

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
 Data File : VU043168.D
 Acq On : 16 Apr 2021 15:05
 Operator : SY/MD
 Sample : M2042-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 FS-SB12A

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82U041221W.M
 Title : SW846 8260

Signal : TIC: VU043168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.691	103	109	122	rVB	7999	11645	1.73%	0.205%
2	2.549	363	376	386	rBV	4566	7856	1.17%	0.138%
3	2.642	394	405	431	rBV	7427	16020	2.39%	0.282%
4	5.096	1156	1168	1182	rBV3	12296	25885	3.86%	0.456%
5	5.298	1213	1231	1244	rBV	109027	230049	34.27%	4.054%
6	5.382	1244	1257	1279	rVB	165369	338598	50.44%	5.967%
7	5.710	1341	1359	1379	rBV	123824	254095	37.85%	4.478%
8	6.256	1513	1529	1553	rBV	251412	466298	69.46%	8.218%
9	6.890	1716	1726	1737	rBV3	5943	11772	1.75%	0.207%
10	7.906	2027	2042	2057	rBV	394998	671283	100.00%	11.830%
11	8.793	2307	2318	2335	rBV2	63139	108271	16.13%	1.908%
12	9.423	2501	2514	2532	rBV	360862	595606	88.73%	10.497%
13	10.349	2793	2802	2812	rBV3	9119	13742	2.05%	0.242%
14	10.491	2835	2846	2856	rBV	33526	50148	7.47%	0.884%
15	10.639	2880	2892	2911	rBV	300472	478491	71.28%	8.433%
16	10.912	2966	2977	2990	rVB	34926	51542	7.68%	0.908%
17	11.031	2996	3014	3026	rBV	47130	77316	11.52%	1.363%
18	11.298	3080	3097	3109	rVB	55089	84923	12.65%	1.497%
19	11.475	3141	3152	3166	rBV	233163	350670	52.24%	6.180%
20	11.697	3213	3221	3229	rVV3	11344	15912	2.37%	0.280%
21	11.751	3229	3238	3247	rVV	22605	32604	4.86%	0.575%
22	11.819	3247	3259	3274	rVV	386732	610730	90.98%	10.763%
23	11.902	3274	3285	3295	rVV	73222	112034	16.69%	1.974%
24	12.105	3332	3348	3361	rBV2	50605	79594	11.86%	1.403%
25	12.192	3367	3375	3391	rBV5	17634	33575	5.00%	0.592%
26	12.382	3422	3434	3444	rVB2	10069	15419	2.30%	0.272%
27	12.472	3452	3462	3468	rBV2	22390	36932	5.50%	0.651%
28	12.578	3483	3495	3503	rBV2	43253	65855	9.81%	1.161%
29	12.690	3521	3530	3542	rBV2	11178	21847	3.25%	0.385%
30	12.893	3580	3593	3604	rBV5	28397	49801	7.42%	0.878%
31	12.980	3609	3620	3629	rVV	35238	52921	7.88%	0.933%
32	13.031	3629	3636	3648	rVB2	8538	14403	2.15%	0.254%
33	13.301	3711	3720	3732	rVB	8721	12426	1.85%	0.219%
34	13.455	3758	3768	3780	rVV2	27338	41903	6.24%	0.738%
35	13.526	3783	3790	3800	rVB5	6426	9584	1.43%	0.169%
36	13.632	3810	3823	3833	rBV5	10859	17610	2.62%	0.310%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\82U041221W.M
Title : SW846 8260

37	14.095	3954	3967	3980	rBV	287638	461130	68.69%	8.127%
38	15.420	4366	4379	4391	rBV	91412	145707	21.71%	2.568%

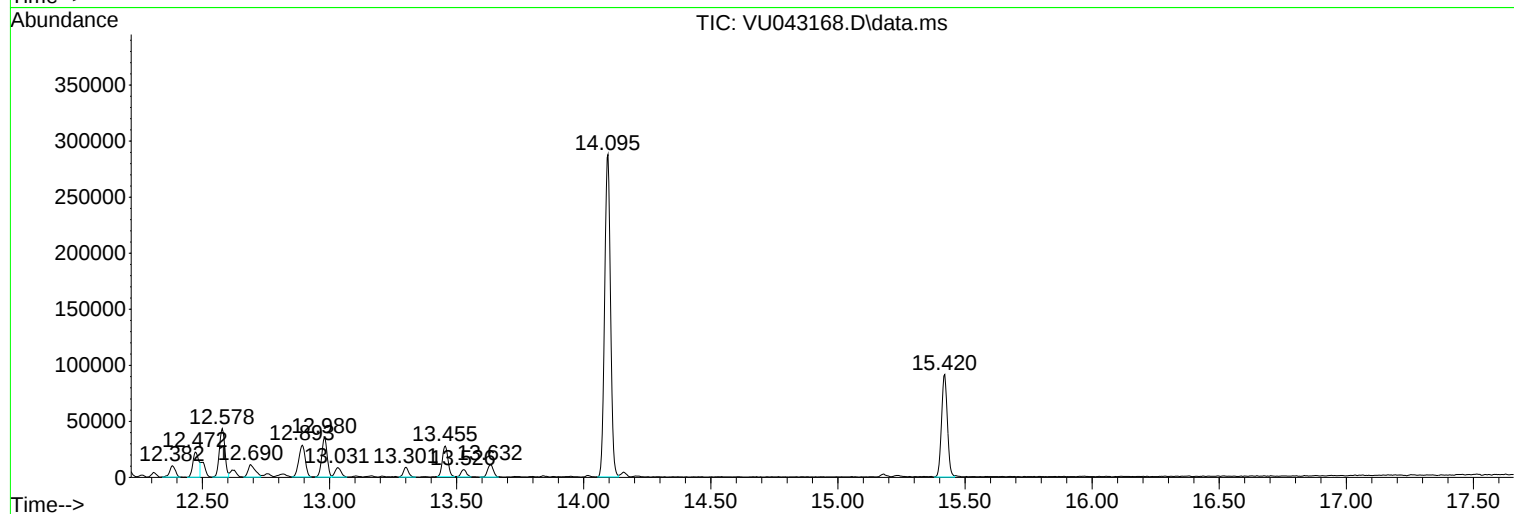
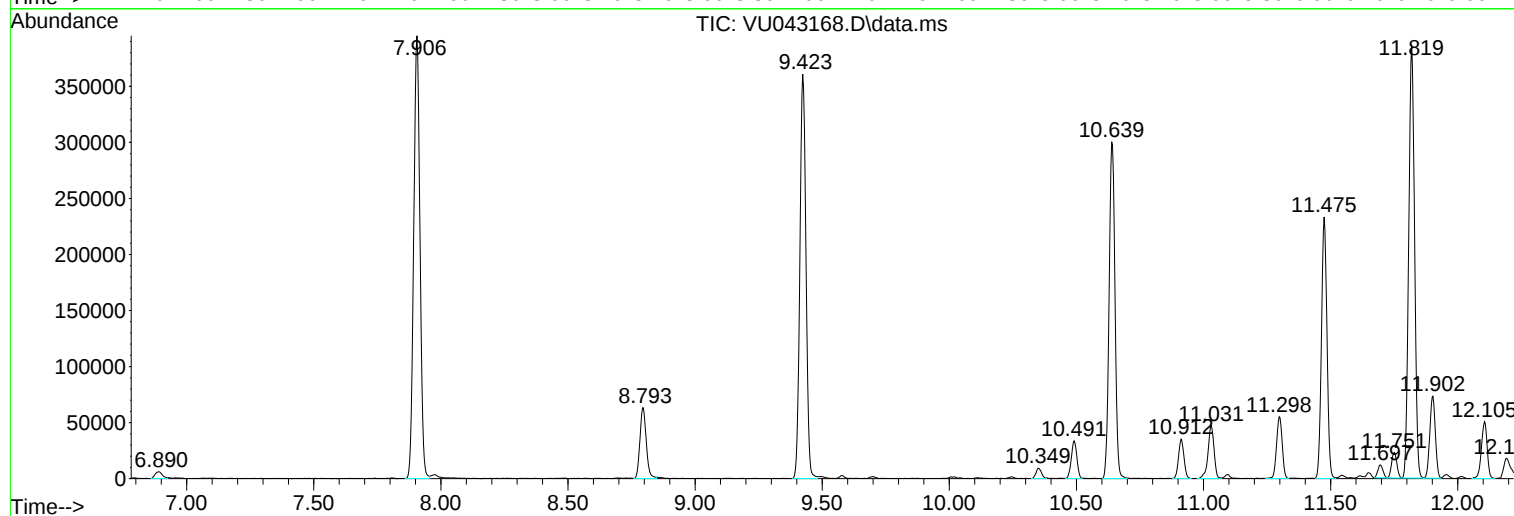
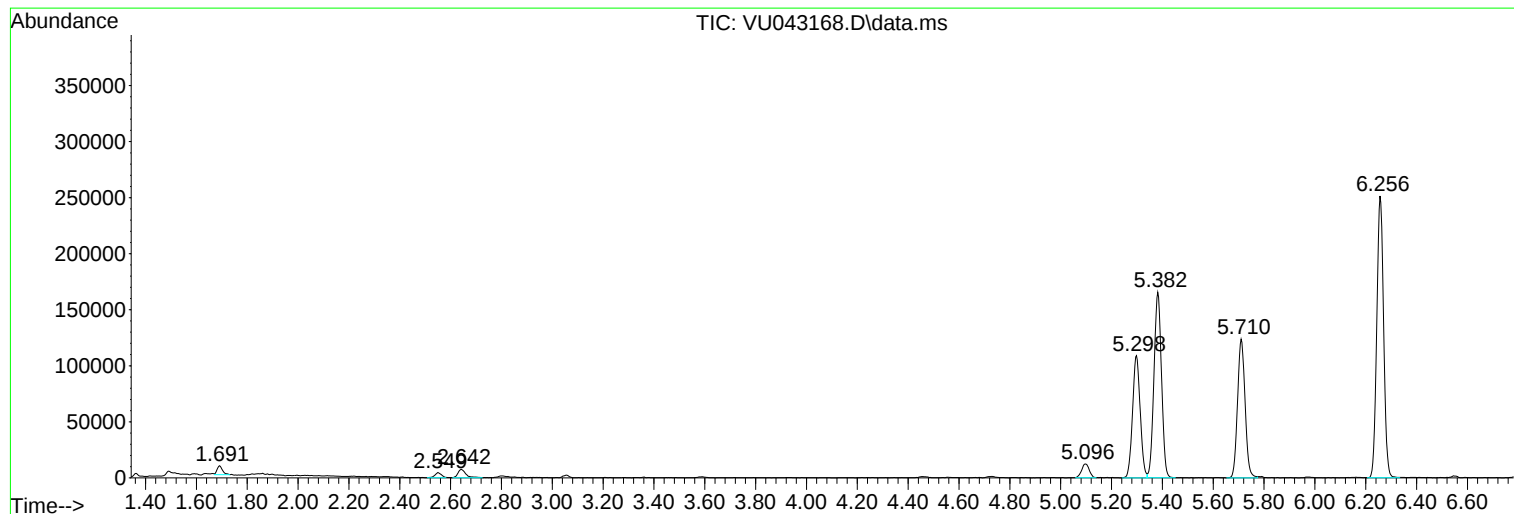
Sum of corrected areas: 5674197

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

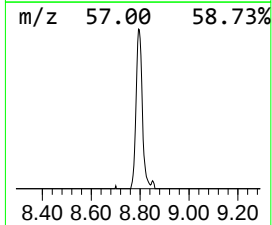
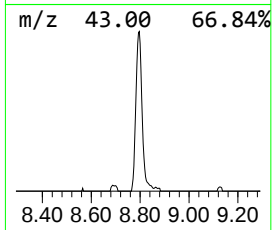
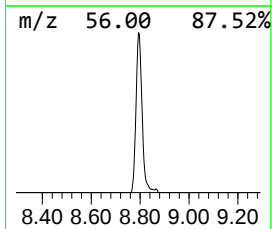
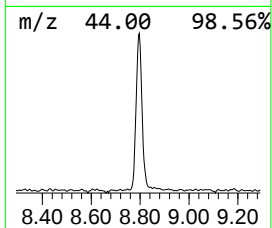
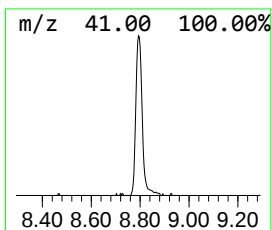
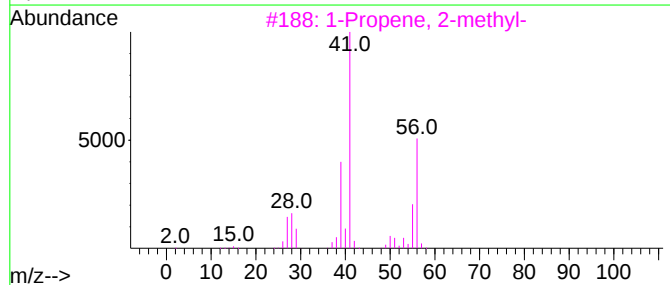
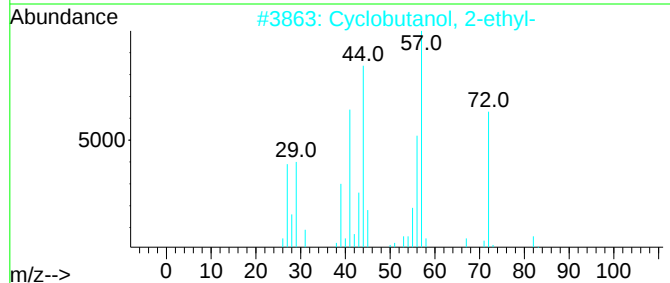
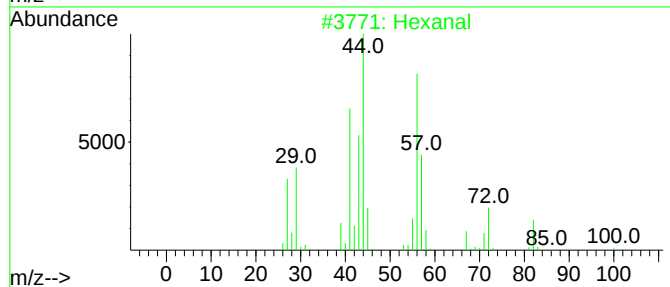
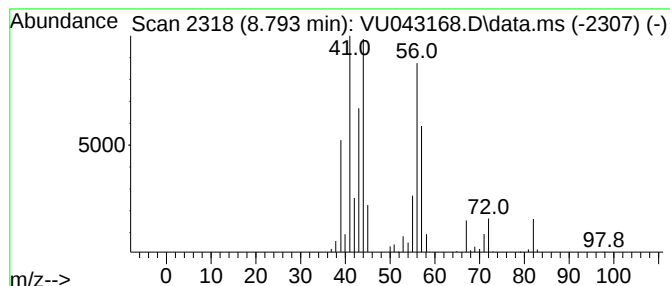
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.793	9.09 ug/l	108271	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	72
2			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	59
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	25
5			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

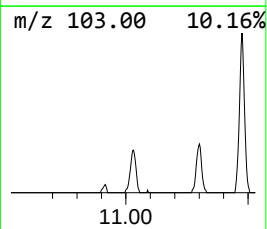
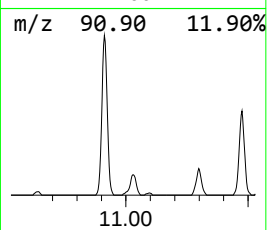
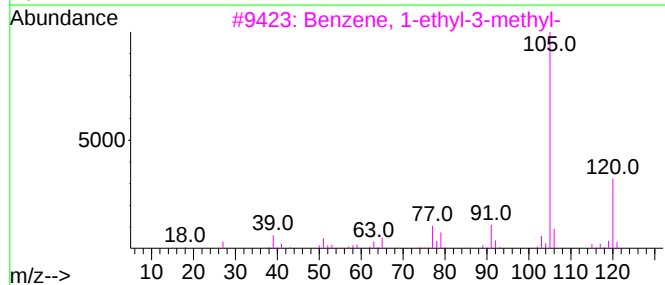
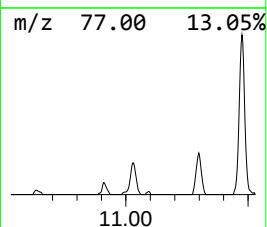
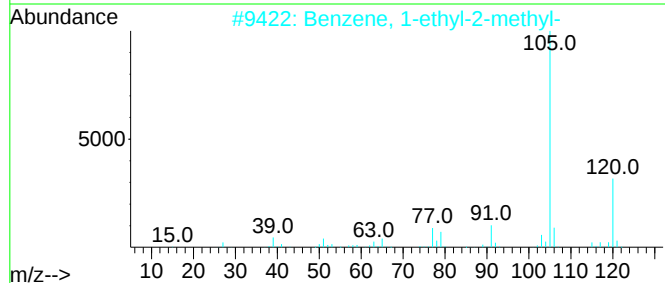
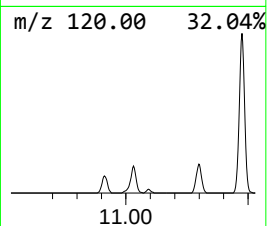
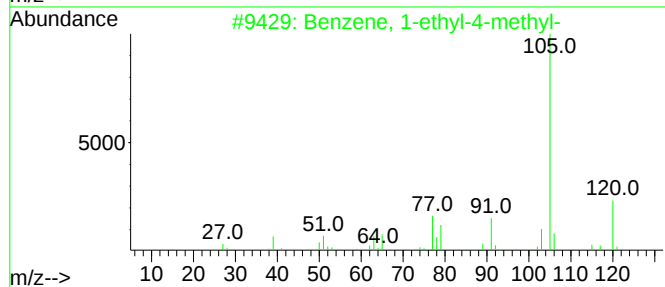
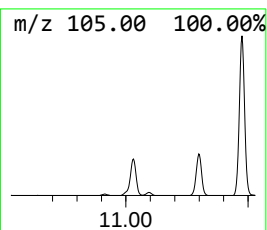
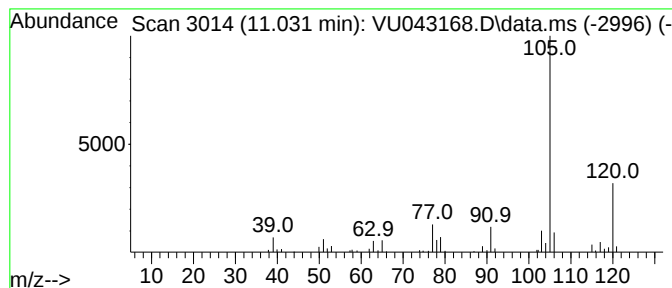
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.031	6.33 ug/l	77316	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

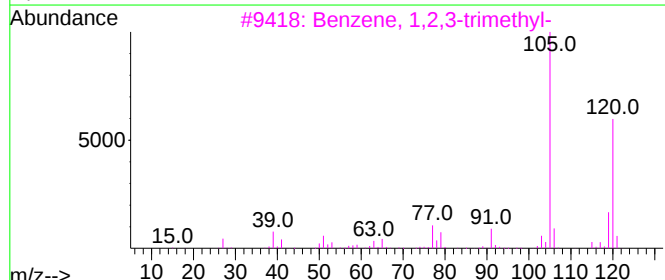
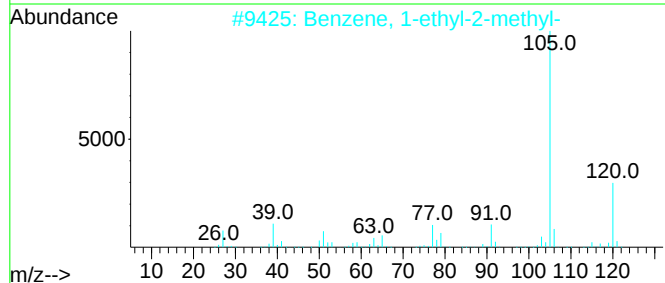
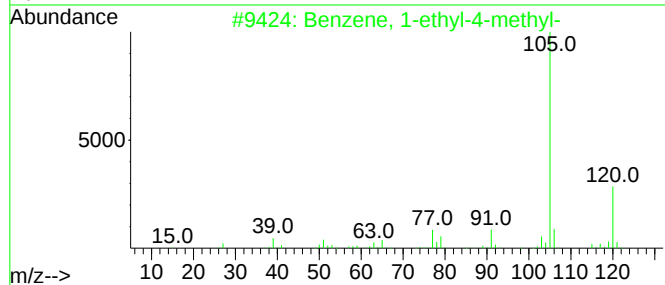
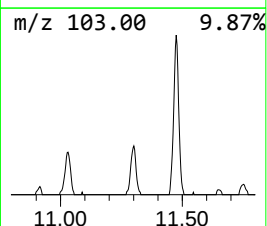
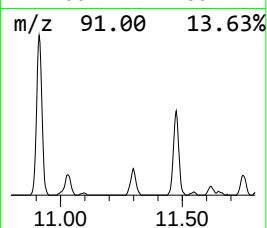
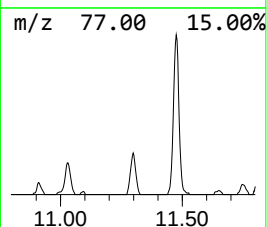
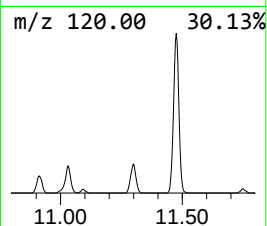
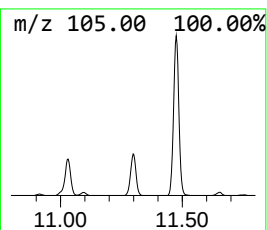
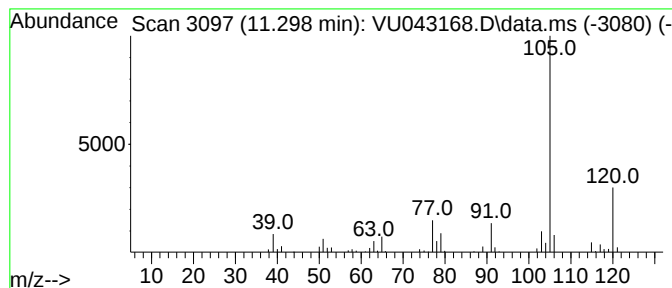
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	6.95 ug/l	84923	1,4-Dichlorobenzene-d4	11.819

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

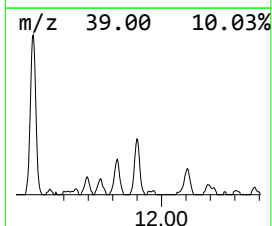
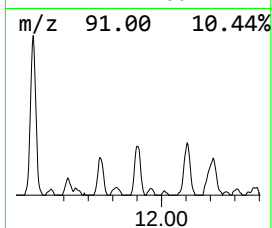
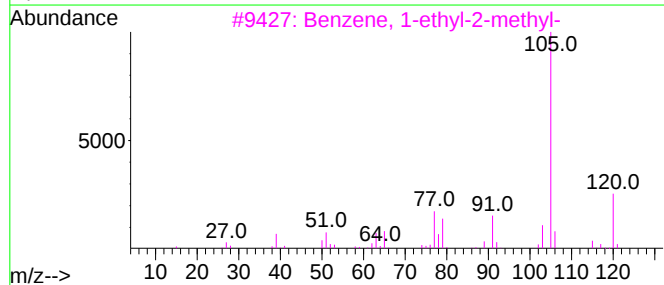
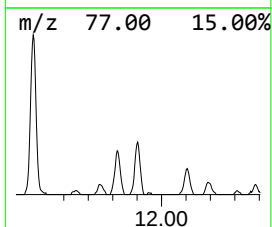
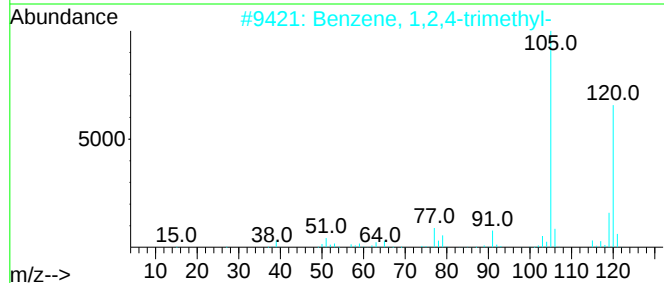
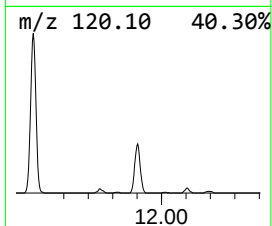
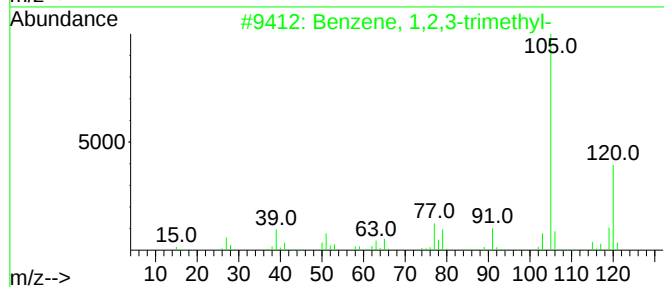
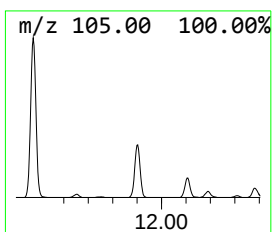
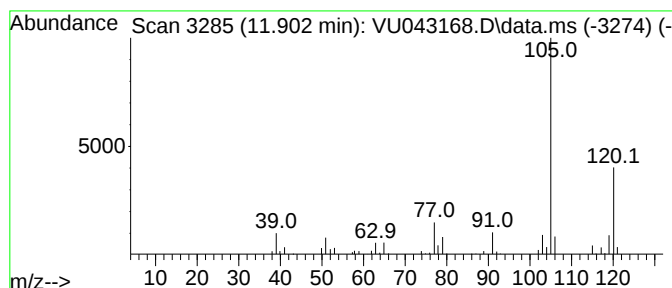
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.903	9.17 ug/l	112034	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

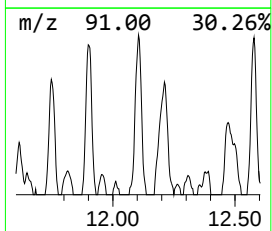
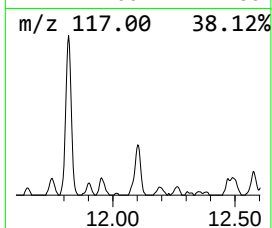
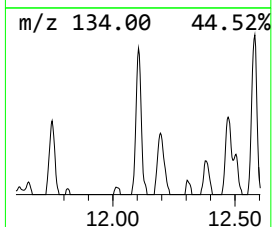
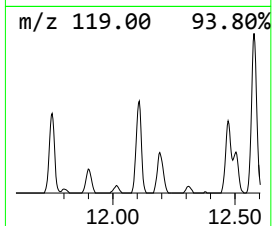
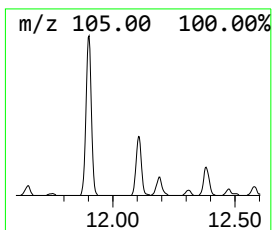
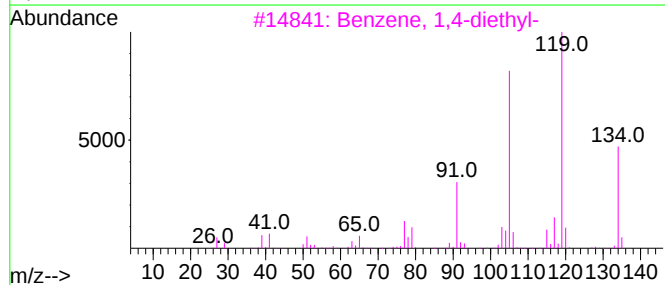
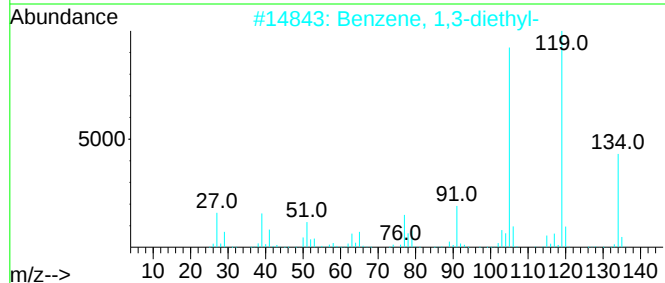
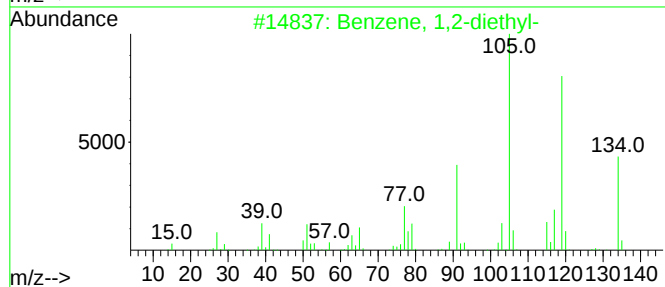
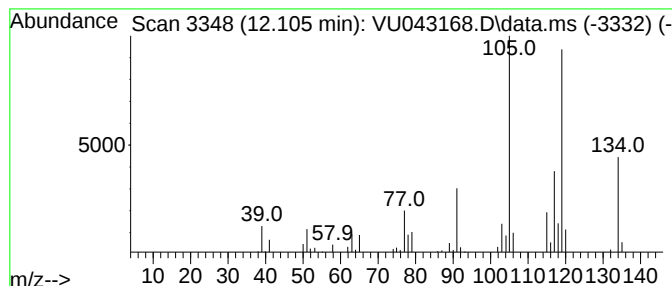
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	6.52 ug/l	79594	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	91
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	76
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	74
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	58
5			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

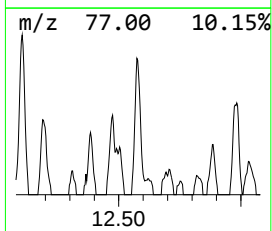
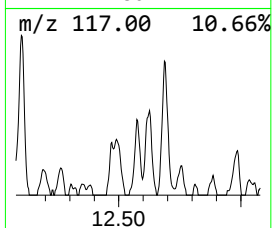
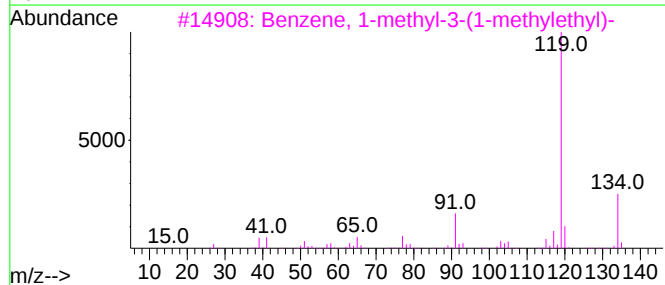
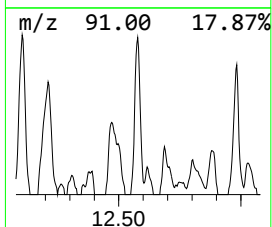
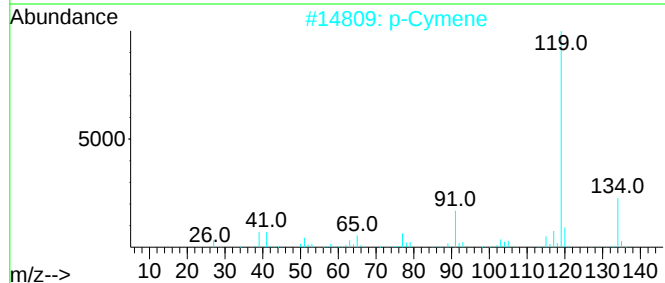
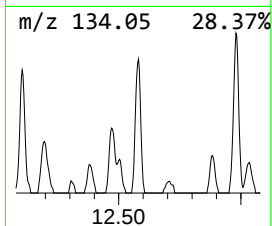
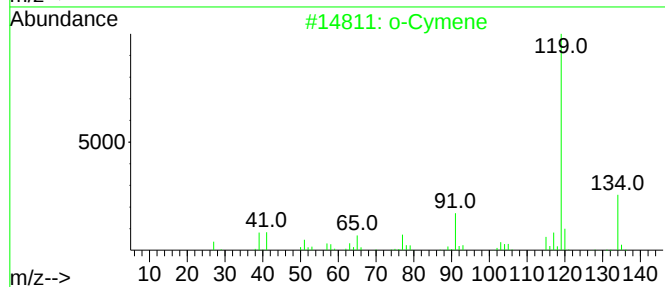
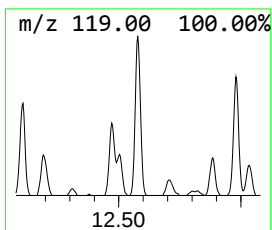
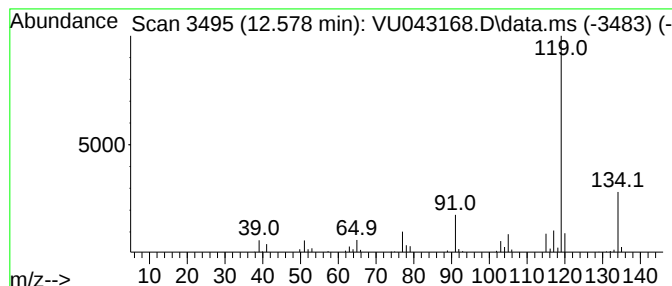
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.578	5.39 ug/l	65855	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			p-Cymene	134	C10H14	000099-87-6	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

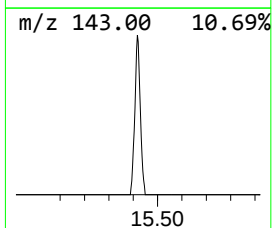
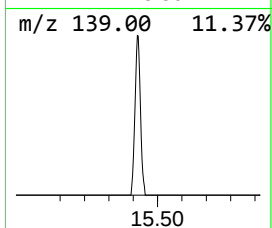
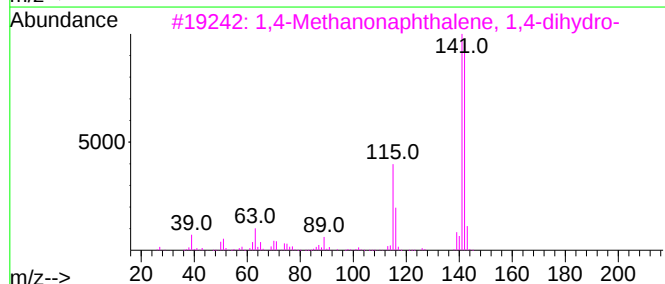
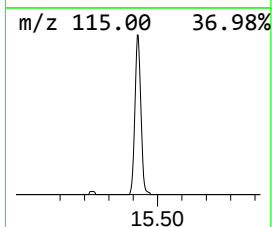
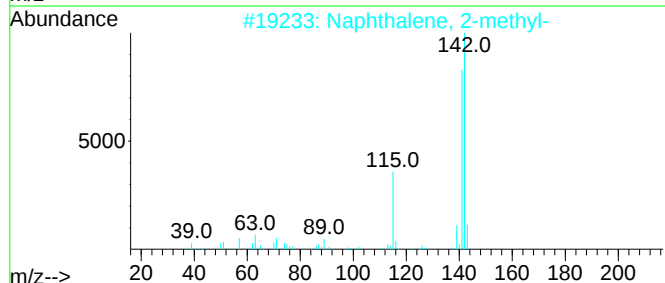
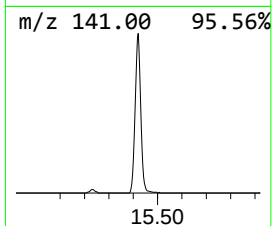
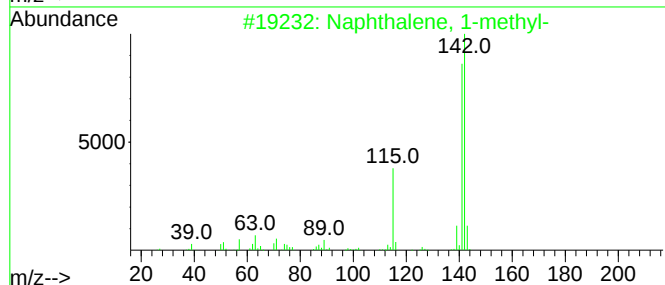
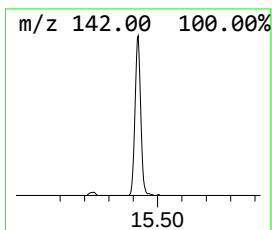
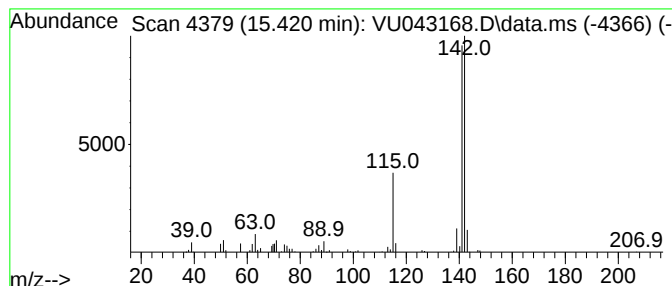
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	11.93 ug/l	145707	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041621\
Data File : VU043168.D
Acq On : 16 Apr 2021 15:05
Operator : SY/MD
Sample : M2042-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB12A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.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
Hexanal	8.793	9.1	ug/l	108271	3	9.423	595606	50.0
Benzene, 1-ethy...	11.031	6.3	ug/l	77316	4	11.819	610730	50.0
Benzene, 1-ethy...	11.298	7.0	ug/l	84923	4	11.819	610730	50.0
Benzene, 1,2,3-...	11.903	9.2	ug/l	112034	4	11.819	610730	50.0
Benzene, 1,2-di...	12.105	6.5	ug/l	79594	4	11.819	610730	50.0
o-Cymene	12.578	5.4	ug/l	65855	4	11.819	610730	50.0
Naphthalene, 1-...	15.420	11.9	ug/l	145707	4	11.819	610730	50.0