

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
 Data File : VU045361.D
 Acq On : 22 Oct 2021 13:49
 Operator : SY/MD
 Sample : M4288-01
 Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 SA-01-101921

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\82U092821W.M
 Title : SW846 8260

Signal : TIC: VU045361.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.304	1215	1233	1243	rBV2	115273	334978	24.14%	3.152%
2	5.372	1243	1254	1281	rVB	304528	749044	53.97%	7.048%
3	5.706	1339	1358	1391	rBV	184440	473387	34.11%	4.454%
4	6.250	1511	1527	1556	rBV	436236	987945	71.19%	9.296%
5	7.902	2025	2041	2058	rBV	704533	1387845	100.00%	13.059%
6	9.427	2500	2515	2542	rBV	518688	1208158	87.05%	11.368%
7	9.578	2553	2562	2575	rBV	8277	14082	1.01%	0.133%
8	9.703	2586	2601	2619	rBV	35871	75065	5.41%	0.706%
9	10.111	2714	2728	2743	rVB3	10866	21547	1.55%	0.203%
10	10.648	2879	2895	2913	rBV	462536	883882	63.69%	8.317%
11	11.822	3244	3260	3275	rBV	709740	1164786	83.93%	10.960%
12	12.063	3325	3335	3345	rBV2	10574	19251	1.39%	0.181%
13	12.330	3408	3418	3427	rBV	14190	20549	1.48%	0.193%
14	13.436	3748	3762	3768	rBV	32398	56118	4.04%	0.528%
15	13.629	3815	3822	3834	rBV6	11164	18138	1.31%	0.171%
16	14.066	3950	3958	3974	rVB3	27654	63752	4.59%	0.600%
17	14.192	3985	3997	4011	rVB8	23208	55891	4.03%	0.526%
18	14.288	4017	4027	4032	rBV6	13041	25185	1.81%	0.237%
19	14.401	4055	4062	4067	rBV	9750	14396	1.04%	0.135%
20	14.452	4070	4078	4085	rVV	60164	82909	5.97%	0.780%
21	14.690	4138	4152	4168	rVB3	61096	128294	9.24%	1.207%
22	14.812	4184	4190	4197	rBV4	11880	19183	1.38%	0.180%
23	14.883	4206	4212	4220	rVB3	20637	28418	2.05%	0.267%
24	15.021	4246	4255	4264	rBV4	58782	101246	7.30%	0.953%
25	15.204	4303	4312	4327	rBV5	105720	288168	20.76%	2.711%
26	15.275	4328	4334	4349	rVB6	48116	91623	6.60%	0.862%
27	15.352	4350	4358	4364	rBV5	30009	48571	3.50%	0.457%
28	15.404	4365	4374	4385	rBV2	170701	262903	18.94%	2.474%
29	15.510	4401	4407	4416	rVB6	39755	60845	4.38%	0.573%
30	15.931	4529	4538	4551	rBV2	136903	360862	26.00%	3.395%
31	16.153	4599	4607	4623	rBV5	85739	166706	12.01%	1.569%
32	16.269	4635	4643	4645	rBV3	139297	179897	12.96%	1.693%
33	16.294	4646	4651	4661	rVB	264089	376614	27.14%	3.544%
34	16.410	4679	4687	4694	rBV3	156152	234374	16.89%	2.205%
35	16.883	4827	4834	4843	rBV	132007	238461	17.18%	2.244%
36	17.137	4905	4913	4923	rVB2	245985	384642	27.72%	3.619%

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SA-01-101921

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\82U092821W.M
Title : SW846 8260

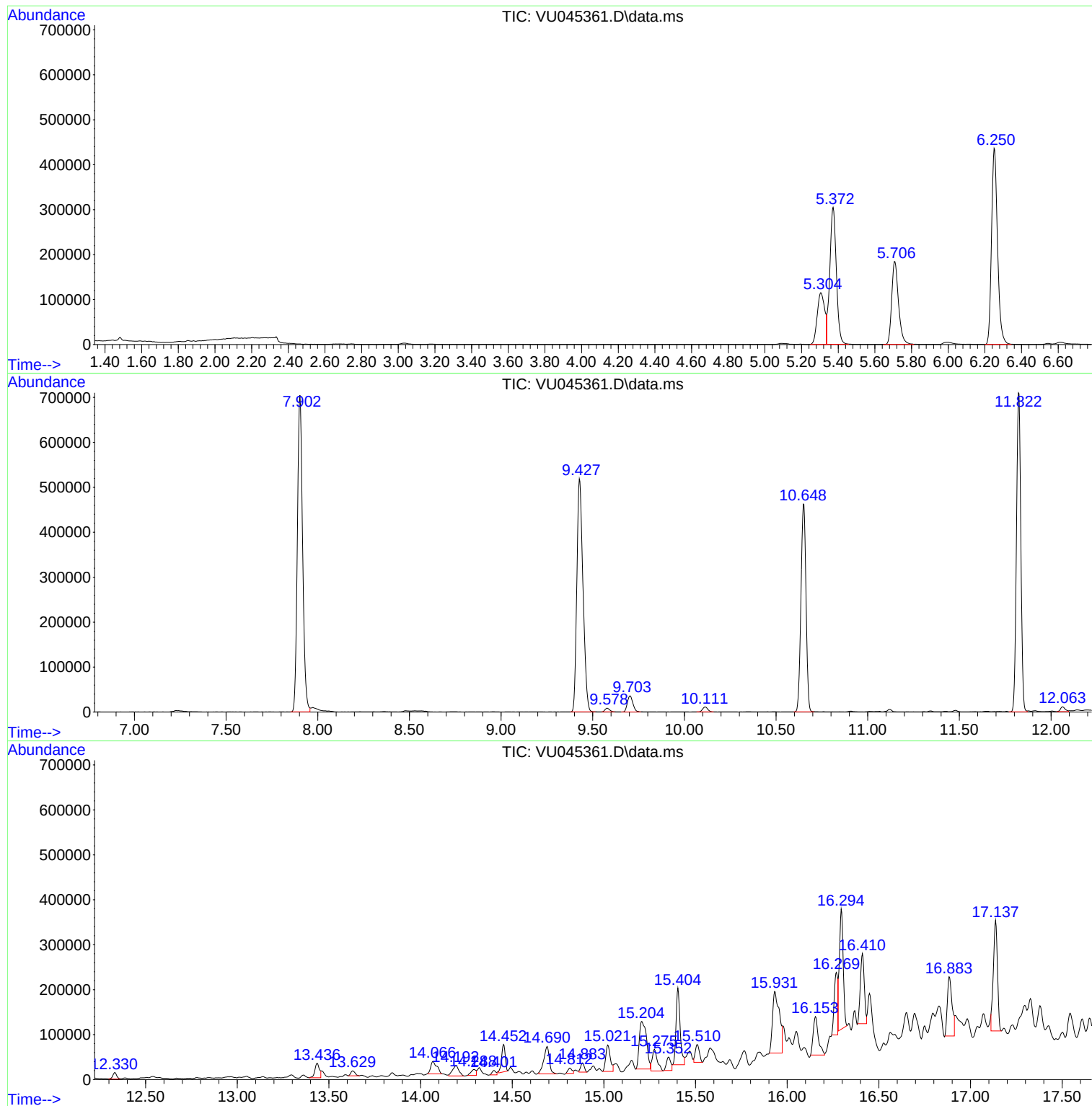
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



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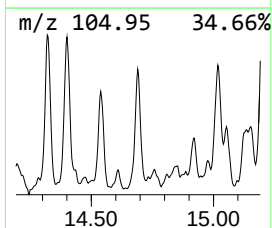
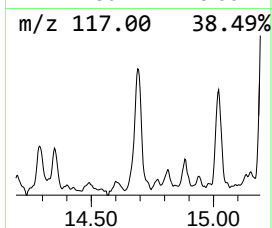
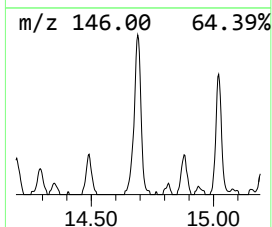
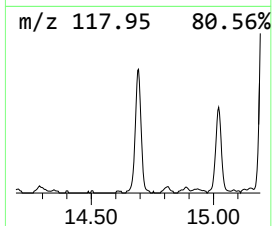
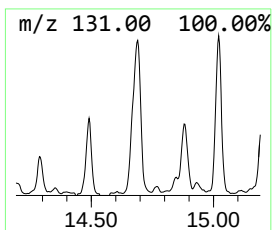
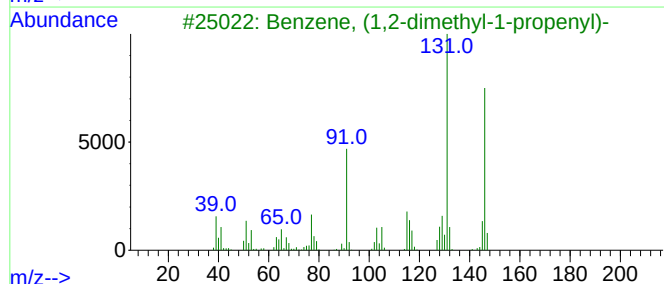
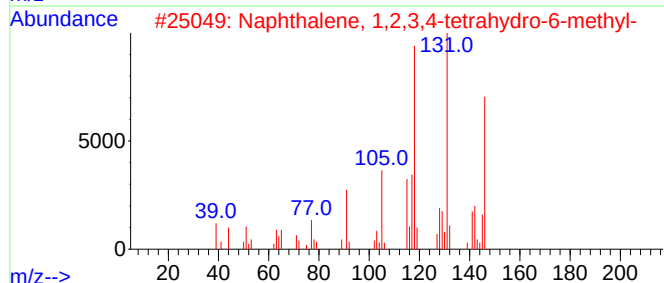
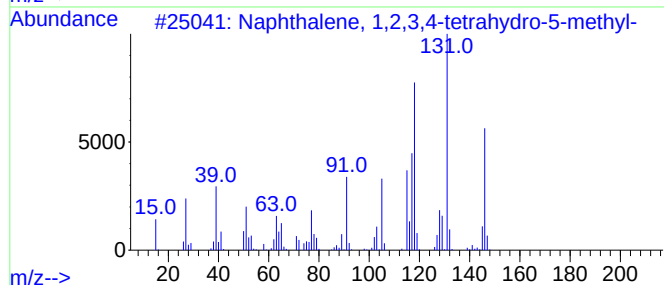
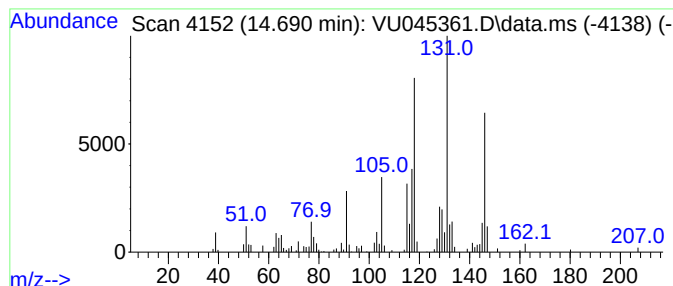
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, 1,2,3,4-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.690	5.51 ug/l	128294	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	87
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	60



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

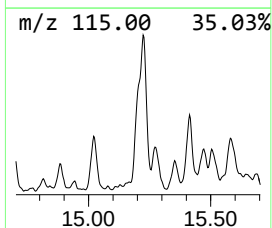
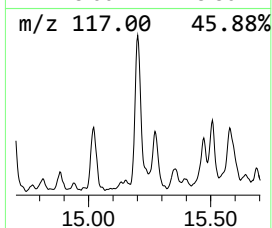
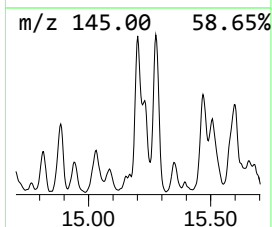
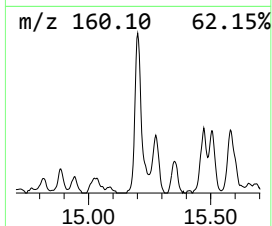
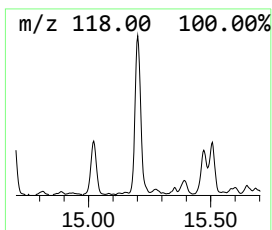
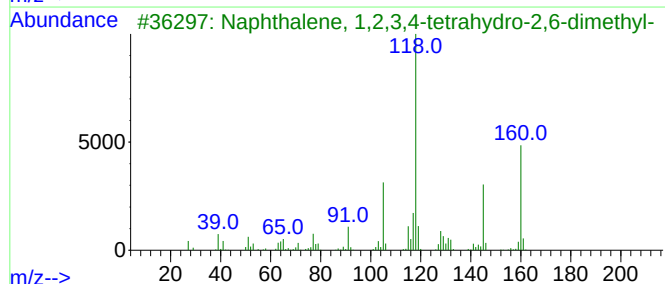
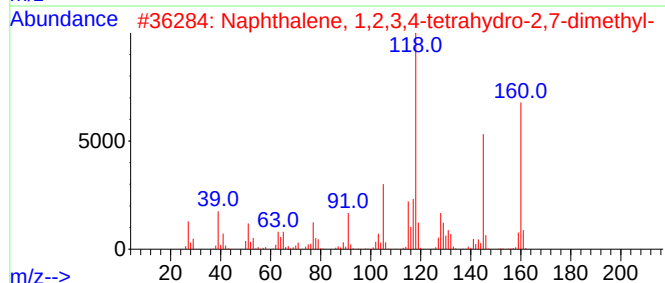
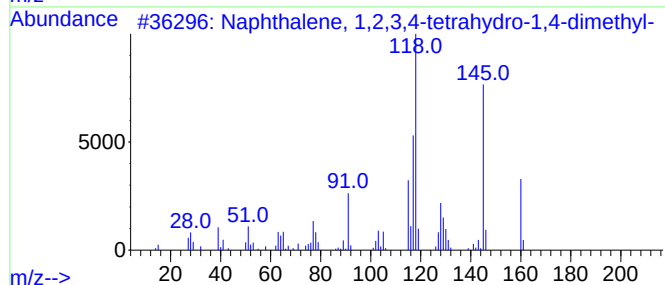
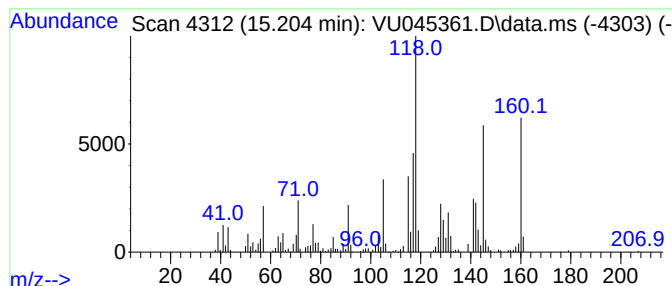
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	12.37 ug/l	288168	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	89
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	64
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	55
4			1(2H)-Naphthalenone, 3,4-dihydro-...	160	C11H12O	014944-23-1	53
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	46



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

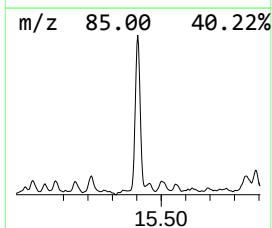
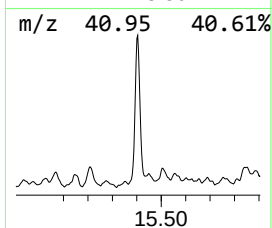
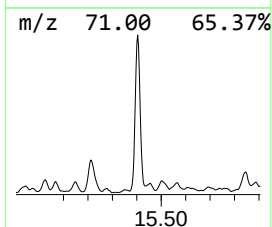
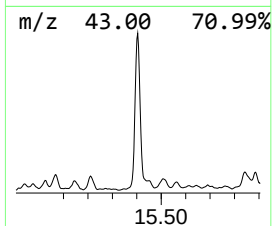
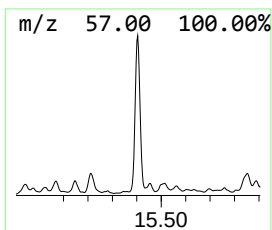
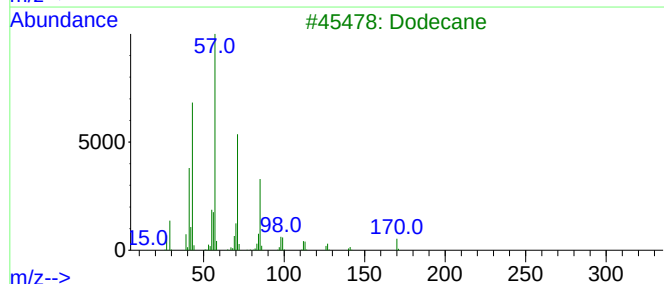
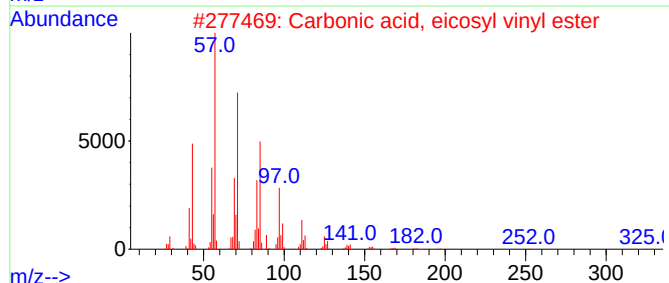
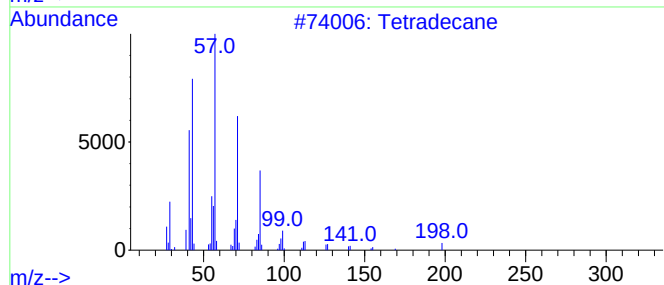
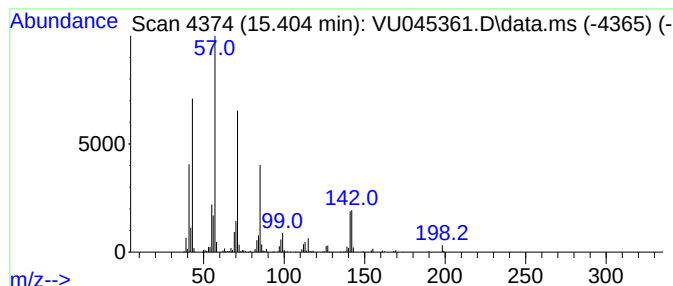
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 3 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	11.29 ug/l	262903	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	98
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	74
3			Dodecane	170	C12H26	000112-40-3	72
4			Tridecane	184	C13H28	000629-50-5	72
5			Hexadecane	226	C16H34	000544-76-3	72



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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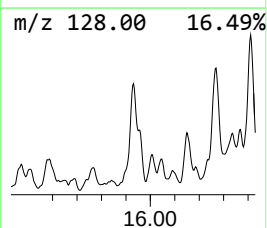
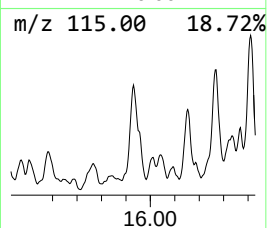
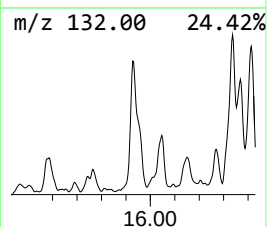
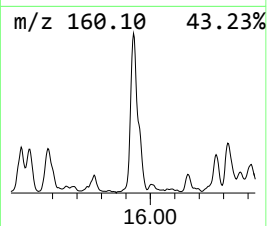
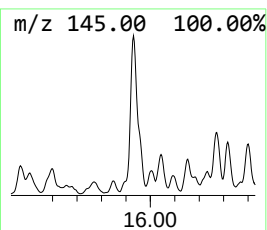
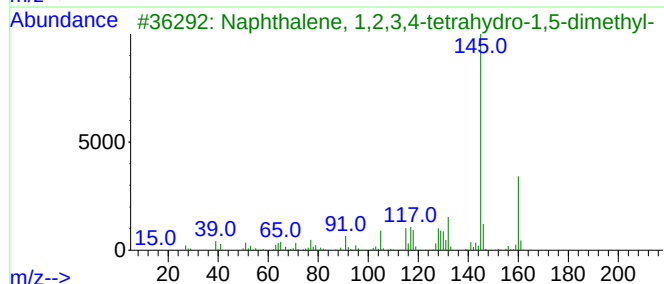
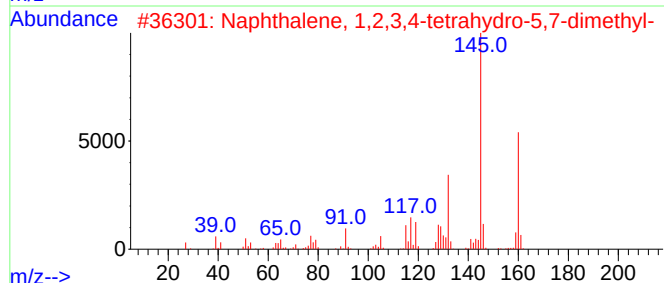
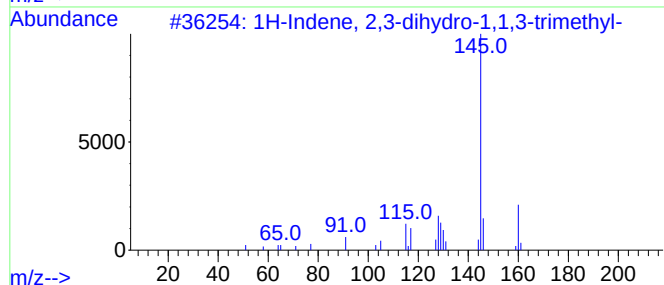
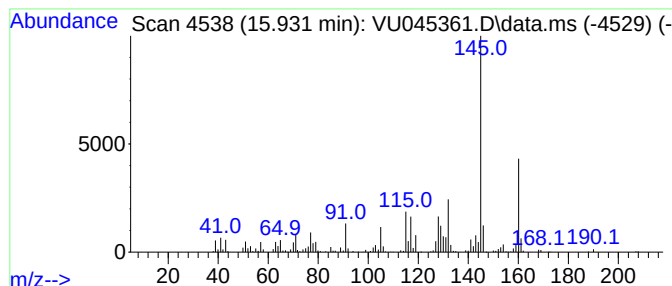
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Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.931	15.49 ug/l	360862	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	94
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	94
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	94
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91



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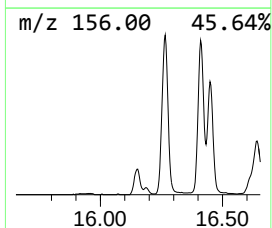
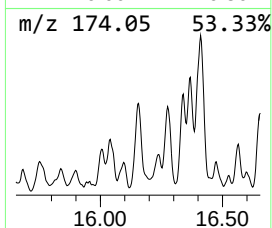
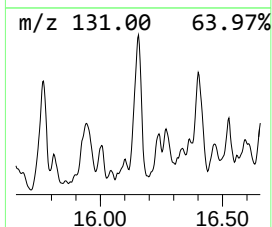
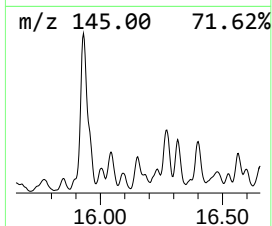
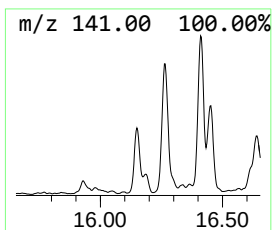
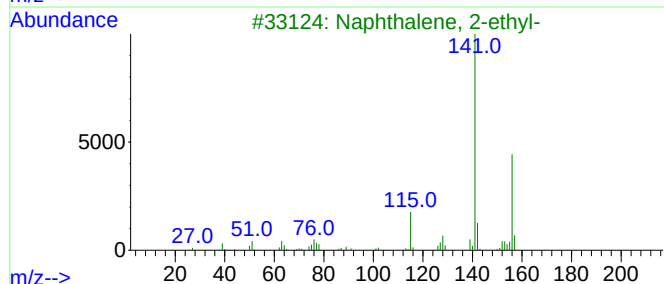
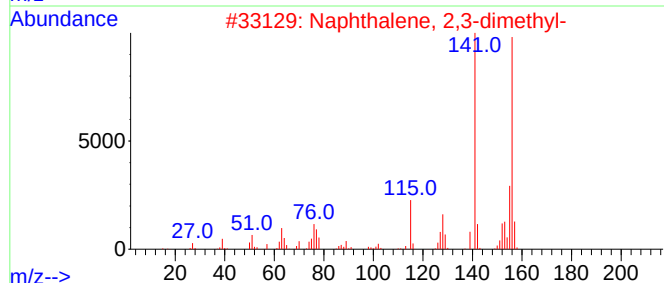
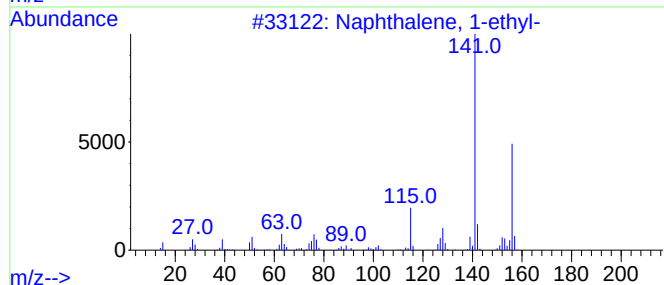
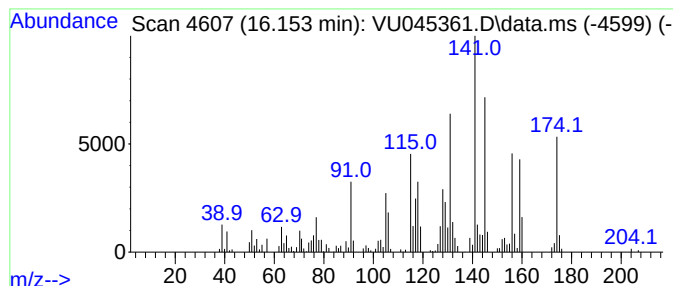
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.153 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.153	7.16 ug/l	166706	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	38
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	38
3			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	38
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	35
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

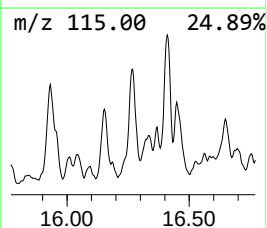
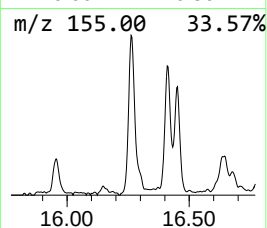
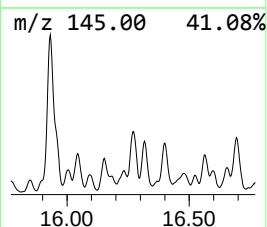
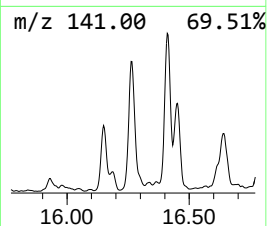
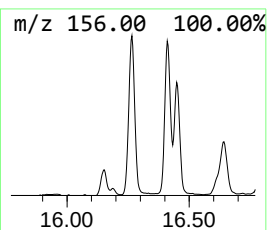
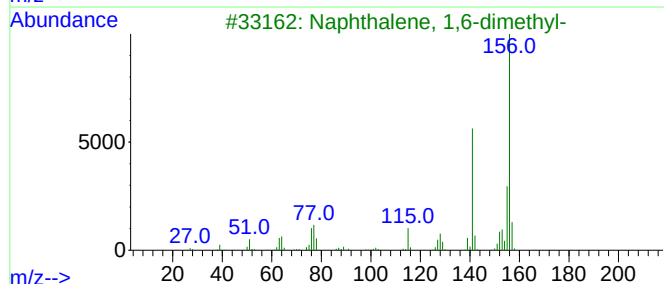
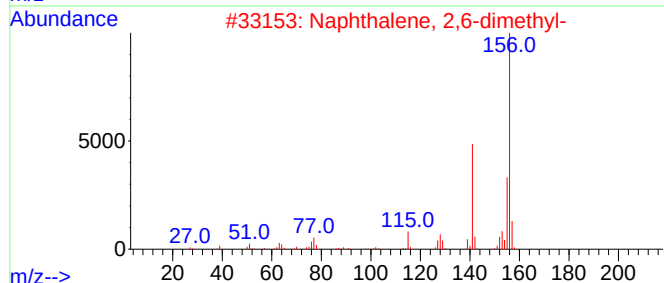
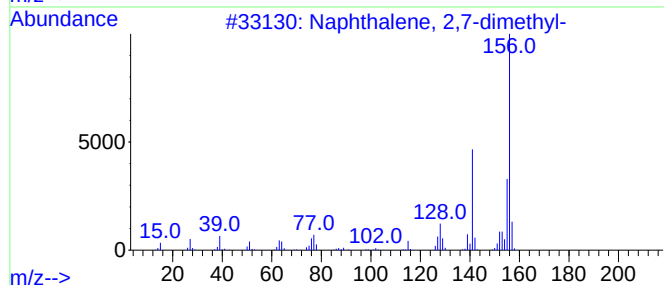
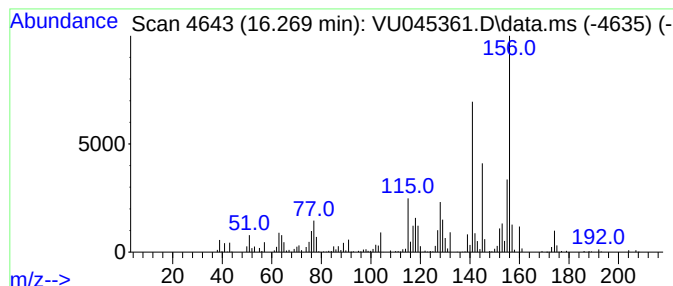
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	7.72 ug/l	179897	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	92
5			Benzene, 2,5-cyclohexadien-1-yl-	156	C12H12	004794-05-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

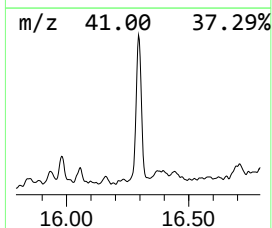
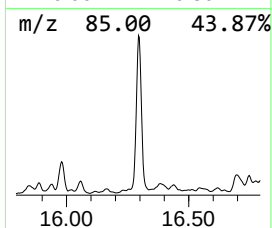
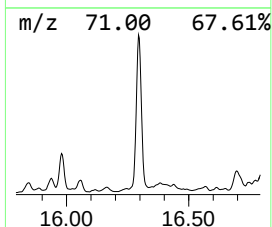
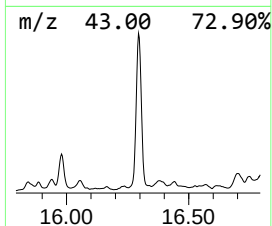
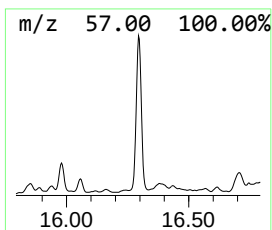
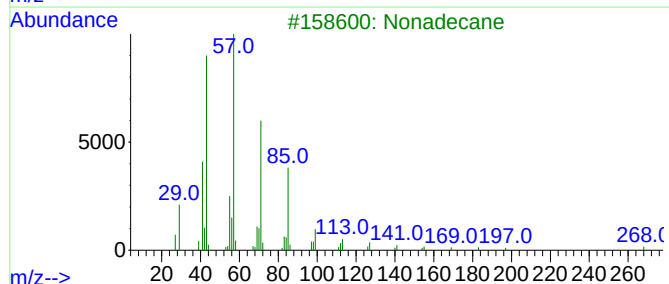
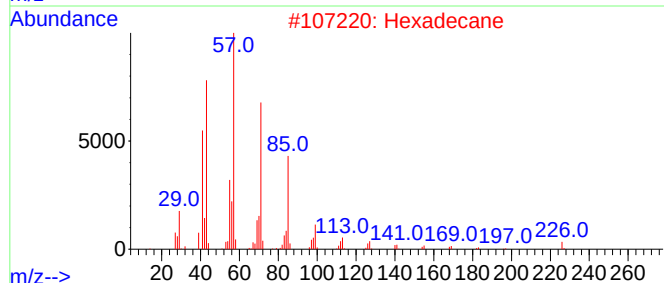
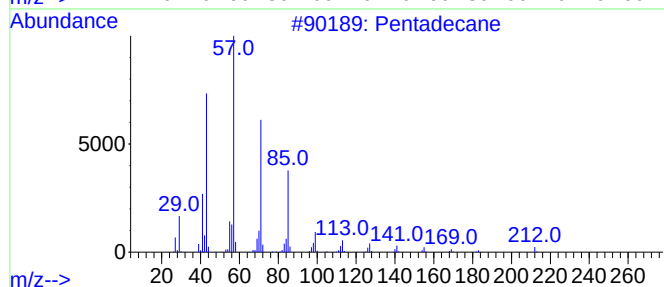
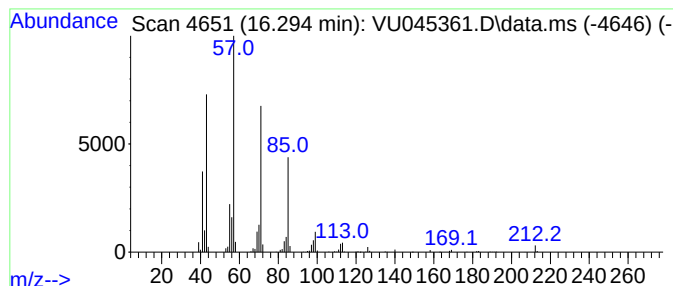
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Quant Title : SW846 8260

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

Peak Number 7 Pentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.294	16.17 ug/l	376614	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	93
2			Hexadecane	226	C16H34	000544-76-3	91
3			Nonadecane	268	C19H40	000629-92-5	91
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	86
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

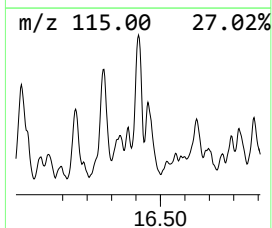
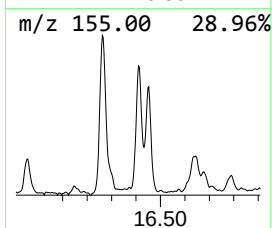
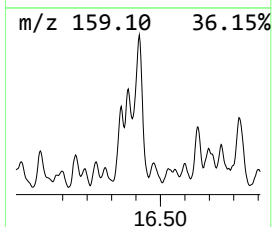
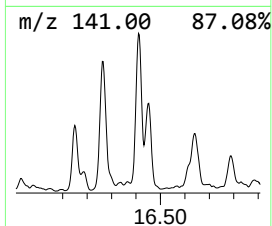
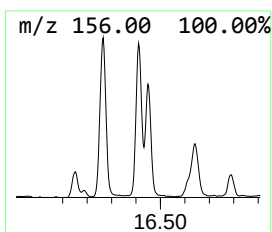
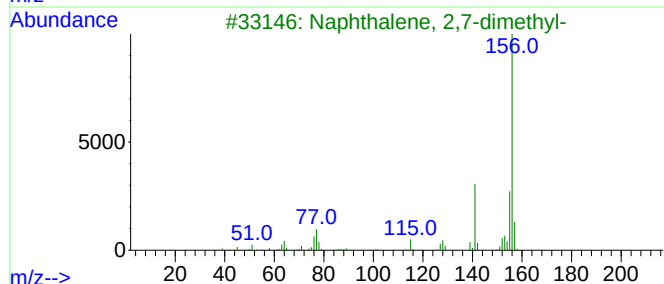
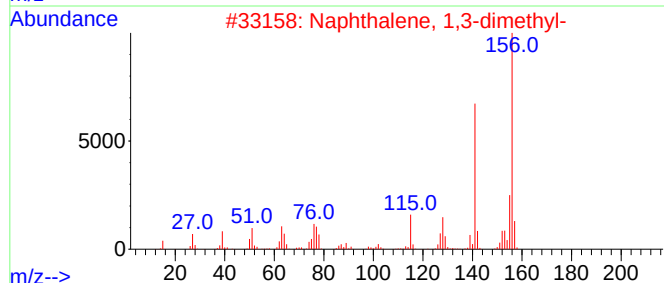
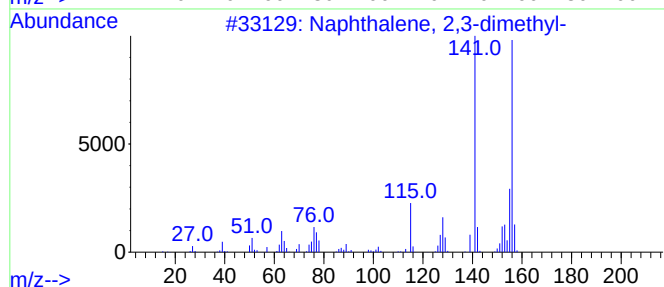
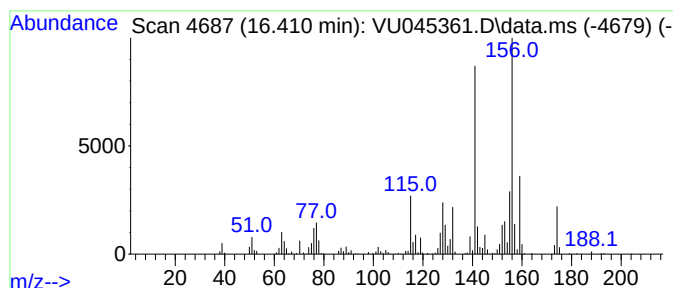
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.410	10.06 ug/l	234374	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

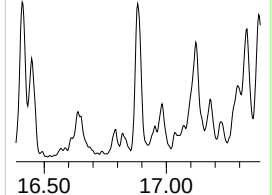
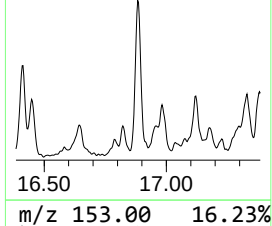
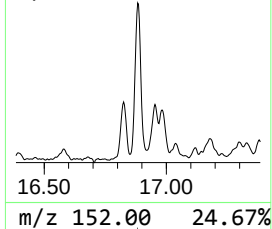
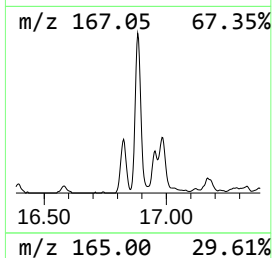
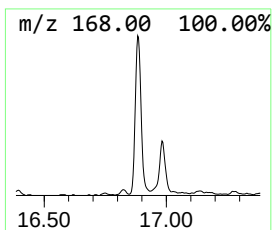
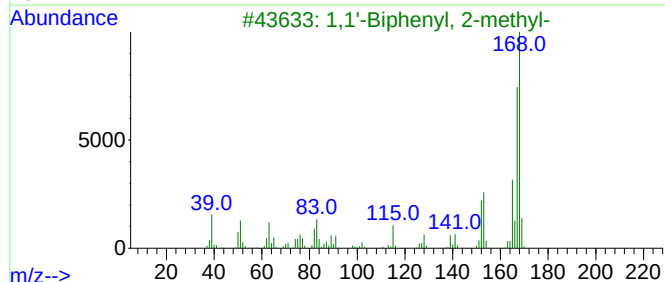
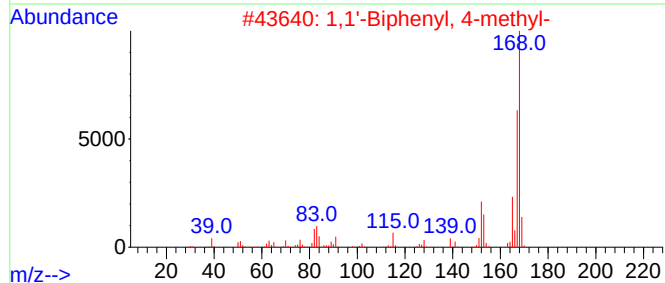
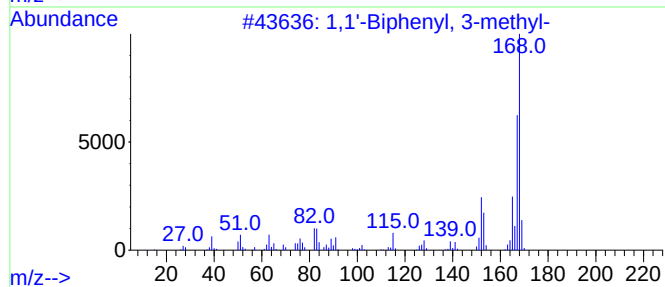
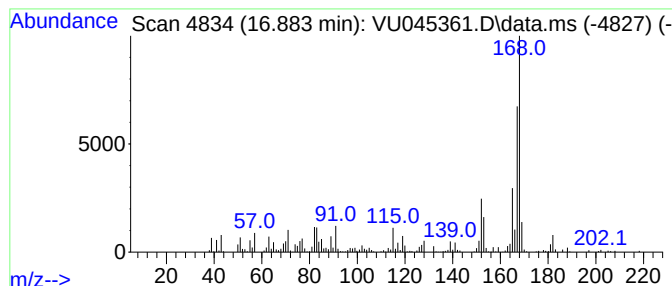
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Quant Title : SW846 8260

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

Peak Number 9 1,1'-Biphenyl, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	10.24 ug/l	238461	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	97		
2	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	96		
3	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	90		
4	Diphenylmethane	168	C13H12	000101-81-5	81		
5	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	62		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

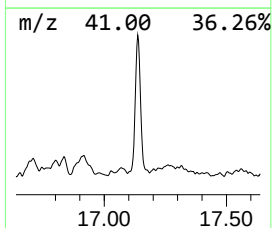
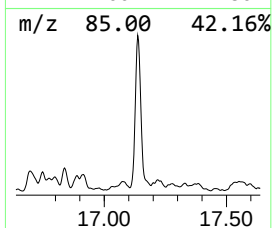
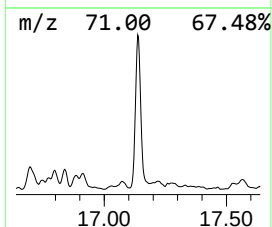
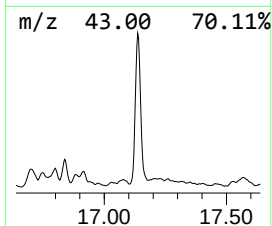
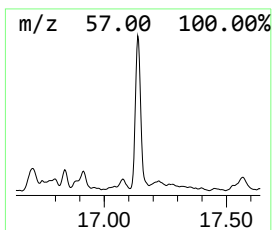
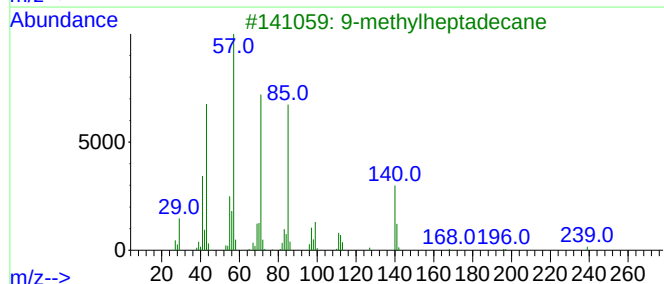
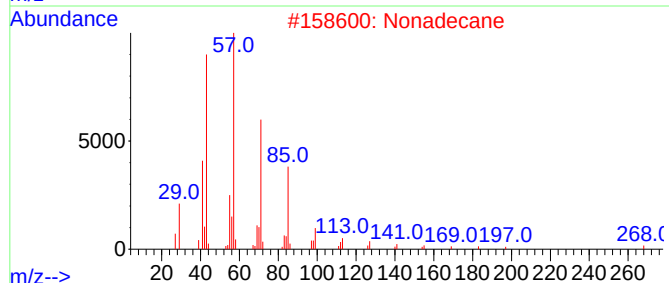
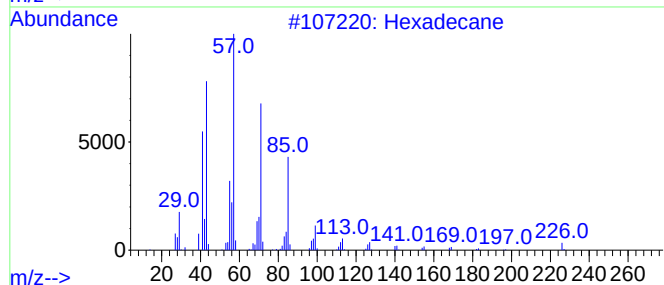
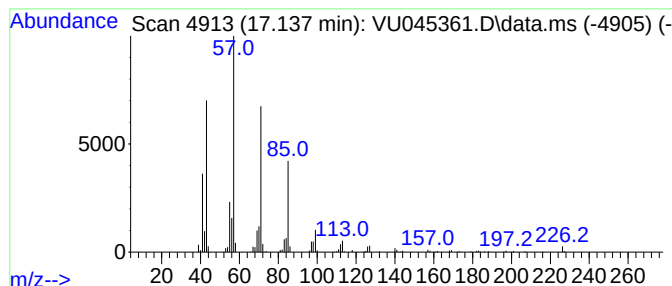
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Quant Title : SW846 8260

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

Peak Number 10 Hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.137	16.51 ug/l	384642	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	96
2			Nonadecane	268	C19H40	000629-92-5	91
3			9-methylheptadecane	254	C18H38	026741-18-4	91
4			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
5			Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045361.D
Acq On : 22 Oct 2021 13:49
Operator : SY/MD
Sample : M4288-01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SA-01-101921

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

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					#	RT	Resp	Conc
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Naphthalene, 1,...	15.204	12.4	ug/l	288168	4	11.825	1164790	50.0
Tetradecane	15.404	11.3	ug/l	262903	4	11.825	1164790	50.0
1H-Indene, 2,3-...	15.931	15.5	ug/l	360862	4	11.825	1164790	50.0
unknown16.153	16.153	7.2	ug/l	166706	4	11.825	1164790	50.0
Naphthalene, 2,...	16.269	7.7	ug/l	179897	4	11.825	1164790	50.0
Pentadecane	16.294	16.2	ug/l	376614	4	11.825	1164790	50.0
Naphthalene, 2,...	16.410	10.1	ug/l	234374	4	11.825	1164790	50.0
1,1'-Biphenyl, ...	16.883	10.2	ug/l	238461	4	11.825	1164790	50.0
Hexadecane	17.137	16.5	ug/l	384642	4	11.825	1164790	50.0