976	2141	2147	2151	rBV	39580	55676	2.22%	0.177%
79	14.263	2188	2194	2197	rBV7	14143	26284	1.05%	0.083%
80	14.427	2216	2221	2226	rBV5	22749	35971	1.43%	0.114%
81	14.537	2234	2239	2242	rBV6	20021	29843	1.19%	0.095%
82	14.653	2253	2258	2262	rBV	19221	32458	1.29%	0.103%

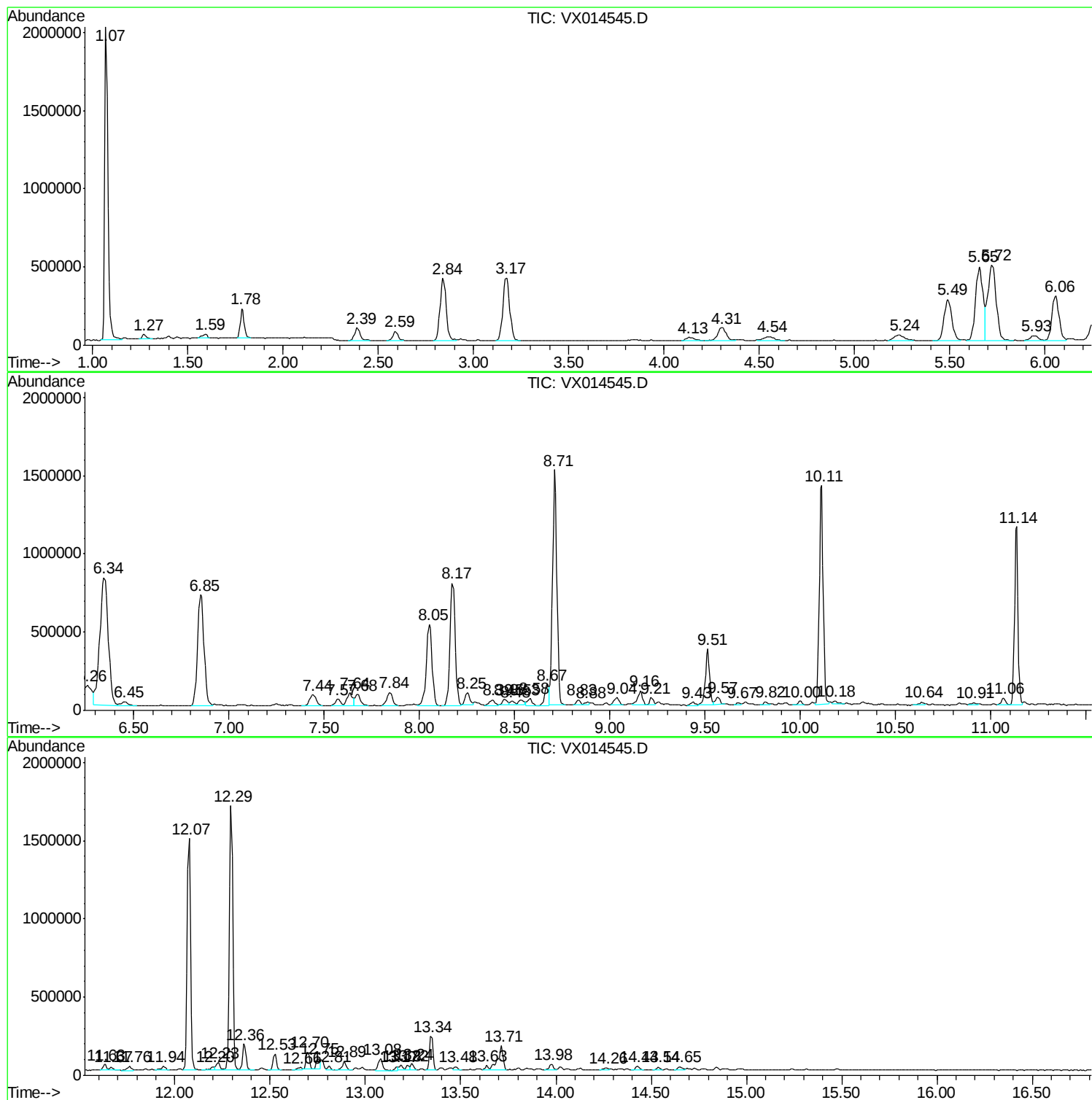
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Instrument :
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ClientSampleId :
MW-1R

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
Quant Title : SW846 8260

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



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Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

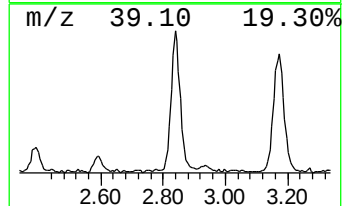
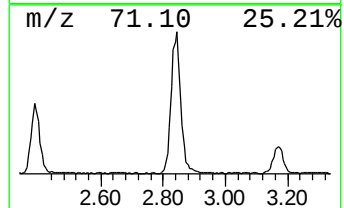
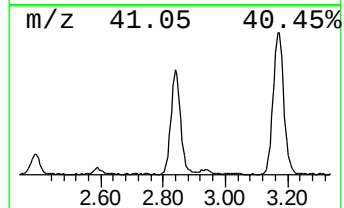
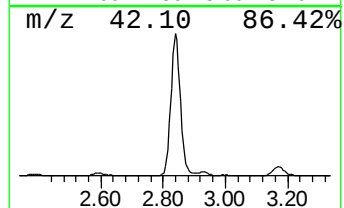
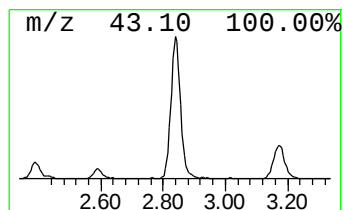
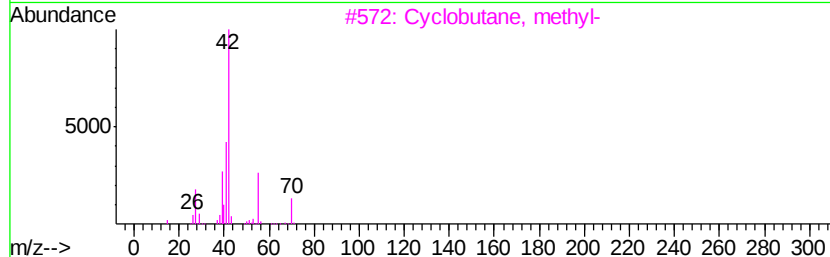
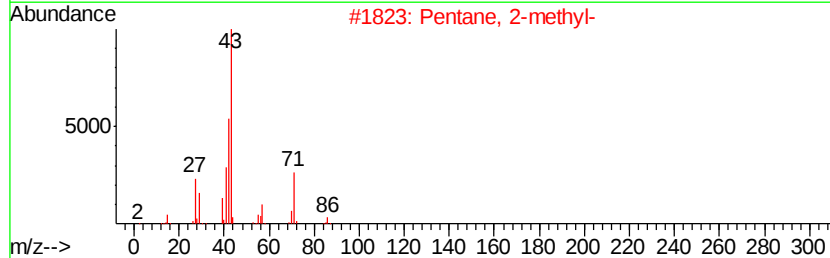
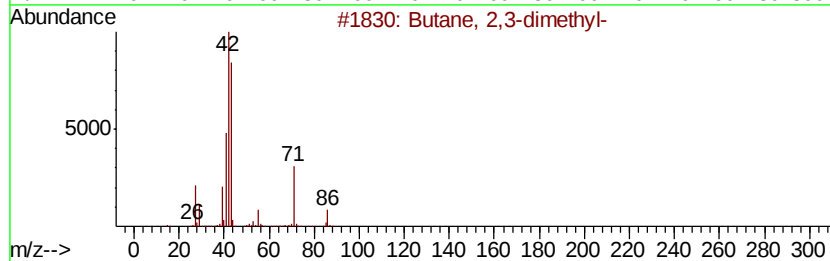
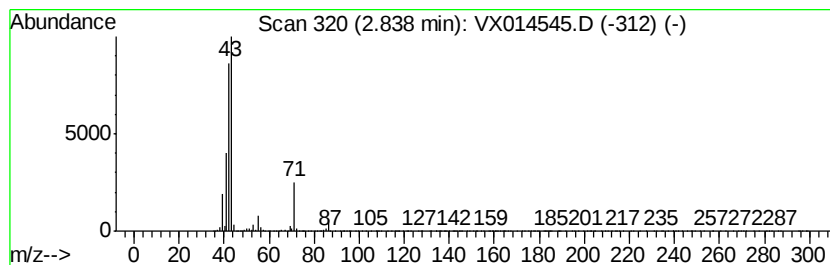
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	34.37 ug/l	899572	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Cyclobutane, methyl-	70	C5H10	000598-61-8	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	38
5		Tetrahydrofuran	72	C4H8O	000109-99-9	36



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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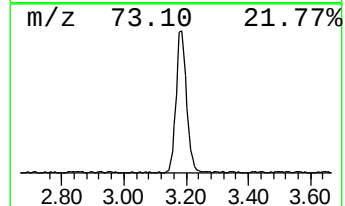
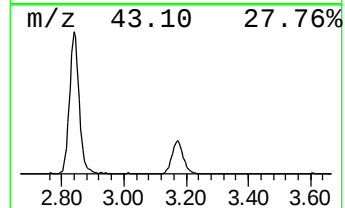
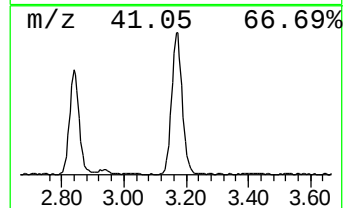
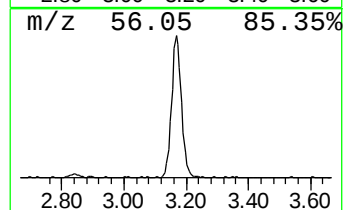
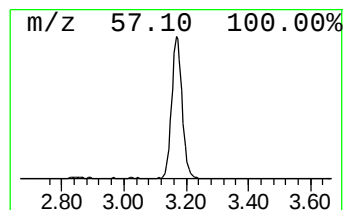
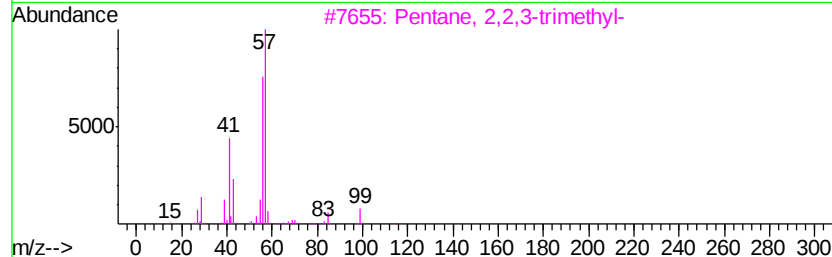
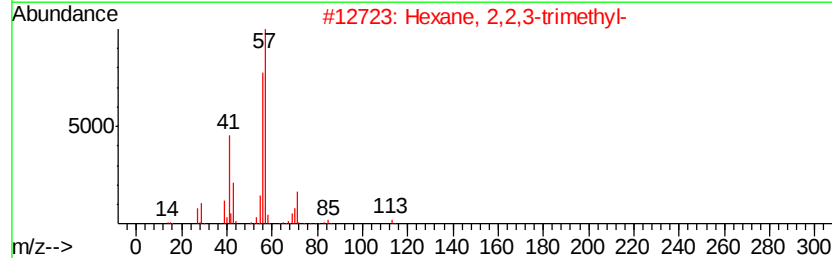
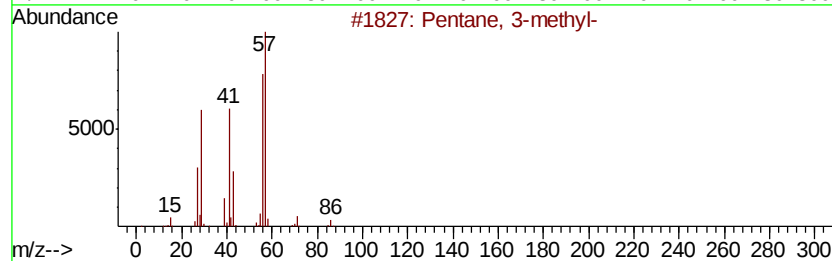
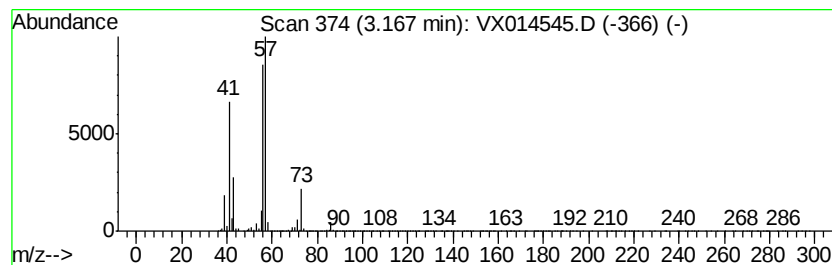
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	38.03 ug/l	995448	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	74
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	45
5		Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	45



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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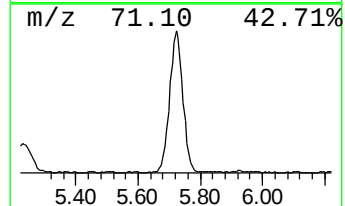
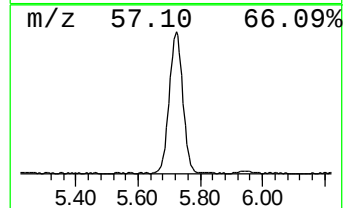
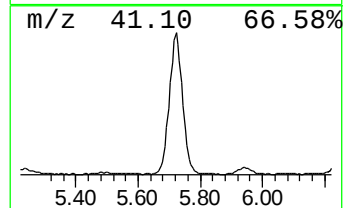
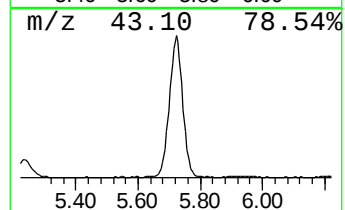
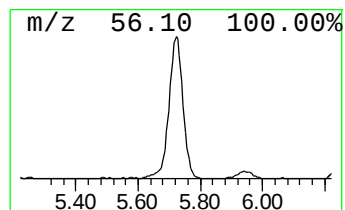
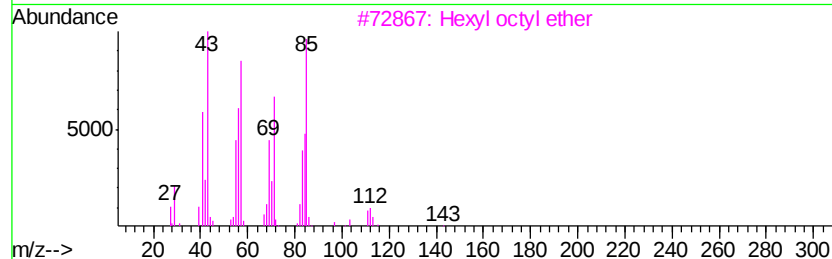
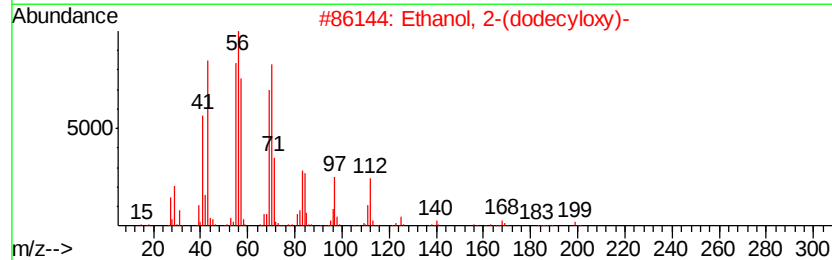
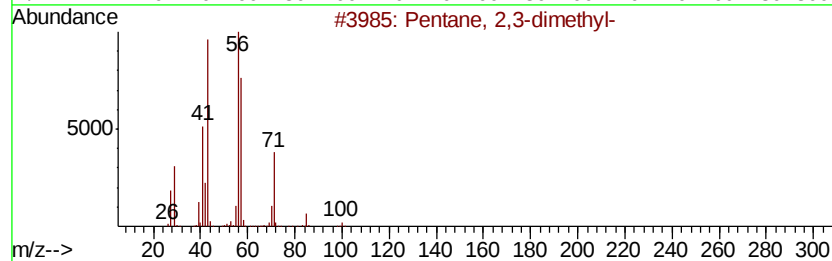
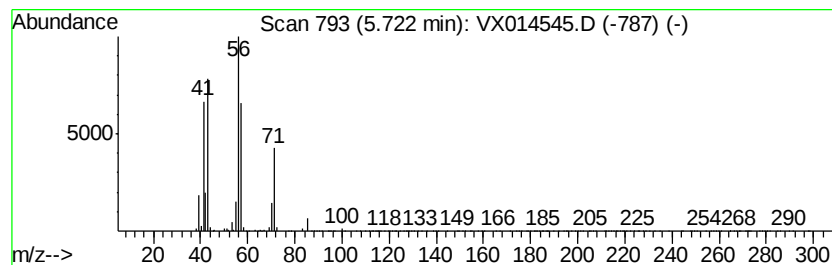
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	55.86 ug/l	1462090	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	78
3		Hexyl octyl ether	214	C14H30O	017071-54-4	59
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5		Heptane	100	C7H16	000142-82-5	38



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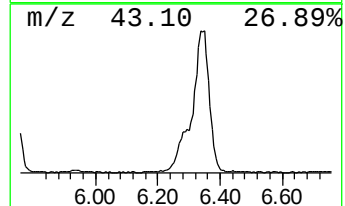
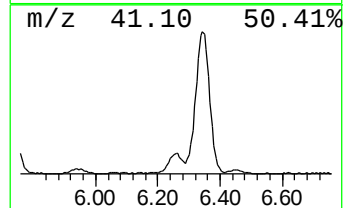
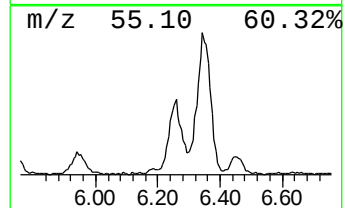
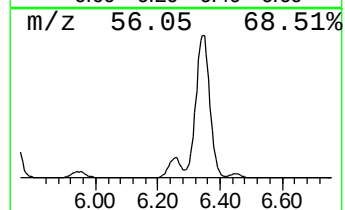
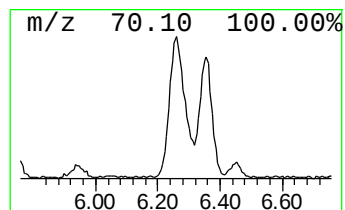
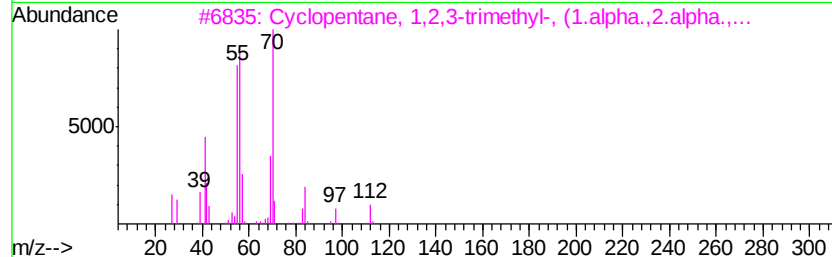
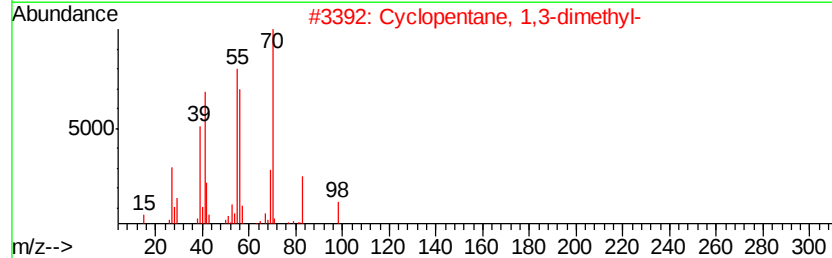
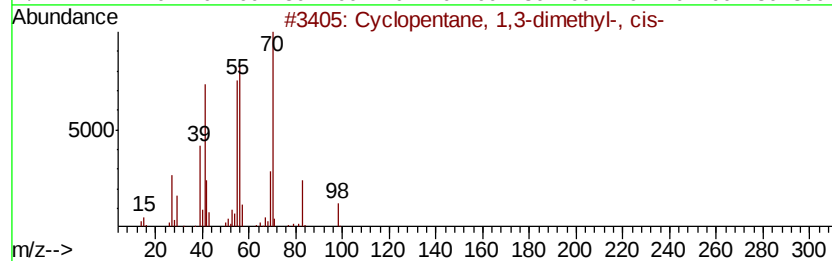
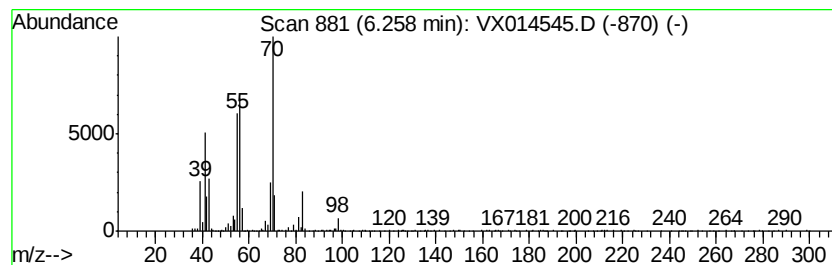
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	11.64 ug/l	389047	1,4-Difluorobenzene	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	91
2		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	90
3		Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	64
4		Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	59
5		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

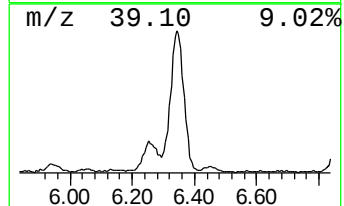
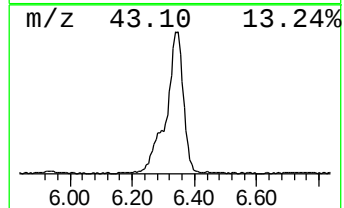
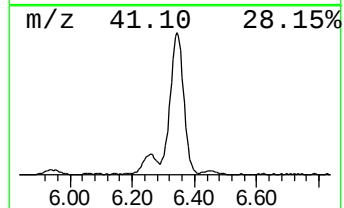
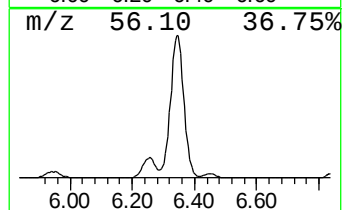
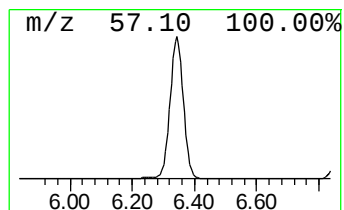
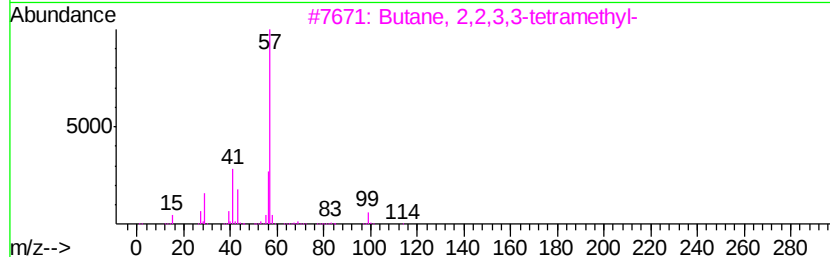
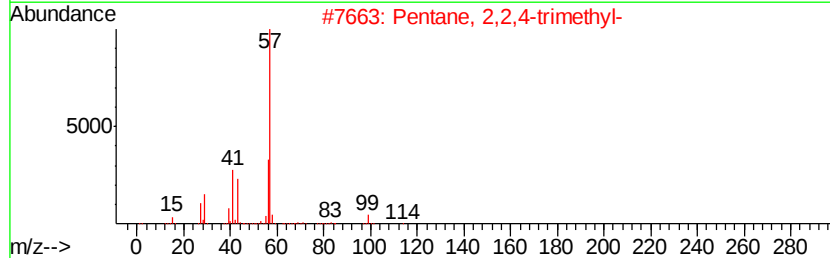
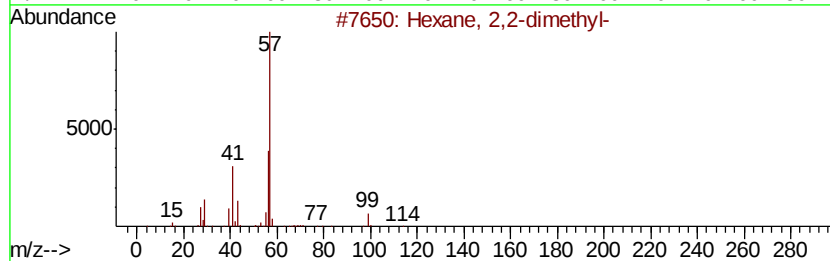
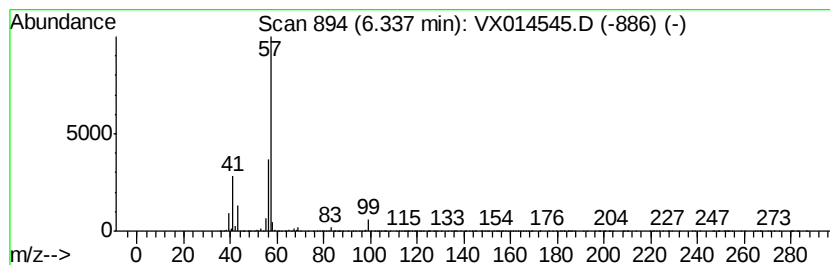
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	75.16 ug/l	2511960	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

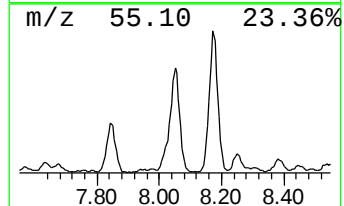
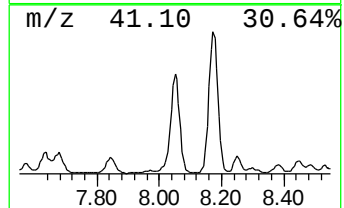
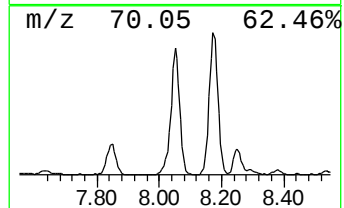
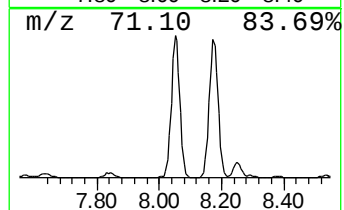
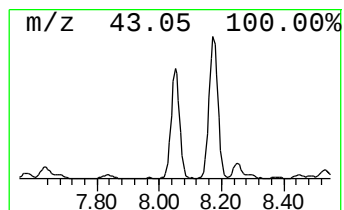
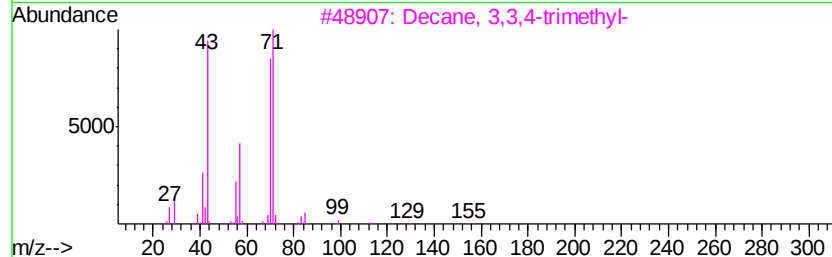
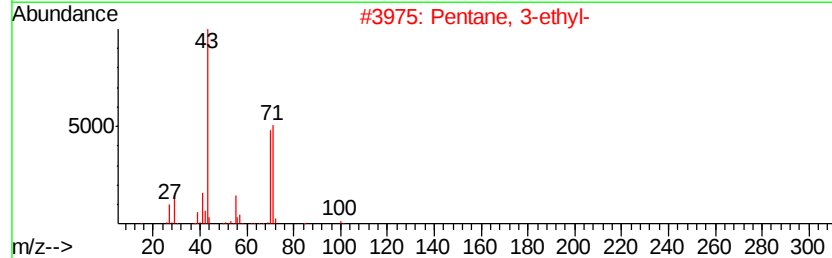
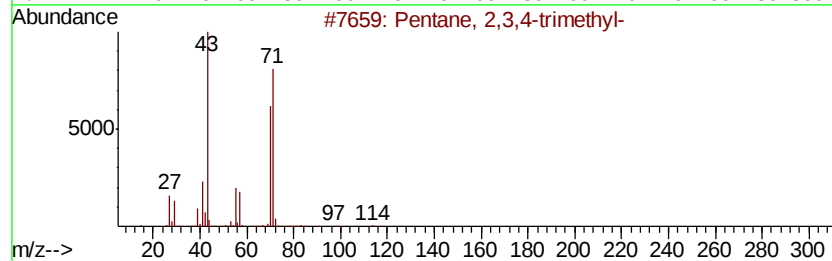
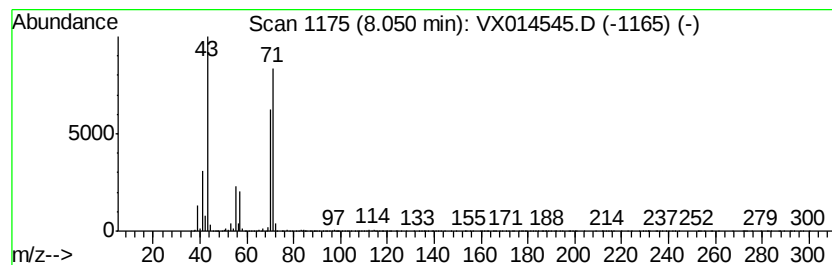
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	32.38 ug/l	1082050	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
4		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

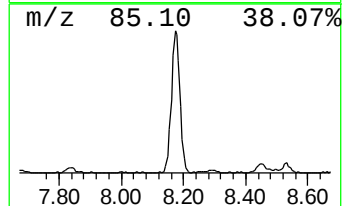
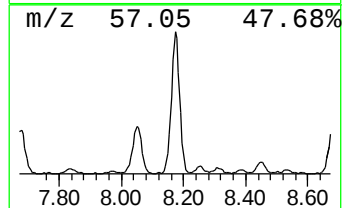
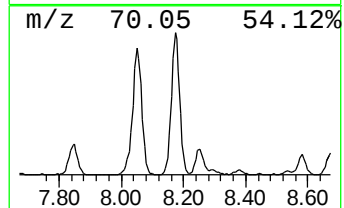
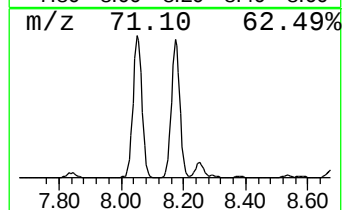
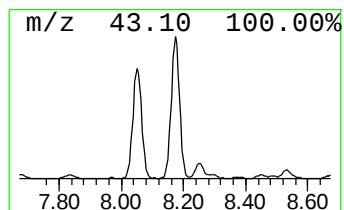
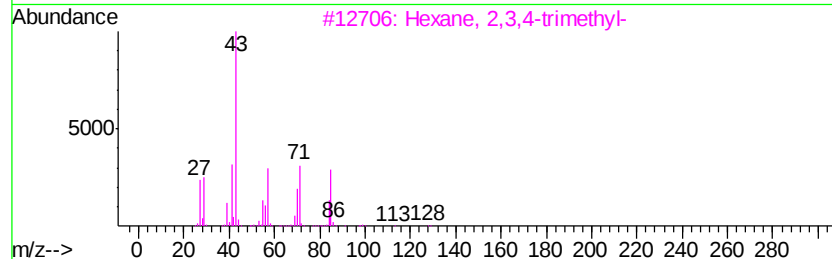
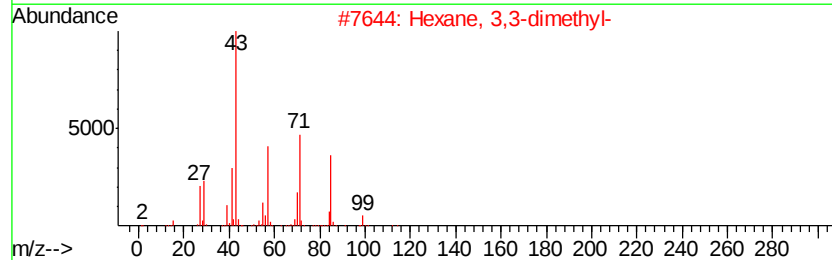
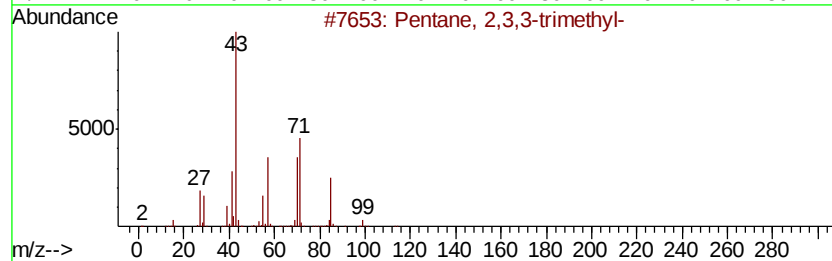
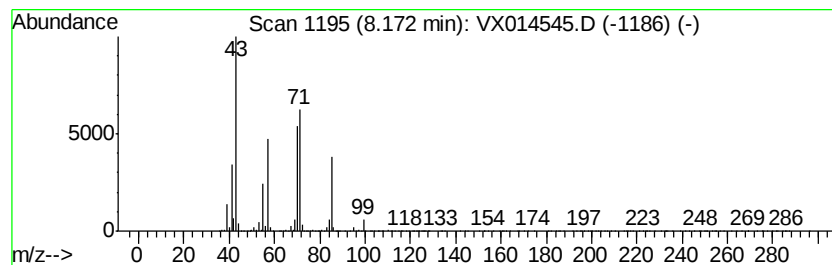
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	45.90 ug/l	1534090	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

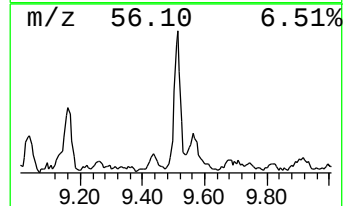
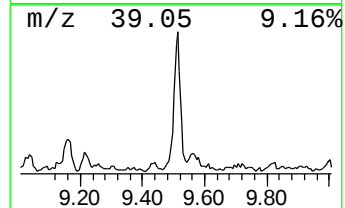
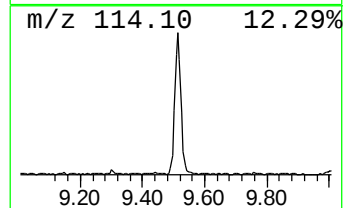
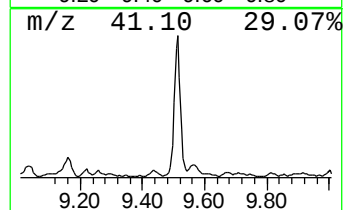
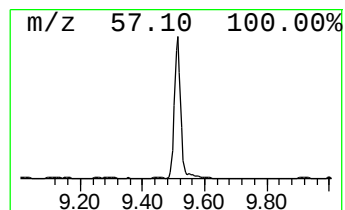
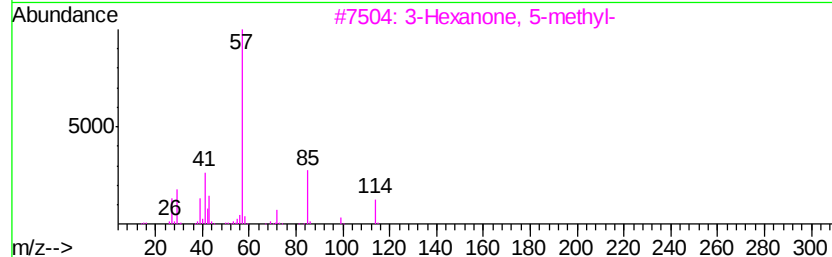
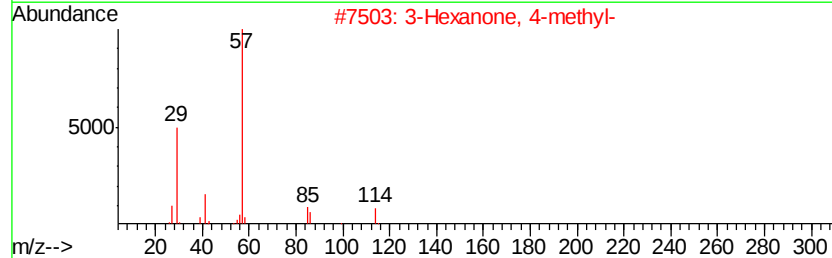
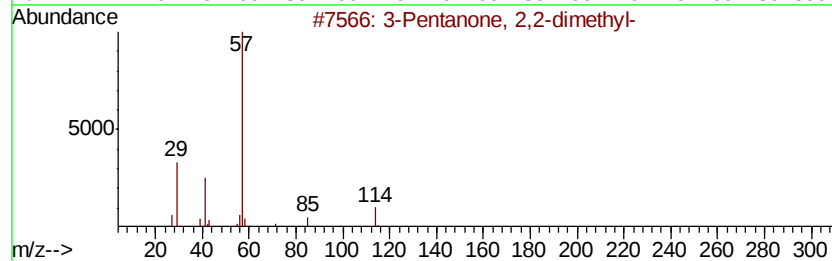
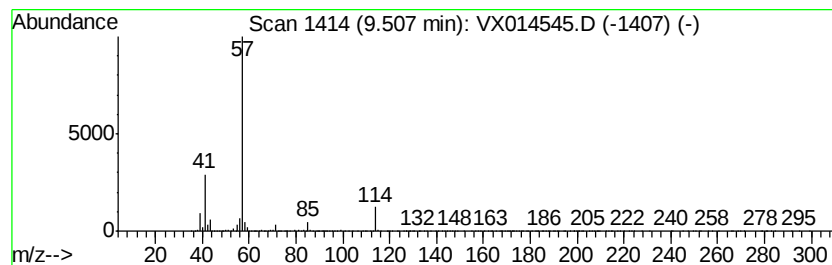
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Quant Title : SW846 8260

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

Peak Number 9 3-Pentanone, 2,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	13.85 ug/l	547157	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	83
2		3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	53
3		3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
4		3,4-Hexanedione	114	C6H10O2	004437-51-8	52
5		3-Heptanone	114	C7H14O	000106-35-4	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

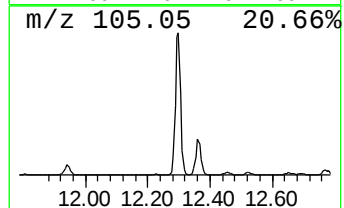
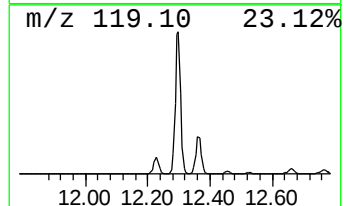
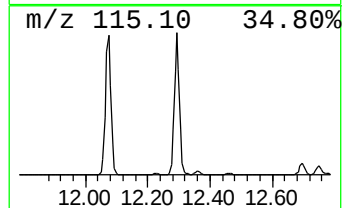
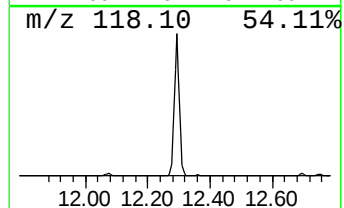
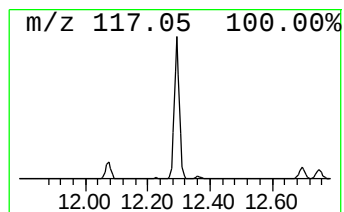
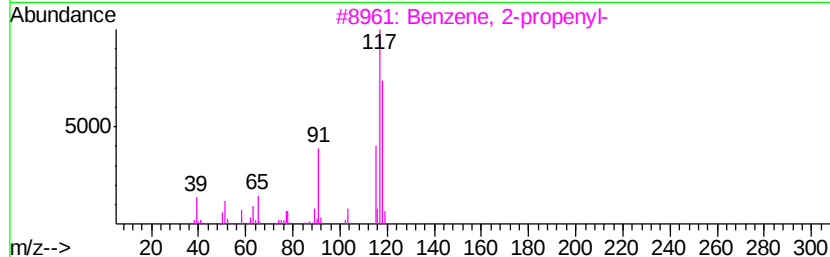
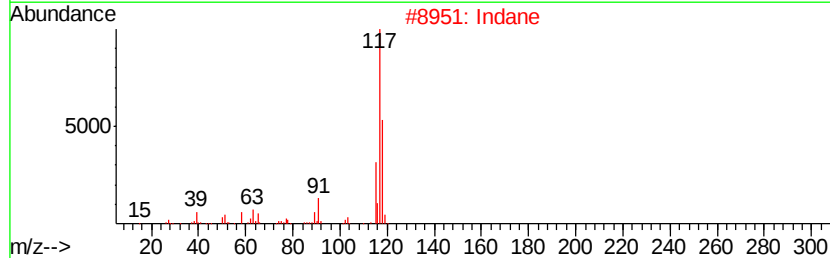
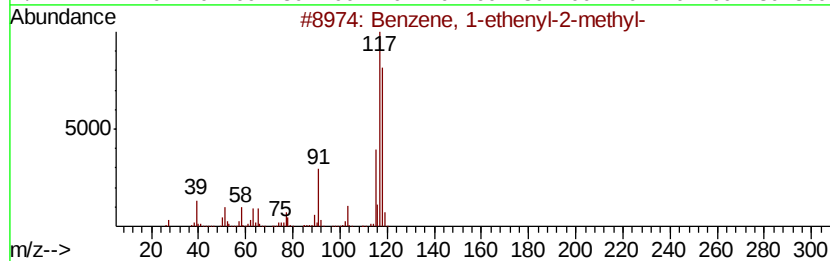
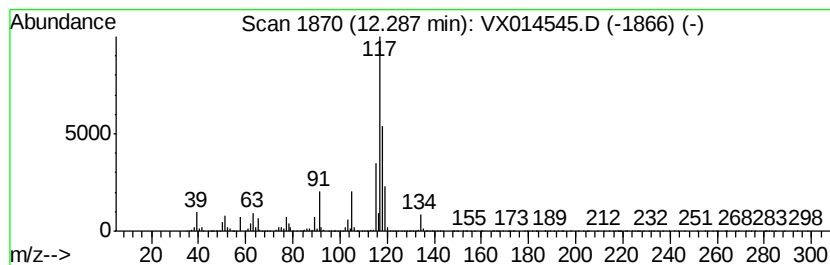
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	57.25 ug/l	2079150	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
2		Indane	118	C9H10	000496-11-7	64
3		Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4		Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5		Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	52



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX011020\
Data File : VX014545.D
Acq On : 10 Jan 2020 18:18
Operator : JC/SP
Sample : L1080-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X010720W.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
Butane, 2,3-dimet...	2.84	34.4	ug/l	899572	1	5.65	1308660	50.0
Pentane, 3-methyl-	3.17	38.0	ug/l	995448	1	5.65	1308660	50.0
Pentane, 2,3-dime...	5.72	55.9	ug/l	1462090	1	5.65	1308660	50.0
Cyclopentane, 1,3...	6.26	11.6	ug/l	389047	2	6.86	1671070	50.0
Hexane, 2,2-dimet...	6.34	75.2	ug/l	2511960	2	6.86	1671070	50.0
Pentane, 2,3,4-tr...	8.05	32.4	ug/l	1082050	2	6.86	1671070	50.0
Pentane, 2,3,3-tr...	8.17	45.9	ug/l	1534090	2	6.86	1671070	50.0
3-Pentanone, 2,2-...	9.51	13.9	ug/l	547157	3	10.11	1975780	50.0
Benzene, 1-etheny...	12.29	57.3	ug/l	2079150	4	12.07	1815960	50.0