

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
 Data File : VU045022.D
 Acq On : 30 Sep 2021 03:27
 Operator : SY/MD
 Sample : M3952-05DL 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 MW-3DL

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
 Title : SW846 8260

Signal : TIC: VU045022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	34	42	53	rVB	104317	110732	2.70%	0.613%
2	1.973	187	197	211	rVB	108066	155742	3.79%	0.863%
3	2.192	255	265	288	rVB	139069	207313	5.05%	1.149%
4	3.083	532	542	551	rVV	66745	121026	2.95%	0.671%
5	3.134	551	558	574	rVB2	34444	69138	1.68%	0.383%
6	3.359	613	628	647	rVB	55802	126228	3.07%	0.699%
7	3.700	718	734	752	rVB	84653	187829	4.58%	1.041%
8	4.533	975	993	1014	rVB	142895	348216	8.48%	1.929%
9	5.292	1212	1229	1242	rBV	179678	382323	9.31%	2.118%
10	5.378	1242	1256	1273	rVV2	437690	1012052	24.65%	5.607%
11	5.594	1308	1323	1331	rBV2	42287	91061	2.22%	0.505%
12	5.706	1345	1358	1367	rBV	212290	413407	10.07%	2.290%
13	5.777	1367	1380	1395	rVV	2039826	4105273	100.00%	22.744%
14	5.851	1395	1403	1413	rVV3	57641	121272	2.95%	0.672%
15	5.922	1415	1425	1435	rVV4	45176	102155	2.49%	0.566%
16	5.993	1435	1447	1459	rVB3	76109	152559	3.72%	0.845%
17	6.134	1480	1491	1503	rBV2	53963	106060	2.58%	0.588%
18	6.253	1514	1528	1552	rVB	473453	914547	22.28%	5.067%
19	6.764	1664	1687	1709	rBV	344299	751079	18.30%	4.161%
20	6.983	1741	1755	1767	rBV	41929	77601	1.89%	0.430%
21	7.076	1767	1784	1796	rVB4	19129	46958	1.14%	0.260%
22	7.237	1825	1834	1852	rVB3	25166	52506	1.28%	0.291%
23	7.857	2015	2027	2030	rBV2	62002	92529	2.25%	0.513%
24	7.899	2030	2040	2053	rVV	750762	1305874	31.81%	7.235%
25	7.973	2053	2063	2073	rVB	103062	169157	4.12%	0.937%
26	8.037	2073	2083	2096	rBV3	16706	42521	1.04%	0.236%
27	8.246	2134	2148	2166	rVB2	46947	92881	2.26%	0.515%
28	8.372	2171	2187	2197	rBV	25231	50974	1.24%	0.282%
29	8.867	2332	2341	2351	rVV	51006	82074	2.00%	0.455%
30	8.928	2351	2360	2371	rVV	29187	47523	1.16%	0.263%
31	9.420	2500	2513	2527	rBV	685540	1117500	27.22%	6.191%
32	9.574	2550	2561	2575	rBV	136677	218383	5.32%	1.210%
33	9.697	2581	2599	2613	rBV	591602	1007788	24.55%	5.583%
34	10.275	2755	2779	2790	rBV6	22176	49554	1.21%	0.275%
35	10.488	2835	2845	2854	rBV2	36770	54645	1.33%	0.303%
36	10.635	2875	2891	2905	rBV	552999	866421	21.11%	4.800%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	10.909	2964	2976	2985	rBV	43731	65691	1.60%	0.364%
38	11.002	2994	3005	3011	rBV	134342	236024	5.75%	1.308%
39	11.092	3022	3033	3054	rVB	102041	170183	4.15%	0.943%
40	11.295	3086	3096	3117	rVB	51822	90200	2.20%	0.500%
41	11.471	3140	3151	3164	rVB	292866	448631	10.93%	2.486%
42	11.745	3219	3236	3245	rBV	31740	52826	1.29%	0.293%
43	11.815	3245	3258	3272	rVV	709147	1126243	27.43%	6.240%
44	11.896	3272	3283	3303	rVB	145135	232149	5.65%	1.286%
45	12.098	3334	3346	3351	rBV2	53314	84518	2.06%	0.468%
46	12.127	3352	3355	3364	rVV	43438	56843	1.38%	0.315%
47	12.192	3364	3375	3395	rVB5	55919	113543	2.77%	0.629%
48	12.468	3451	3461	3465	rBV	29257	42708	1.04%	0.237%
49	12.500	3466	3471	3481	rVV	37178	52915	1.29%	0.293%
50	12.574	3482	3494	3502	rVV	38189	60986	1.49%	0.338%
51	12.684	3517	3528	3550	rVB3	51285	110459	2.69%	0.612%
52	13.031	3626	3636	3650	rVB	32459	50154	1.22%	0.278%
53	13.455	3758	3768	3781	rVB3	68404	120193	2.93%	0.666%
54	14.089	3950	3965	3988	rVB	47298	82573	2.01%	0.457%

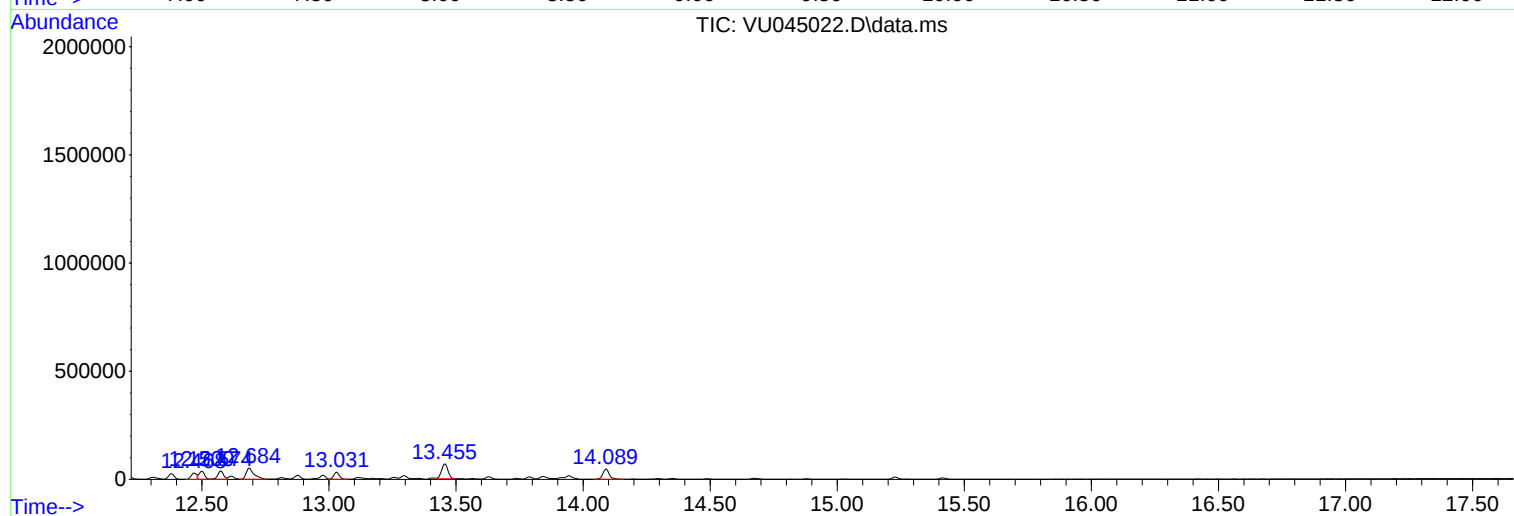
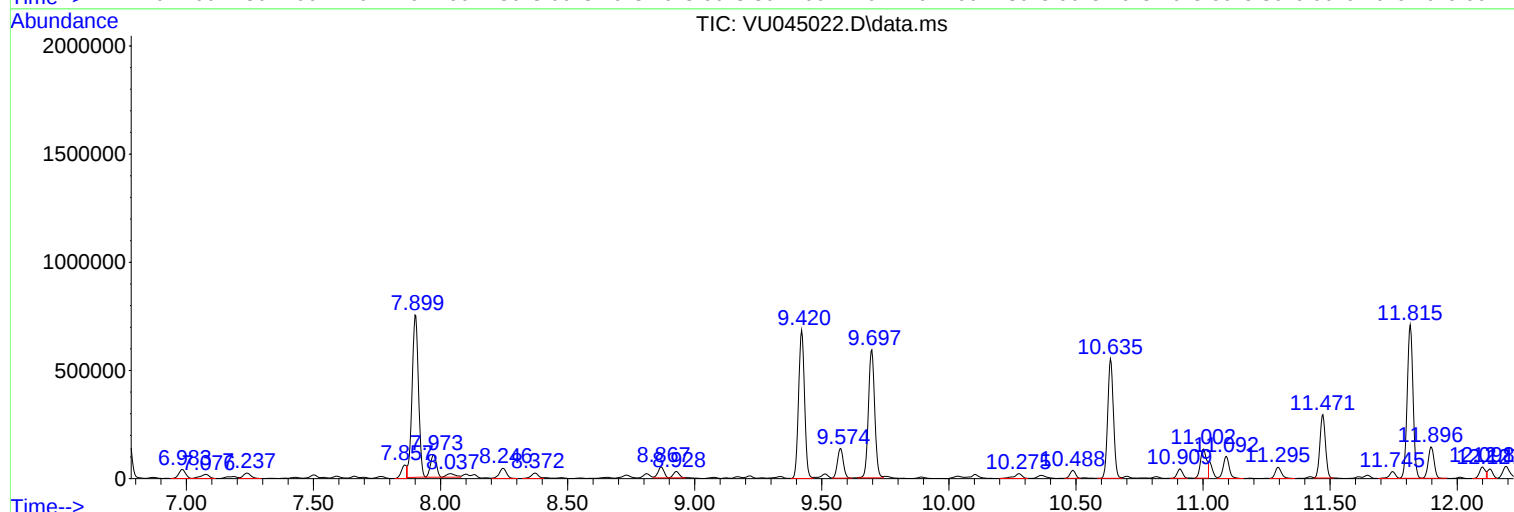
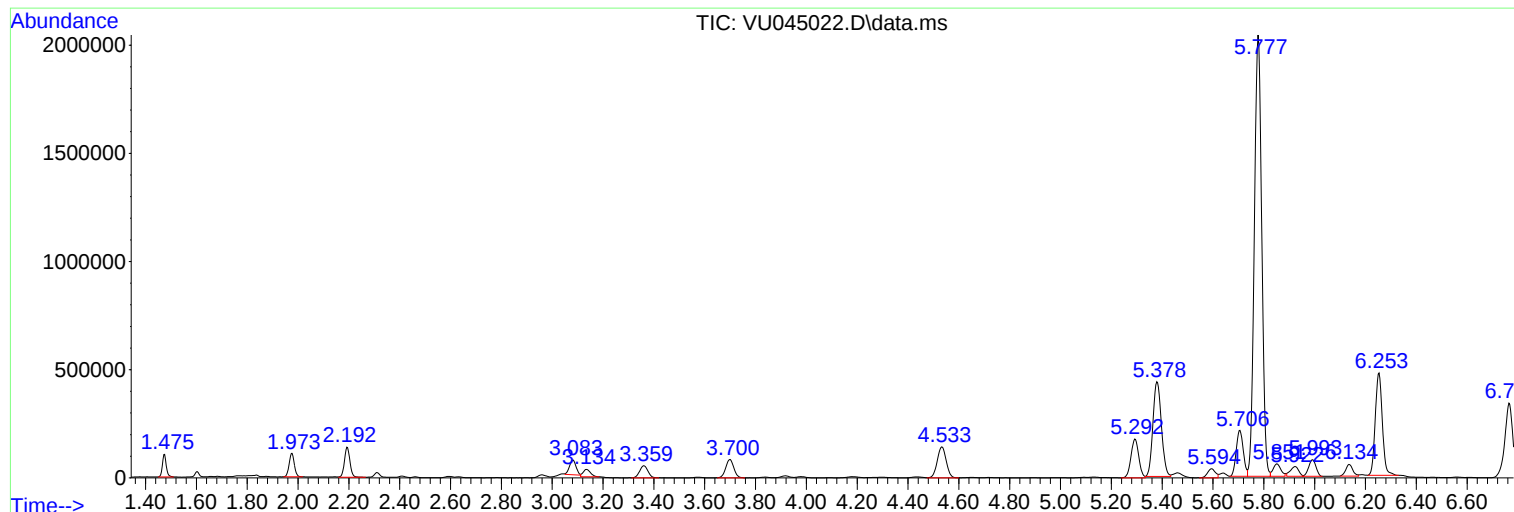
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

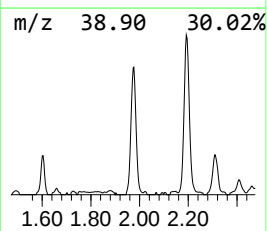
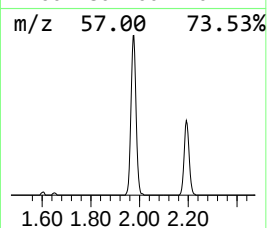
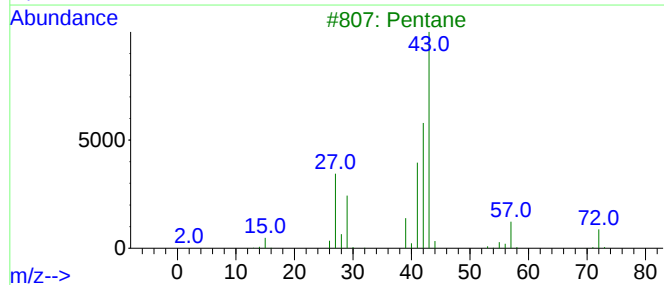
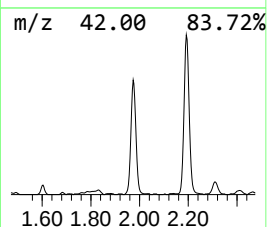
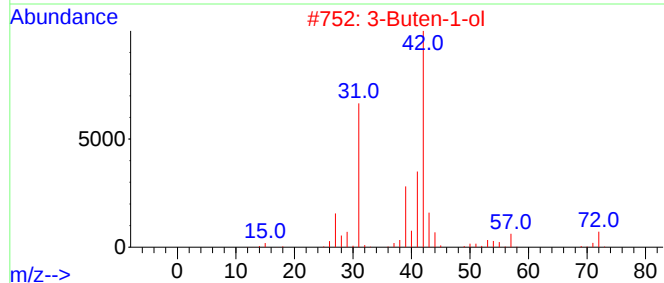
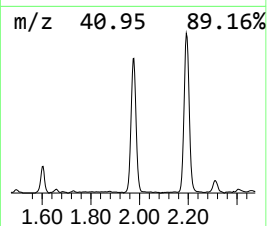
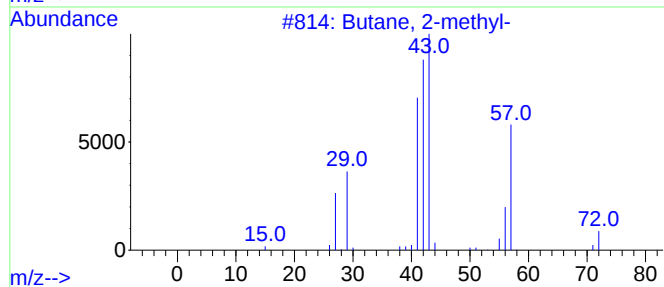
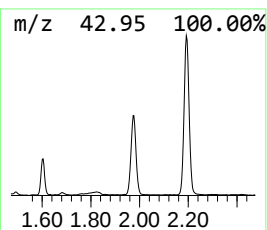
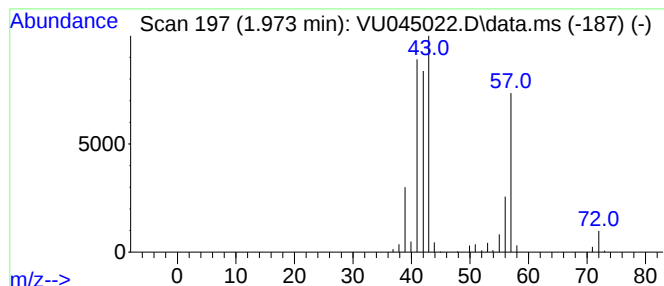
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.973	7.69 ug/l	155742	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-		72	C5H12	000078-78-4	87	
2	3-Buten-1-ol		72	C4H8O	000627-27-0	43	
3	Pentane		72	C5H12	000109-66-0	42	
4	2,5-Furandione, dihydro-3-methyl-		114	C5H6O3	004100-80-5	17	
5	Butane, 1-chloro-2-methyl-		106	C5H11Cl	000616-13-7	12	



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-3DL

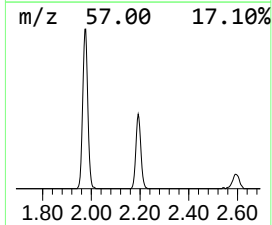
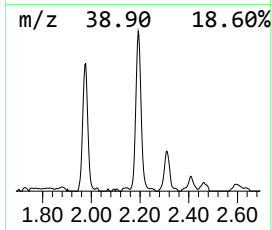
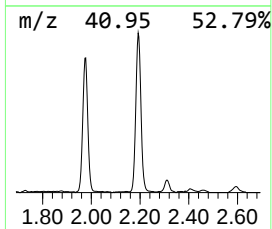
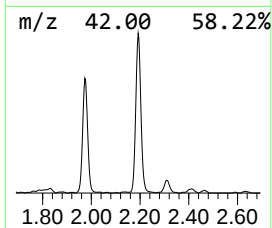
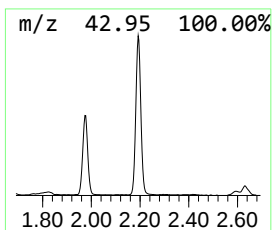
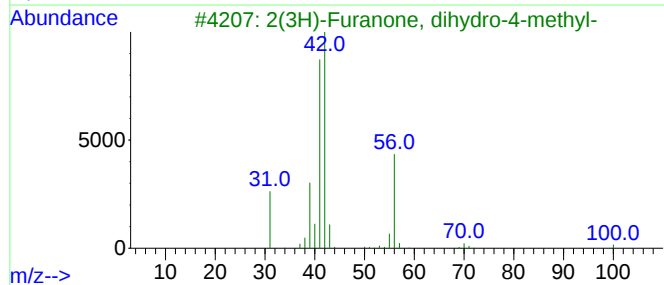
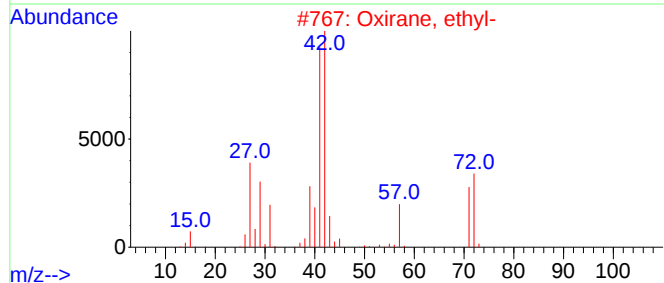
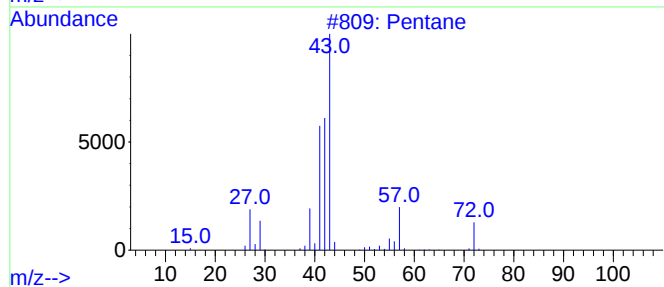
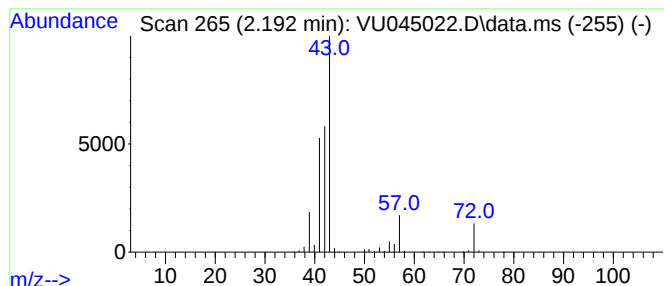
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.192	10.24 ug/l	207313	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	17
5			1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

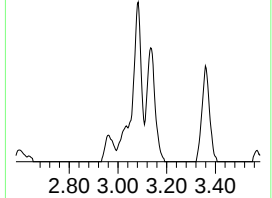
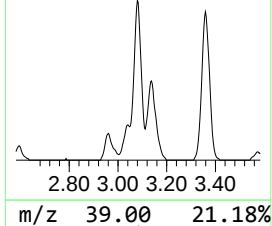
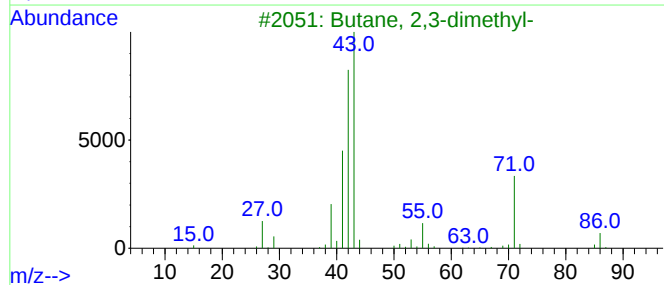
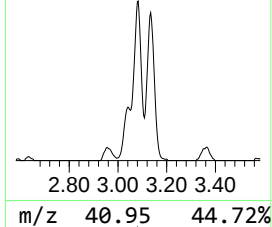
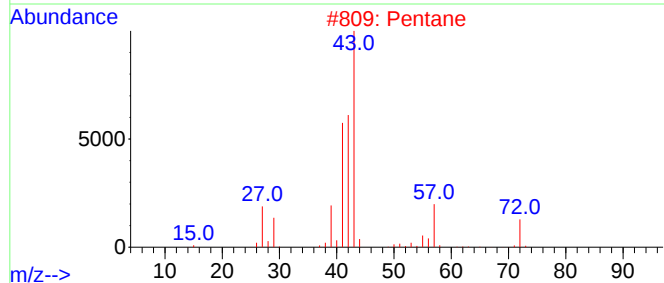
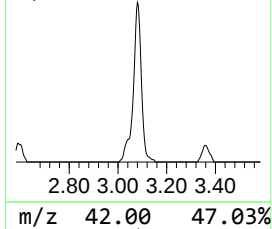
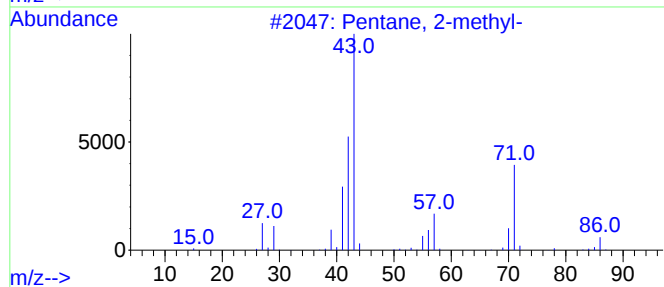
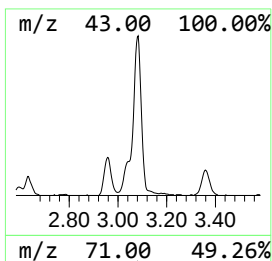
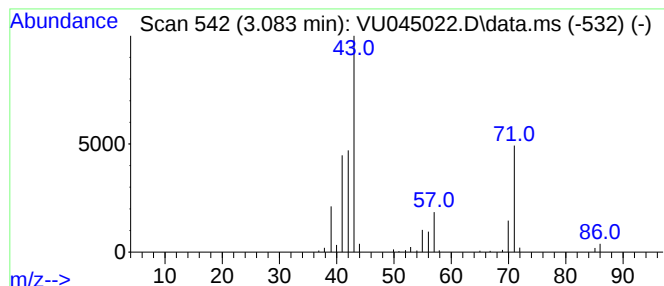
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.083	5.98 ug/l	121026	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane	72	C5H12	000109-66-0	43
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38
4			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	28



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ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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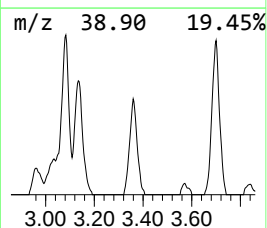
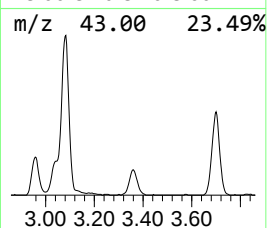
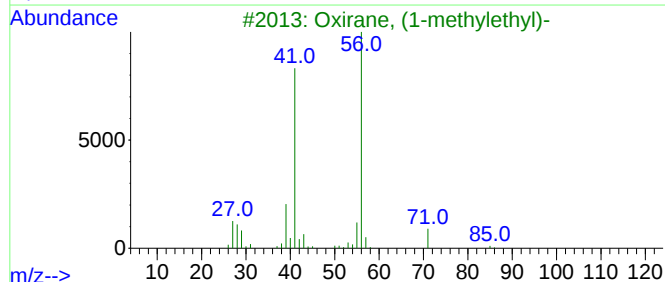
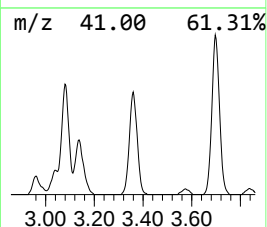
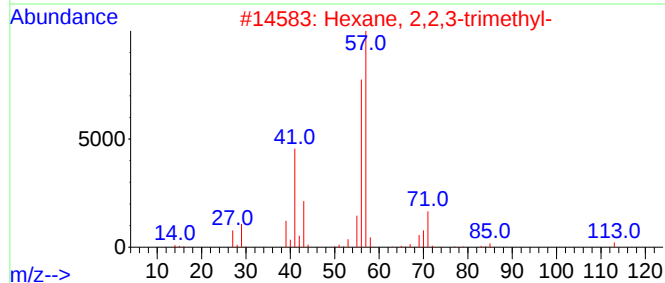
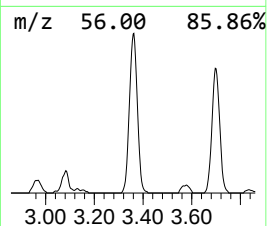
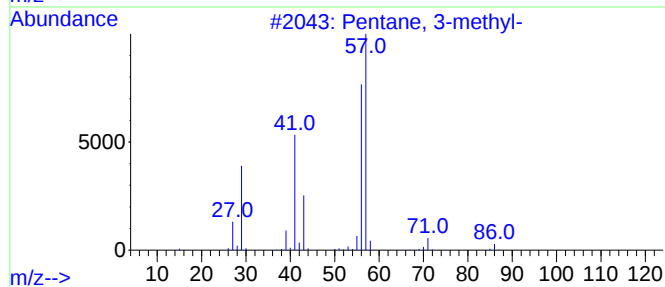
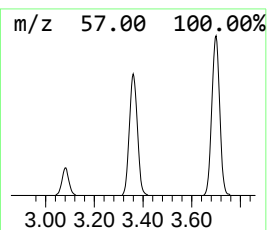
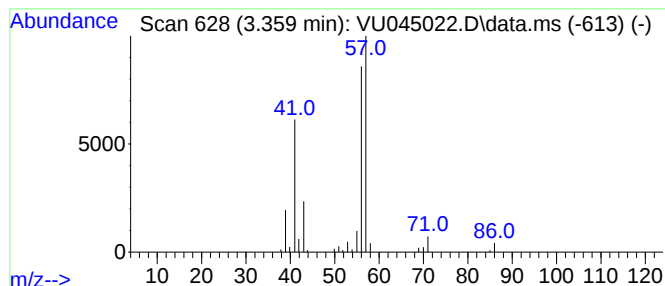
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.359	6.24 ug/l	126228	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



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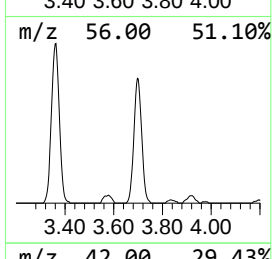
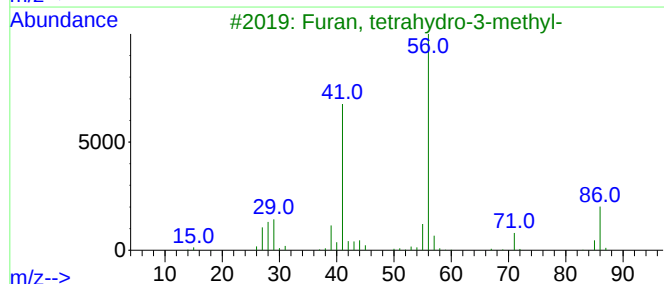
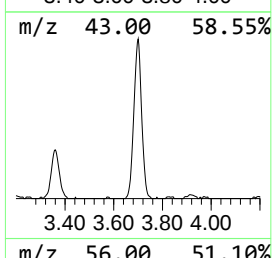
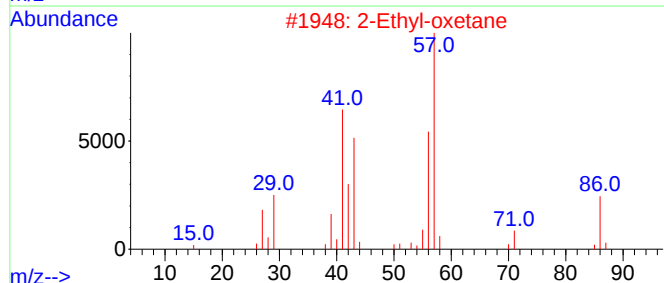
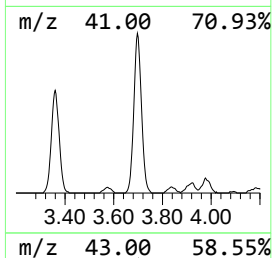
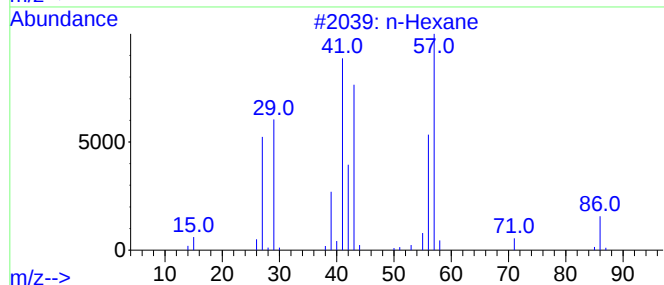
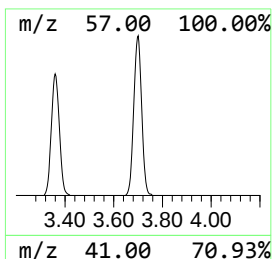
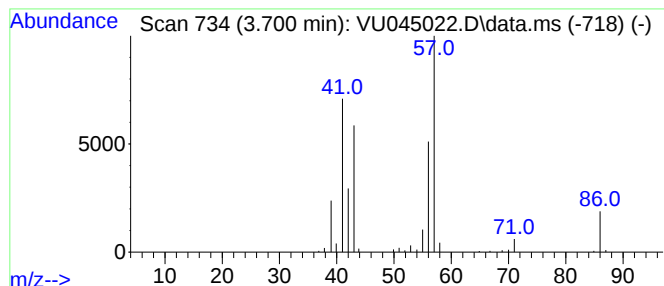
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.700	9.28 ug/l	187829	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	83
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	80
3			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	47
4			Pentane, 3-methyl-	86	C6H14	000096-14-0	42
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

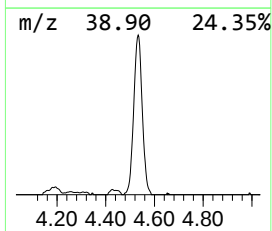
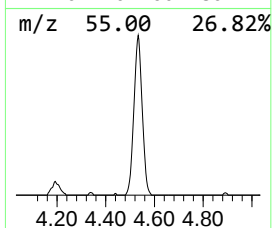
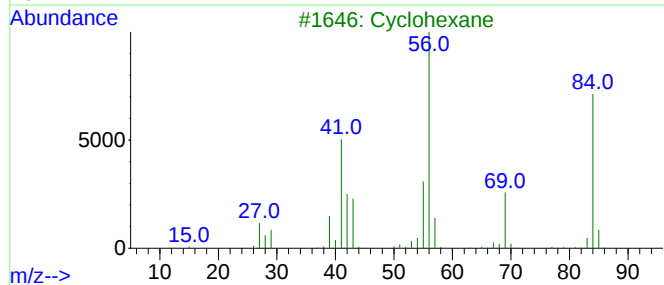
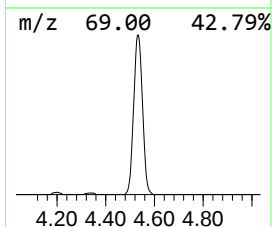
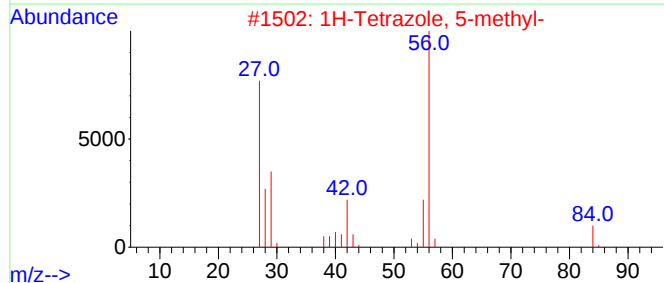
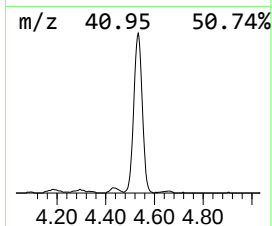
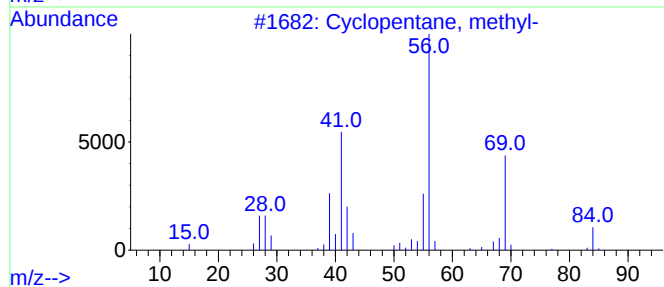
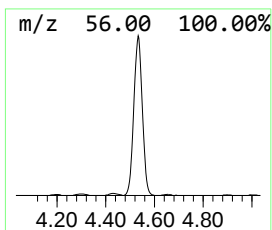
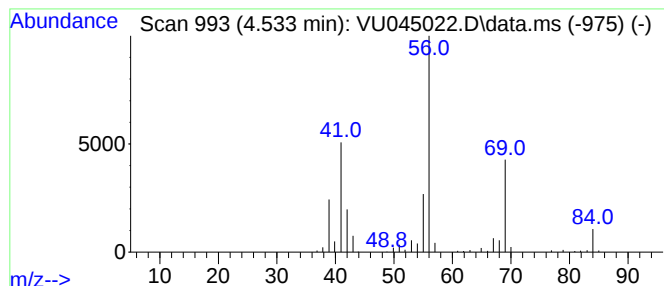
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.533	17.20 ug/l	348216	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			Cyclohexane	84	C6H12	000110-82-7	64
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Cyclobutane	56	C4H8	000287-23-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

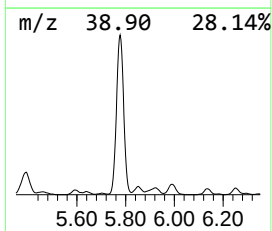
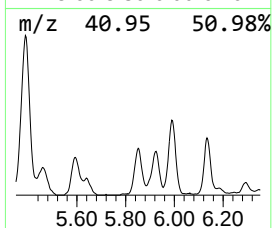
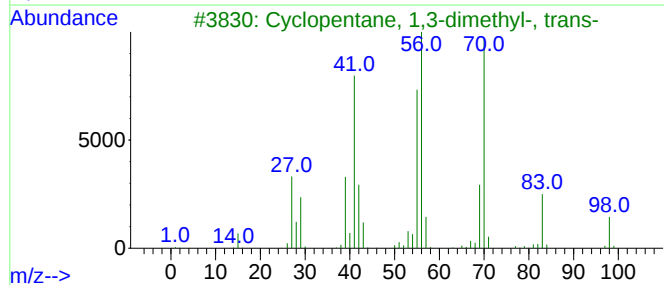
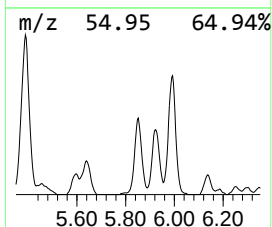
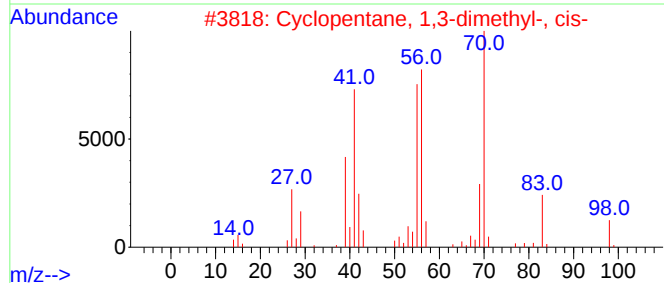
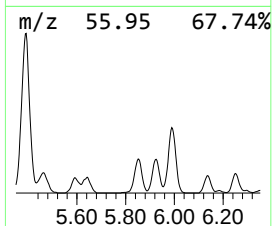
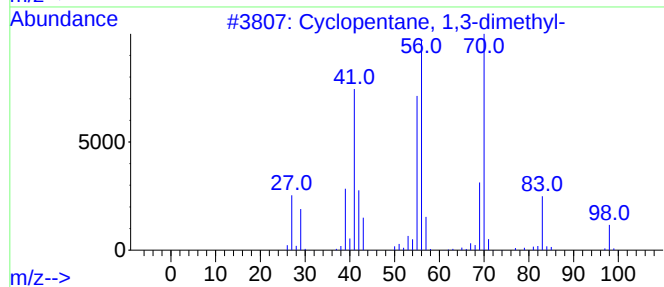
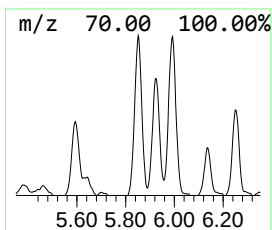
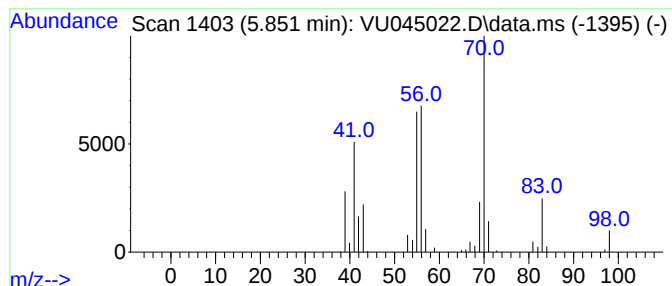
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentane, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	6.63 ug/l	121272	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	91
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	90
3			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	90
4			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	64
5			1-Heptene, 3-methyl-	112	C8H16	004810-09-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

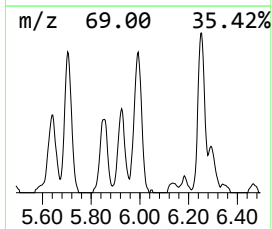
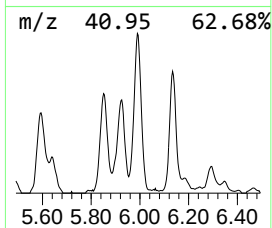
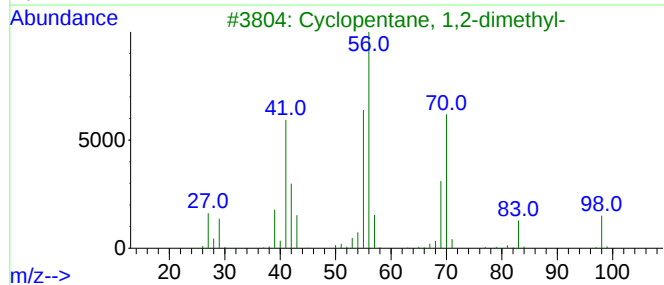
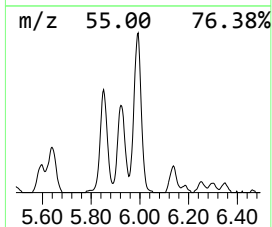
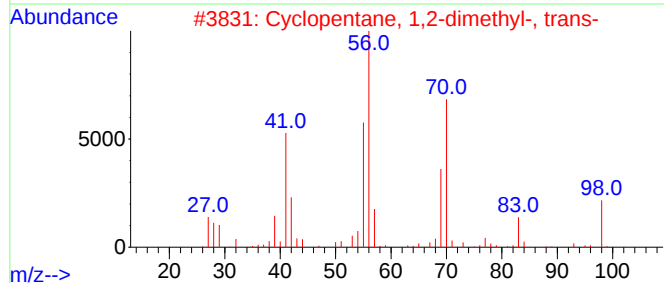
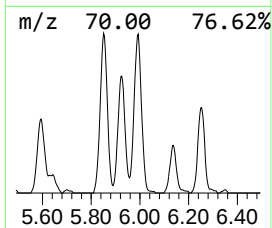
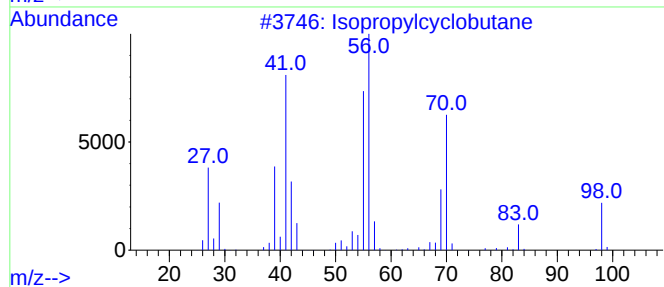
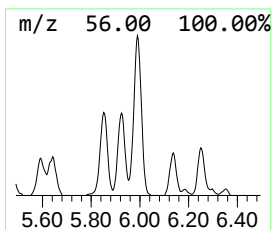
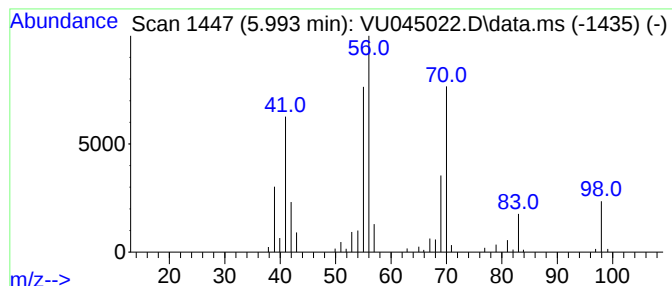
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Isopropylcyclobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.993	8.34 ug/l	152559	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropylcyclobutane	98	C7H14	000872-56-0	94
2			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
3			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87
4			Cycloheptane	98	C7H14	000291-64-5	83
5			1-Heptene	98	C7H14	000592-76-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

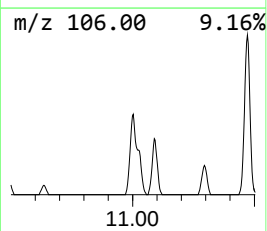
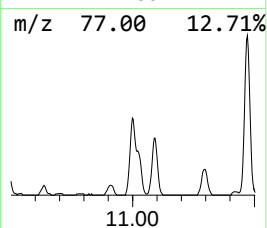
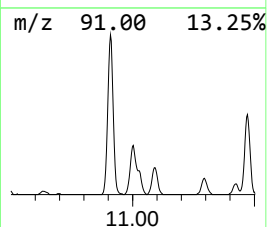
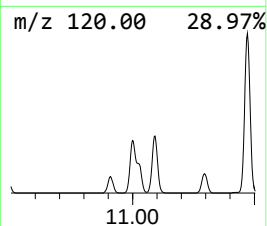
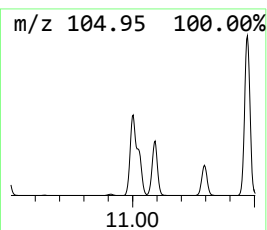
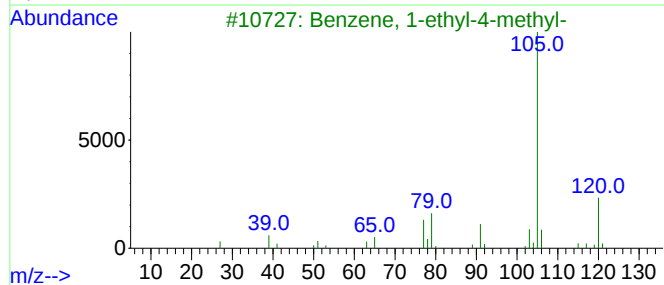
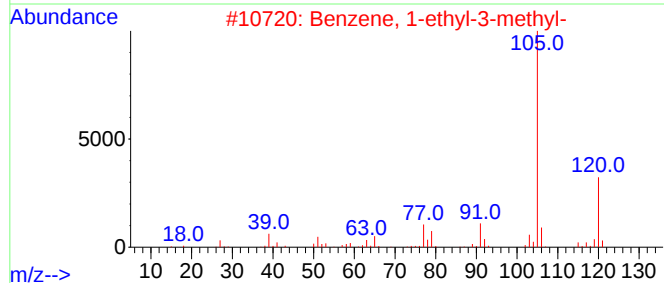
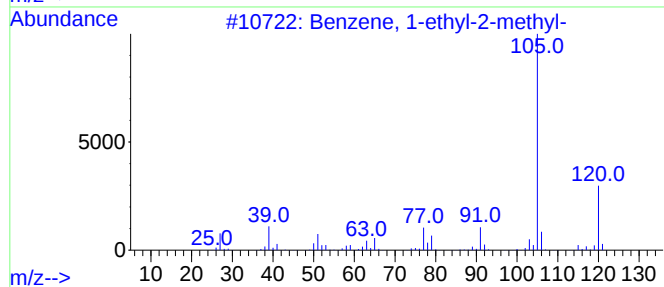
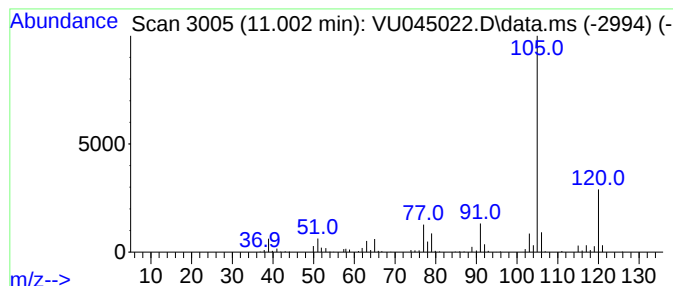
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.002	10.48 ug/l	236024	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

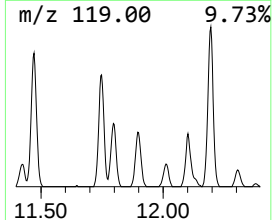
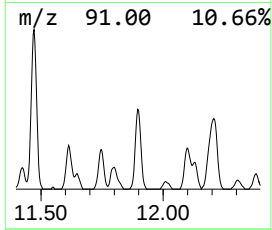
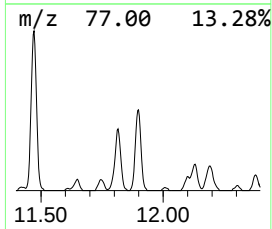
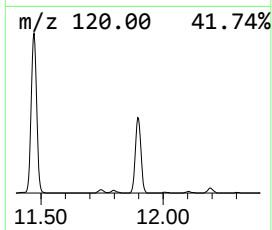
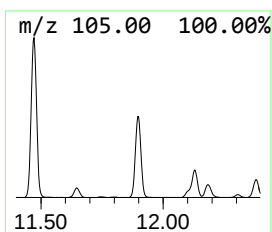
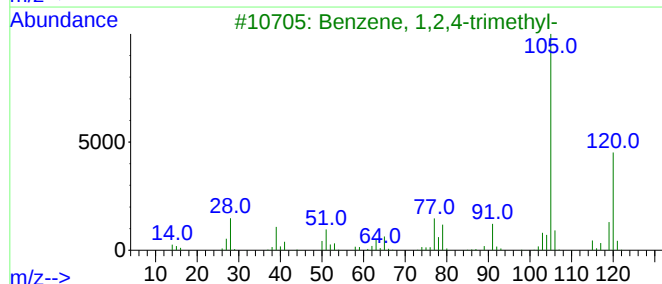
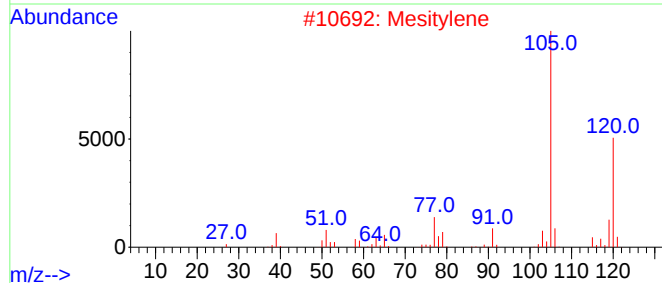
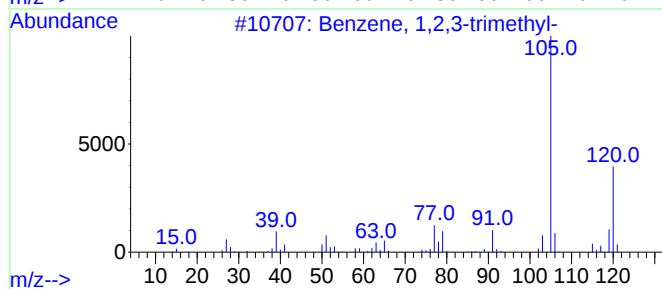
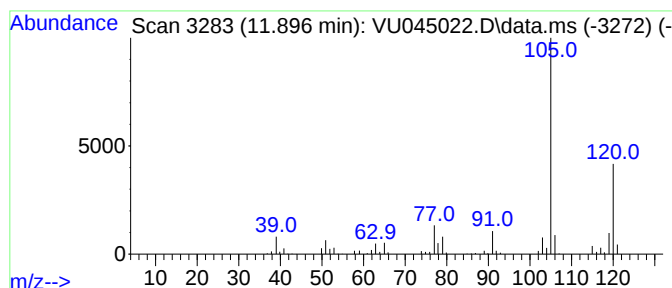
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	10.31 ug/l	232149	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045022.D
Acq On : 30 Sep 2021 03:27
Operator : SY/MD
Sample : M3952-05DL 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-3DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane	2.192	10.2	ug/l	207313	1	5.375	1012050	50.0
Pentane, 2-methyl-	3.083	6.0	ug/l	121026	1	5.375	1012050	50.0
Pentane, 3-methyl-	3.359	6.2	ug/l	126228	1	5.375	1012050	50.0
n-Hexane	3.700	9.3	ug/l	187829	1	5.375	1012050	50.0
Cyclopentane, m...	4.533	17.2	ug/l	348216	1	5.375	1012050	50.0
Cyclopentane, 1...	5.851	6.6	ug/l	121272	2	6.253	914547	50.0
Isopropylcyclob...	5.993	8.3	ug/l	152559	2	6.253	914547	50.0
Benzene, 1-ethy...	11.002	10.5	ug/l	236024	4	11.816	1126240	50.0
Benzene, 1,2,3-...	11.896	10.3	ug/l	232149	4	11.816	1126240	50.0