

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
 Data File : VU042861.D
 Acq On : 31 Mar 2021 16:40
 Operator : SY/MD
 Sample : M1828-04
 Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 FS-SB14(5-6)

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\82U032421W.M
 Title : SW846 8260

Signal : TIC: VU042861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.295	1214	1230	1244	rBV	109568	235504	33.32%	4.645%
2	5.378	1244	1256	1274	rVB	182200	373395	52.83%	7.364%
3	5.710	1344	1359	1374	rBV	127019	259840	36.76%	5.124%
4	6.256	1514	1529	1550	rBV	261398	498502	70.53%	9.831%
5	7.906	2024	2042	2057	rBV	407562	706775	100.00%	13.939%
6	7.976	2057	2064	2077	rVB3	7140	12692	1.80%	0.250%
7	9.426	2499	2515	2536	rBV	367095	639687	90.51%	12.616%
8	9.578	2554	2562	2573	rVB2	5268	7879	1.11%	0.155%
9	9.703	2590	2601	2612	rBV	9955	16698	2.36%	0.329%
10	10.645	2881	2894	2915	rBV	324569	536945	75.97%	10.589%
11	10.899	2962	2973	2986	rVB	38192	62687	8.87%	1.236%
12	11.475	3141	3152	3167	rVB4	9797	15787	2.23%	0.311%
13	11.822	3248	3260	3273	rBV	444202	696391	98.53%	13.734%
14	12.333	3409	3419	3428	rBV7	5416	8862	1.25%	0.175%
15	12.848	3570	3579	3588	rBV10	5133	8255	1.17%	0.163%
16	13.060	3636	3645	3654	rVB10	9620	17074	2.42%	0.337%
17	13.137	3661	3669	3680	rVB8	6042	10084	1.43%	0.199%
18	13.307	3704	3722	3730	rBV8	4867	12505	1.77%	0.247%
19	13.439	3755	3763	3768	rBV	24903	40250	5.69%	0.794%
20	13.539	3786	3794	3801	rBV10	6236	9521	1.35%	0.188%
21	13.593	3803	3811	3817	rBV2	29559	47187	6.68%	0.931%
22	13.735	3849	3855	3867	rVB10	8470	14448	2.04%	0.285%
23	13.986	3919	3933	3934	rBV10	13178	23813	3.37%	0.470%
24	14.005	3936	3939	3946	rVB5	13667	15148	2.14%	0.299%
25	14.053	3947	3954	3958	rBV5	17139	24421	3.46%	0.482%
26	14.095	3959	3967	3977	rVV	115077	171198	24.22%	3.376%
27	14.195	3989	3998	4013	rBV5	36431	74330	10.52%	1.466%
28	14.458	4072	4080	4087	rBV	52064	70648	10.00%	1.393%
29	15.230	4308	4320	4330	rBV3	74213	133722	18.92%	2.637%
30	15.417	4370	4378	4397	rVB2	62045	120414	17.04%	2.375%
31	16.156	4603	4608	4614	rBV2	7195	7705	1.09%	0.152%
32	16.201	4616	4622	4634	rVB7	14772	24977	3.53%	0.493%
33	16.269	4636	4643	4650	rBV	17412	26843	3.80%	0.529%
34	16.417	4681	4689	4696	rBV	30704	50043	7.08%	0.987%
35	16.552	4724	4731	4737	rBV	5521	7771	1.10%	0.153%
36	16.626	4746	4754	4757	rBV9	7328	10571	1.50%	0.208%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

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\82U032421W.M
Title : SW846 8260

37	16.793	4798	4806	4815	rBV5	6440	9968	1.41%	0.197%
38	16.892	4829	4837	4847	rBV5	4934	7918	1.12%	0.156%
39	17.108	4894	4904	4916	rVB2	25896	44340	6.27%	0.874%
40	17.281	4951	4958	4968	rBV4	8704	15756	2.23%	0.311%

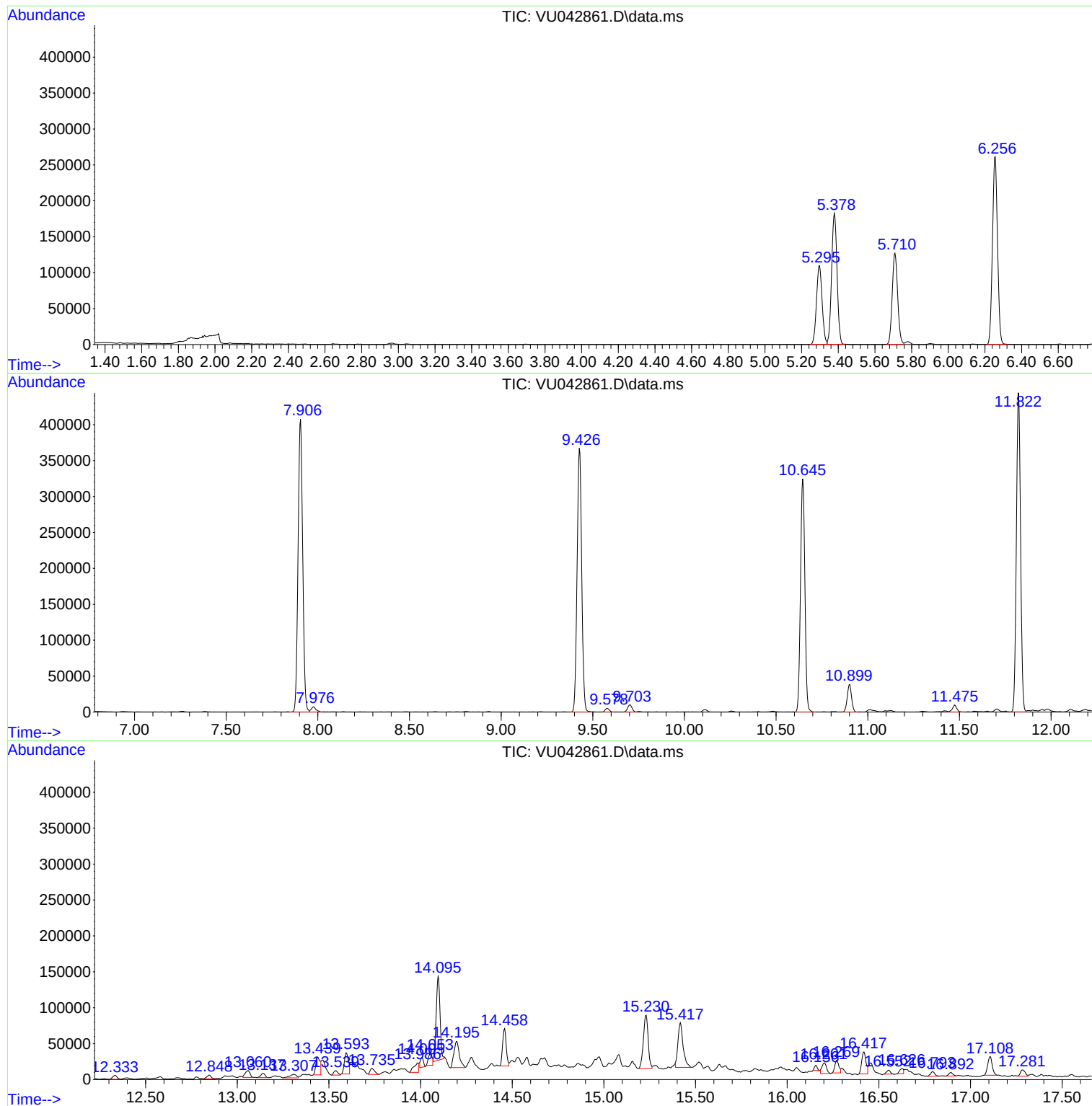
Sum of corrected areas: 5070554

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

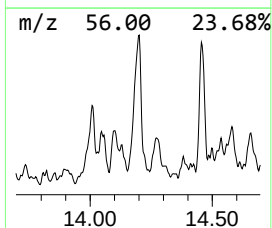
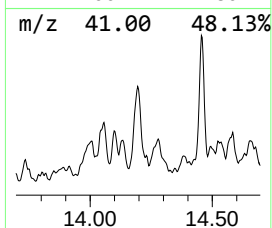
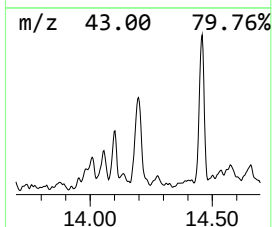
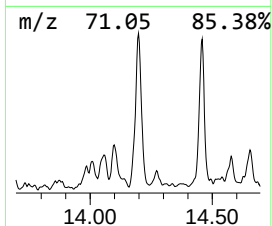
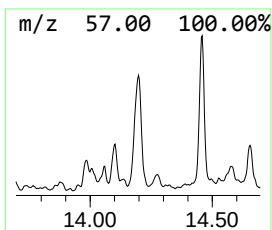
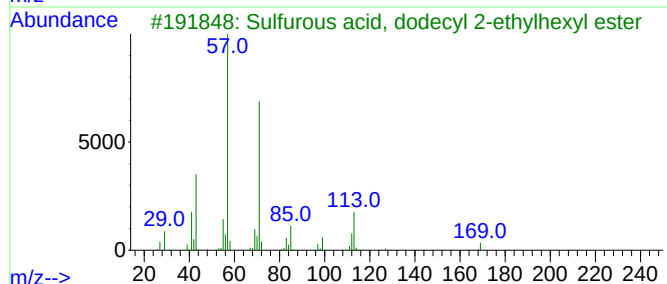
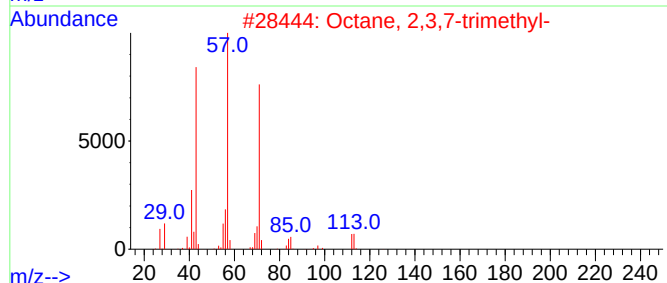
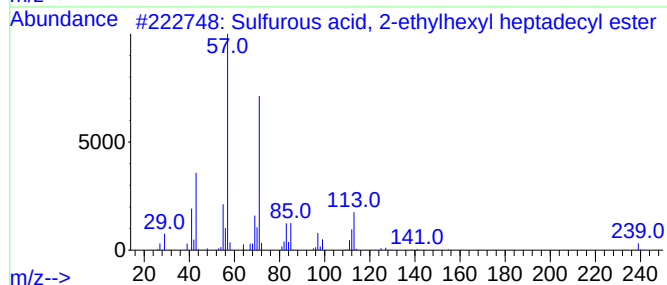
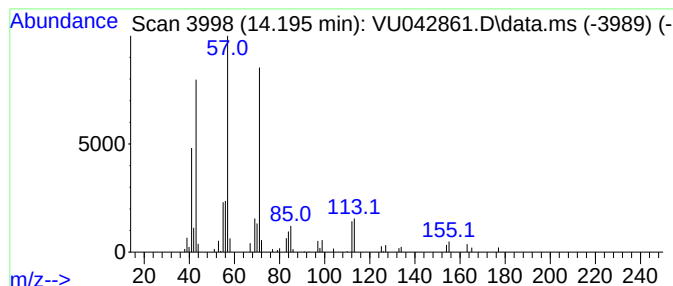
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfurous acid, 2-ethylhexy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	5.34 ug/l	74330	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	72
2			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	72
3			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	64
5			Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

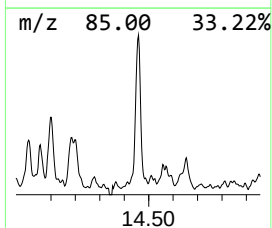
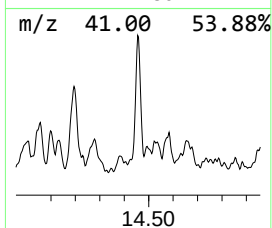
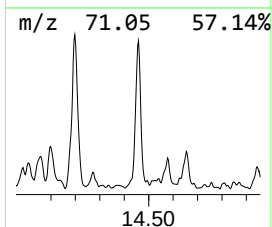
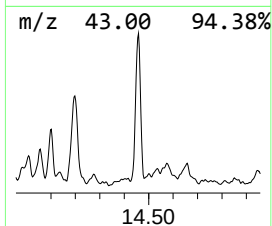
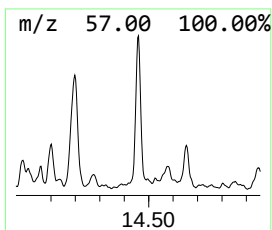
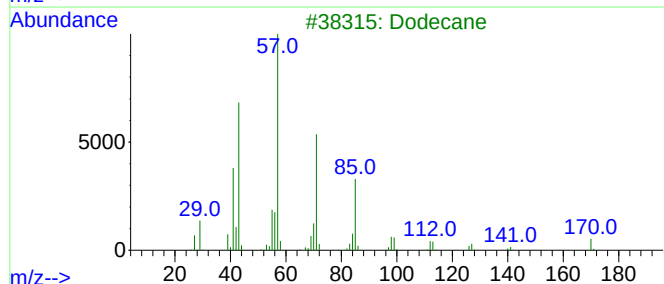
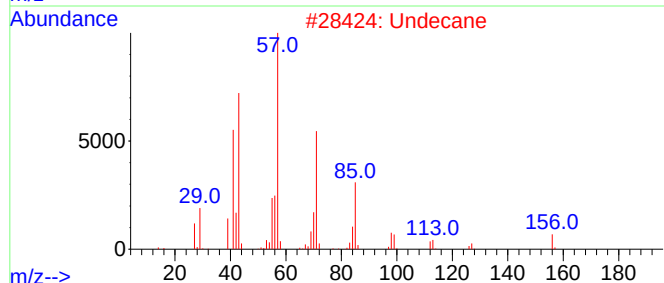
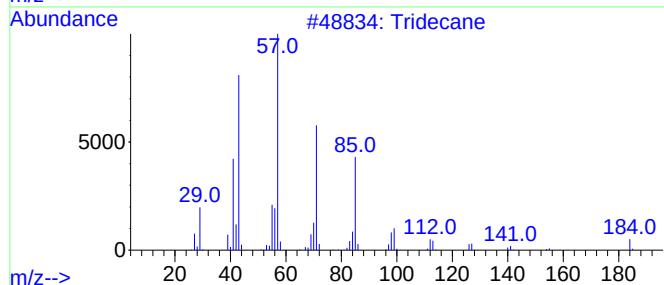
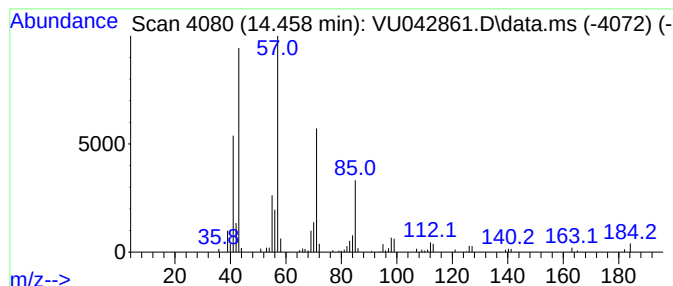
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 2 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.458	5.07 ug/l	70648	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Undecane	156	C11H24	001120-21-4	86
3			Dodecane	170	C12H26	000112-40-3	86
4			Hexadecane	226	C16H34	000544-76-3	80
5			Tetradecane	198	C14H30	000629-59-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

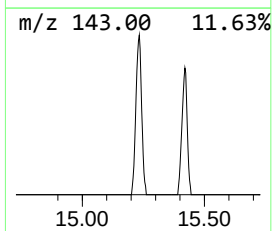
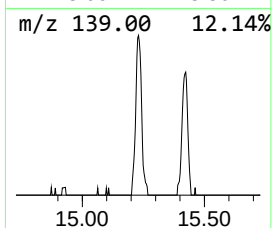
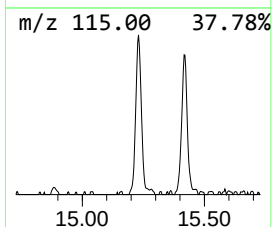
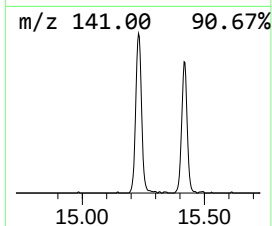
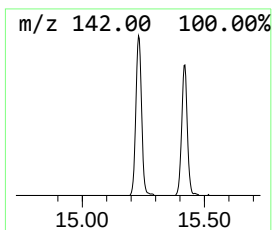
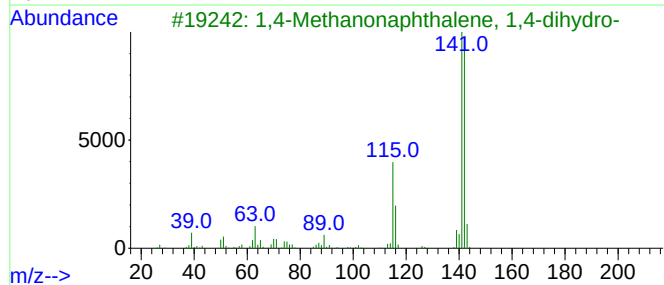
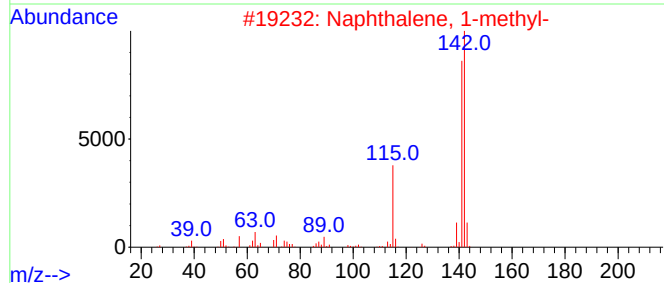
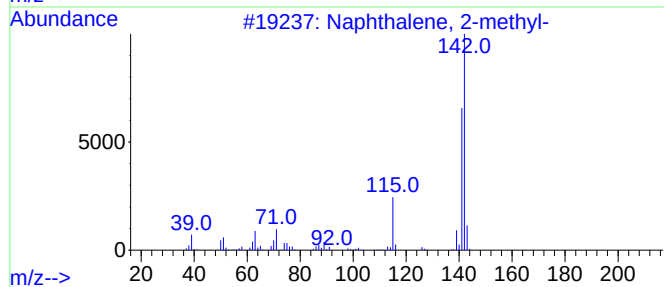
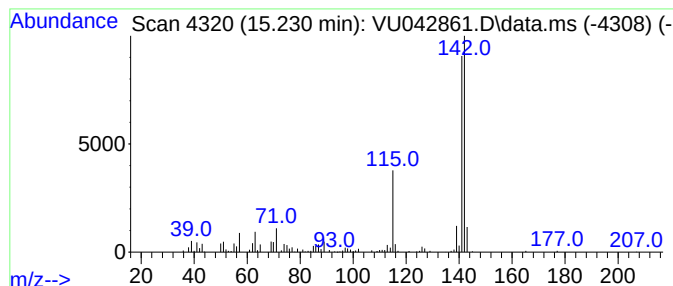
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.230	9.60 ug/l	133722	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

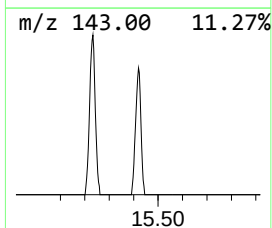
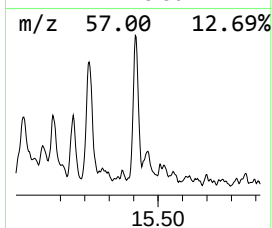
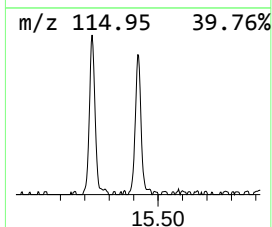
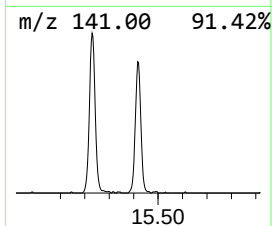
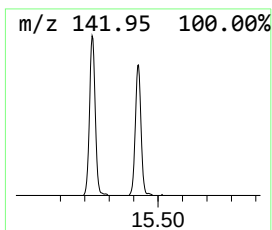
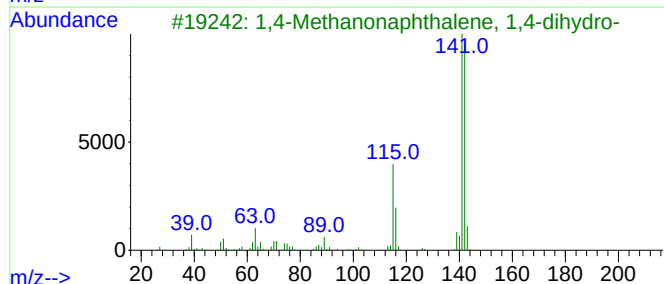
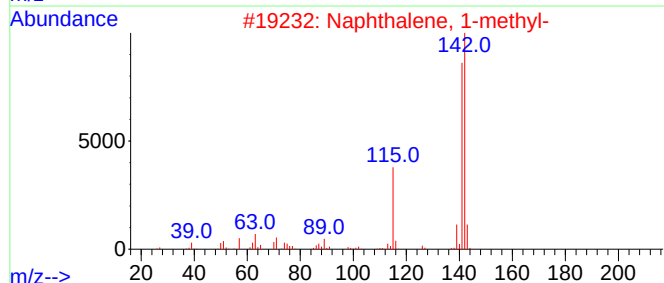
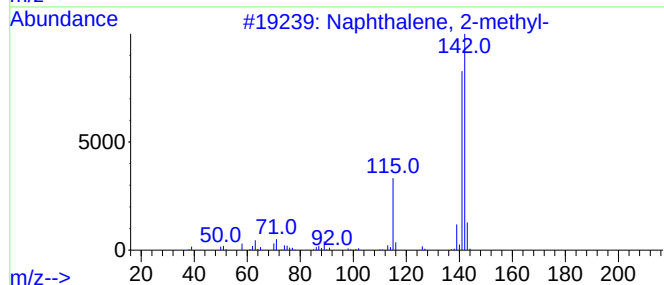
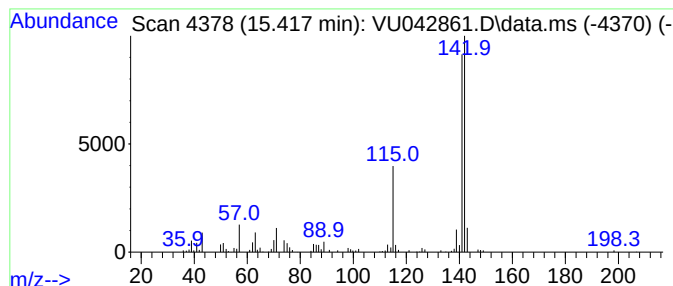
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.417	8.65 ug/l	120414	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042861.D
Acq On : 31 Mar 2021 16:40
Operator : SY/MD
Sample : M1828-04
Misc : 6.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FS-SB14(5-6)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.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
Sulfurous acid,...	14.195	5.3	ug/l	74330	4	11.822	696391	50.0
Tridecane	14.458	5.1	ug/l	70648	4	11.822	696391	50.0
Naphthalene, 1-...	15.230	9.6	ug/l	133722	4	11.822	696391	50.0
1,4-Methanonaph...	15.417	8.7	ug/l	120414	4	11.822	696391	50.0