

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
 Data File : VX034342.D
 Acq On : 06 Mar 2023 12:12
 Operator : JC/MD
 Sample : 01744-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 72-11939

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_X\Method\82X021723W.M
 Title : SW846 8260

Signal : TIC: VX034342.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.618	67	87	88	rBV10	17896	81815	6.39%	0.942%
2	2.947	298	305	311	rBV2	6859	16588	1.29%	0.191%
3	5.385	692	705	719	rBV	140473	413671	32.29%	4.765%
4	5.544	720	731	746	rVB	242439	692810	54.07%	7.980%
5	5.952	787	798	812	rBV	159013	428986	33.48%	4.941%
6	6.757	919	930	946	rBV	387831	931767	72.72%	10.733%
7	8.647	1233	1240	1254	rBV	812845	1281239	100.00%	14.758%
8	10.055	1465	1471	1484	rBV	767694	1068890	83.43%	12.312%
9	11.085	1634	1640	1654	rBV	612925	832004	64.94%	9.584%
10	12.024	1788	1794	1805	rBV	824850	1039151	81.11%	11.970%
11	13.774	2075	2081	2089	rBV	196656	248674	19.41%	2.864%
12	14.640	2218	2223	2234	rVB	227953	299513	23.38%	3.450%
13	14.780	2241	2246	2254	rVB	144051	180007	14.05%	2.073%
14	15.207	2309	2316	2321	rBV	60658	81586	6.37%	0.940%
15	15.377	2336	2344	2347	rBV	26455	42461	3.31%	0.489%
16	15.475	2354	2360	2370	rVB	63573	111378	8.69%	1.283%
17	15.615	2374	2383	2386	rBV	70999	116335	9.08%	1.340%
18	15.652	2386	2389	2396	rVB	40750	59988	4.68%	0.691%
19	15.835	2410	2419	2430	rVB2	22267	56041	4.37%	0.646%
20	15.987	2437	2444	2451	rBV	9178	17263	1.35%	0.199%
21	16.091	2454	2461	2467	rBV	24616	41566	3.24%	0.479%
22	16.194	2473	2478	2485	rVB3	7275	13033	1.02%	0.150%
23	16.328	2491	2500	2510	rBV	223094	421412	32.89%	4.854%
24	16.530	2528	2533	2539	rBV3	8614	19209	1.50%	0.221%
25	16.597	2539	2544	2549	rVV4	9049	16944	1.32%	0.195%
26	16.688	2549	2559	2573	rVB	72850	169101	13.20%	1.948%

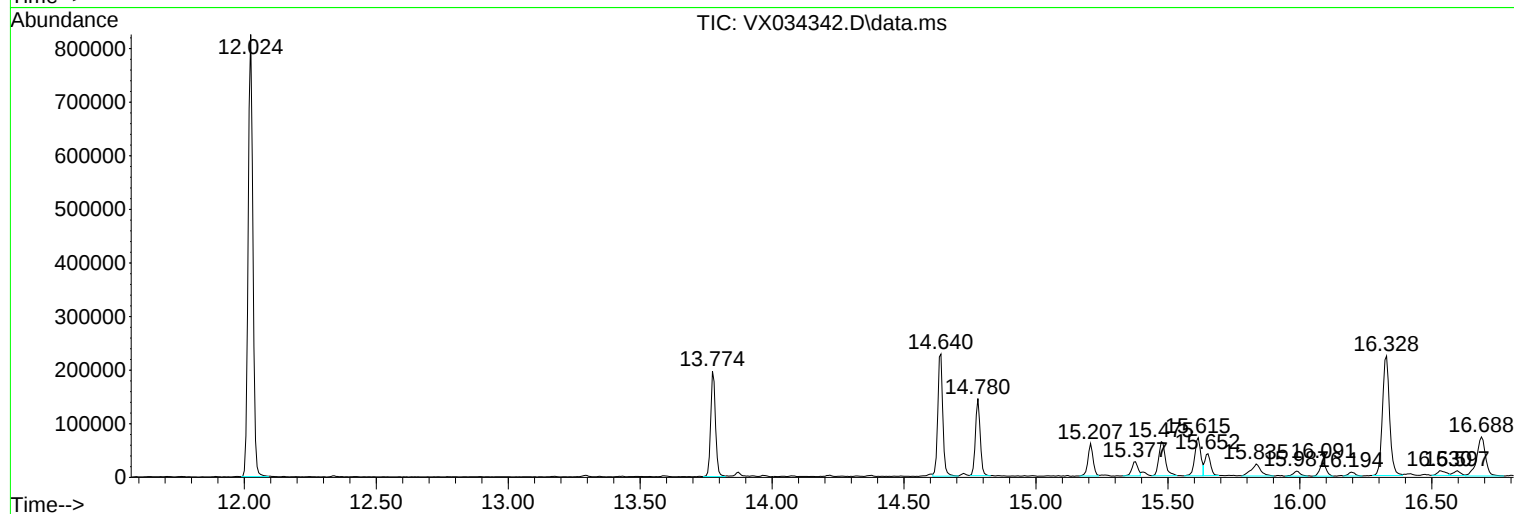
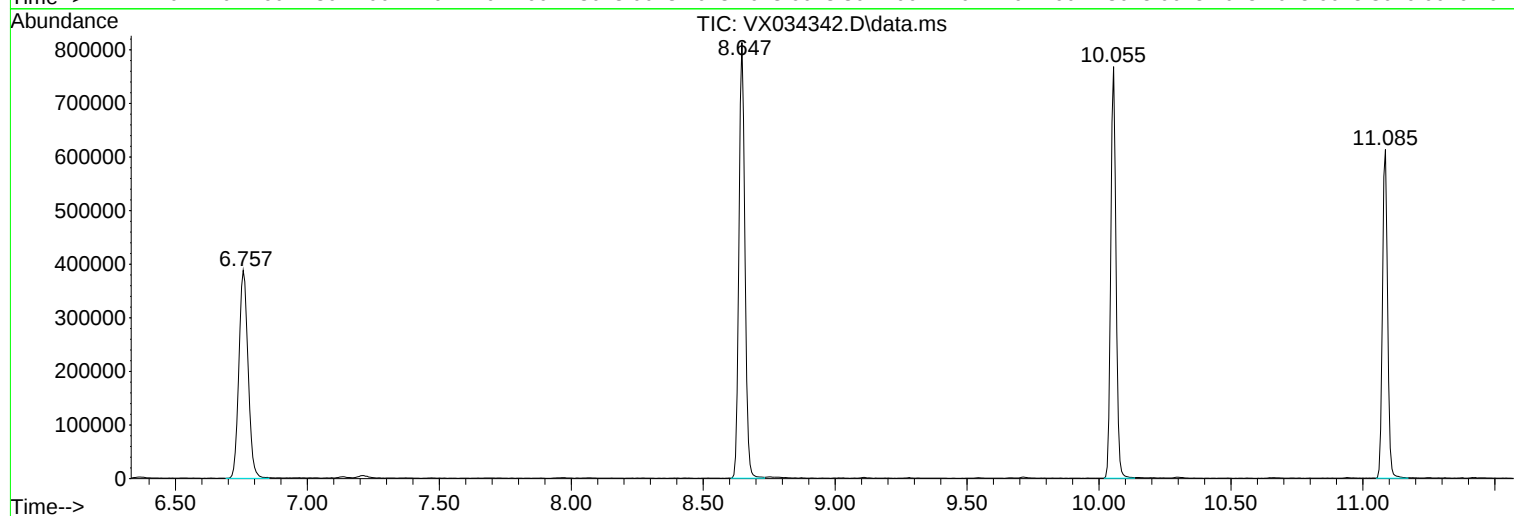
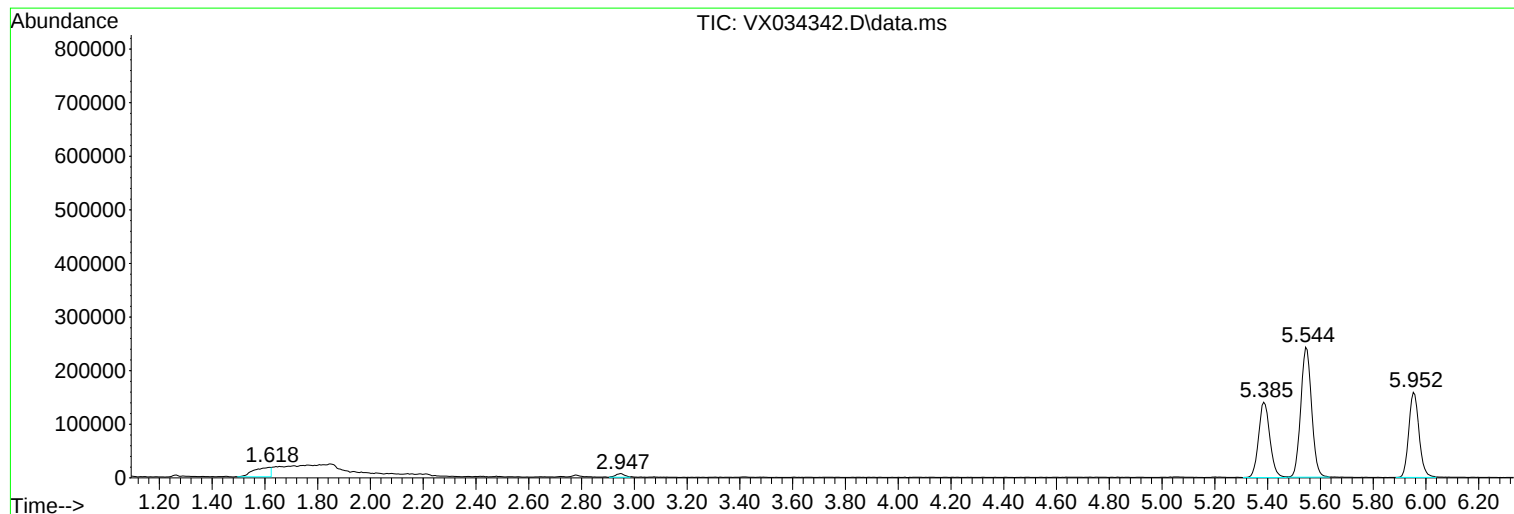
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Instrument :
MSVOA_X
ClientSampleId :
72-11939

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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



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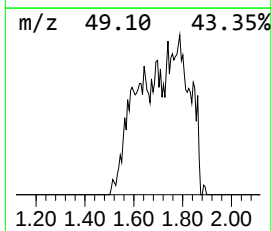
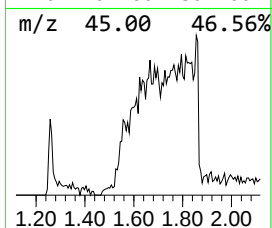
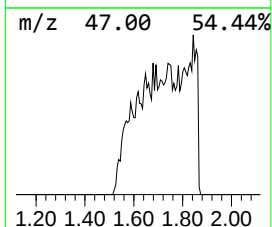
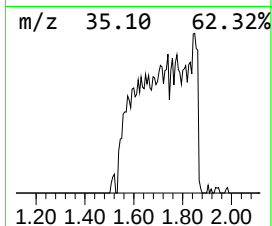
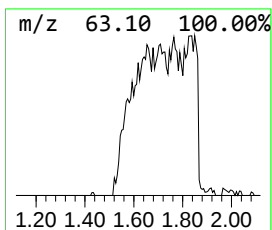
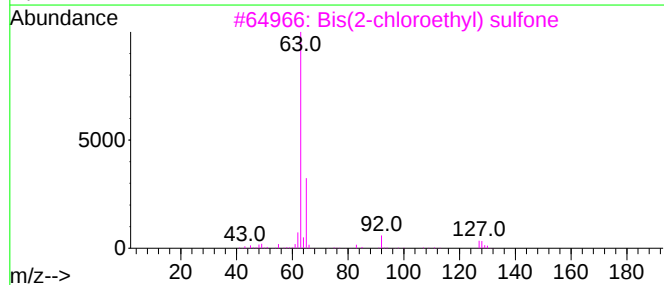
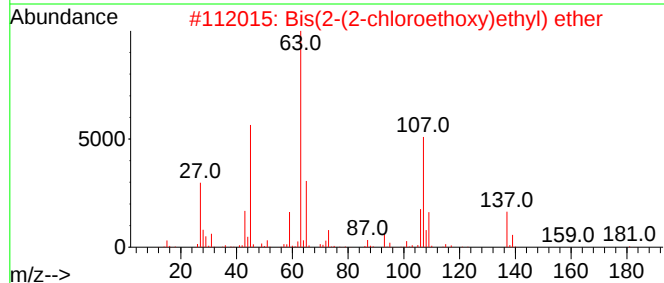
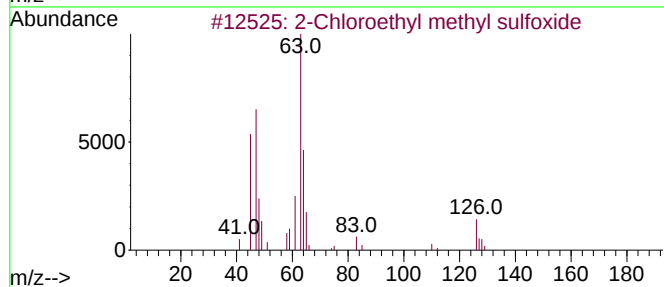
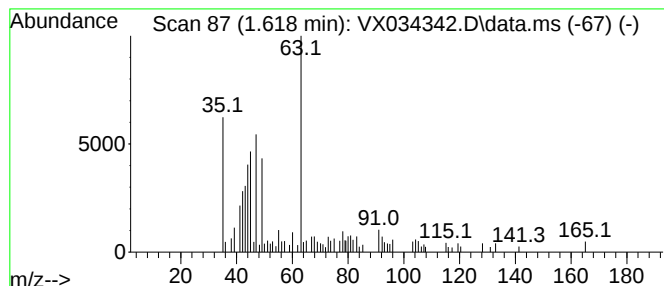
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.168 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.618	5.90 ug/l	81815	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	33
2		Bis(2-(2-chloroethoxy)ethyl) ether	230	C8H16Cl2O3	000638-56-2	25
3		Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	23
4		Silane, bis(fluoromethyl)dimethyl-	124	C4H10F2Si	065864-63-3	16
5		(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	9



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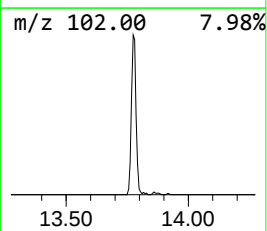
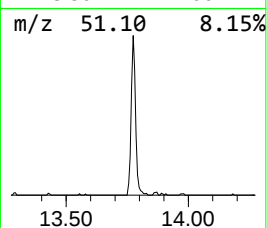
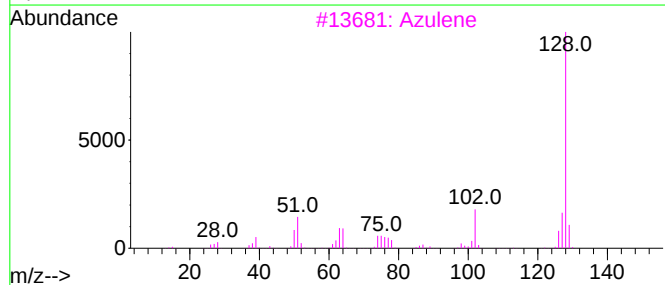
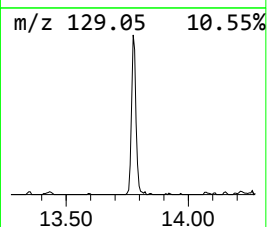
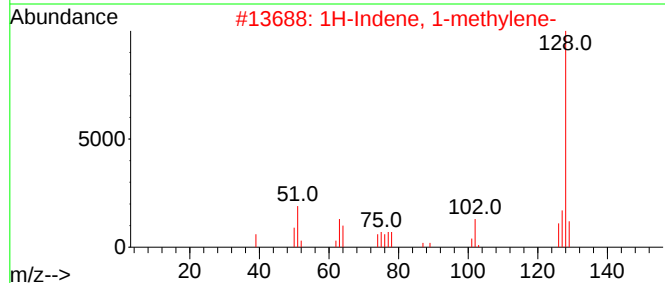
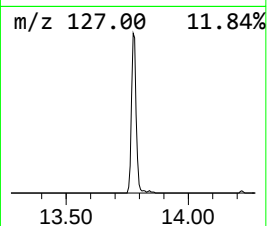
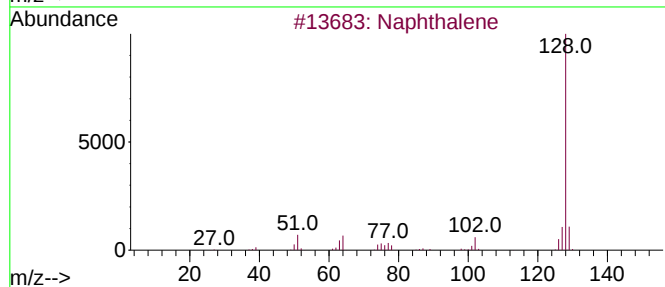
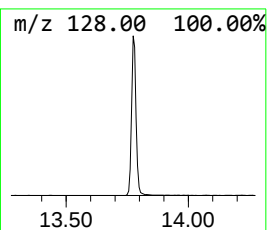
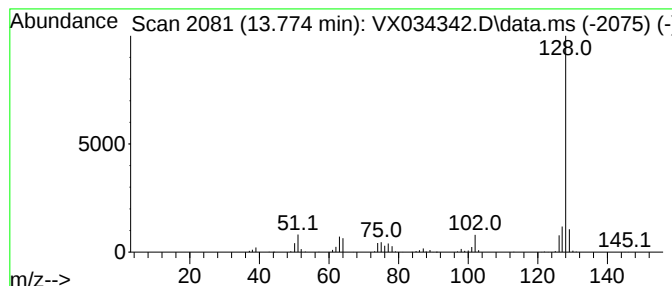
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 2 1H-Indene, 1-methylene- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	11.97 ug/l	248674	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	94
3			Azulene	128	C10H8	000275-51-4	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
5			1,2-Benzenedicarbonitrile	128	C8H4N2	000091-15-6	53



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Instrument :
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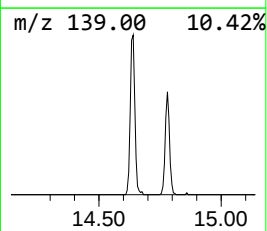
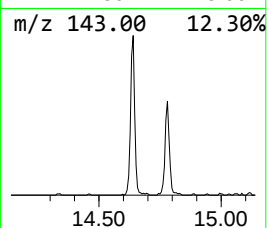
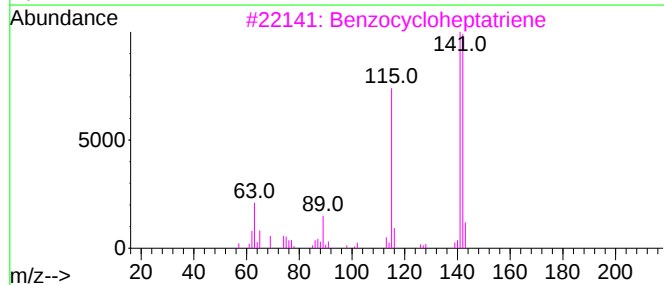
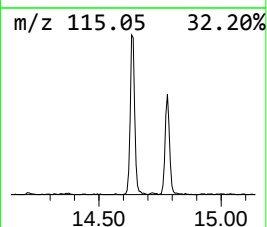
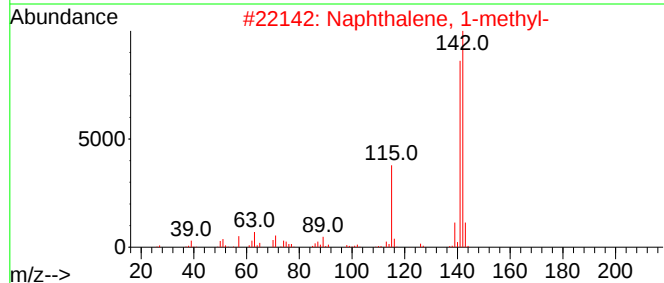
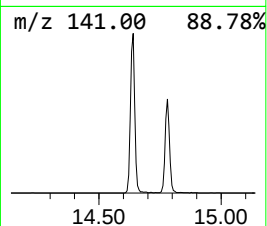
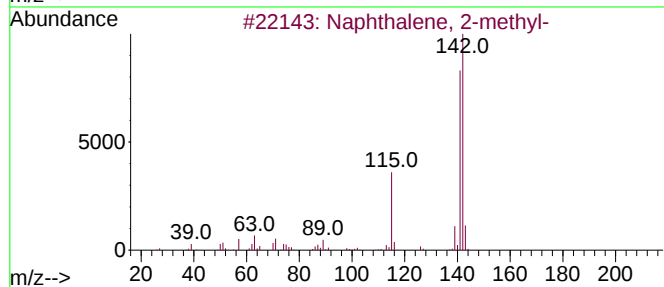
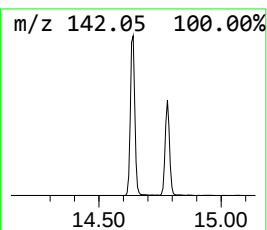
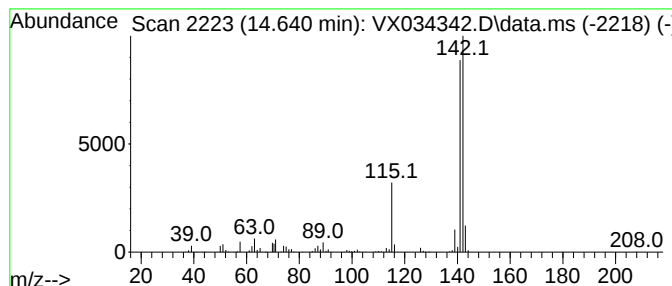
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	14.41 ug/l	299513	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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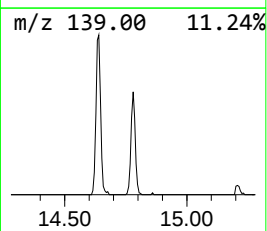
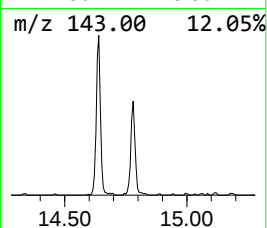
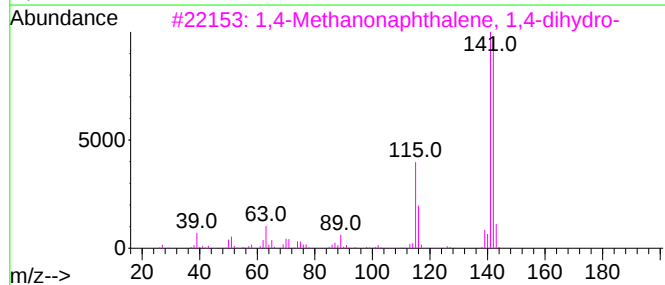
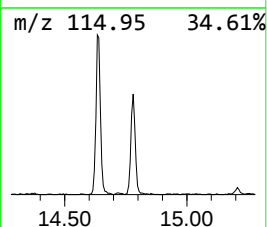
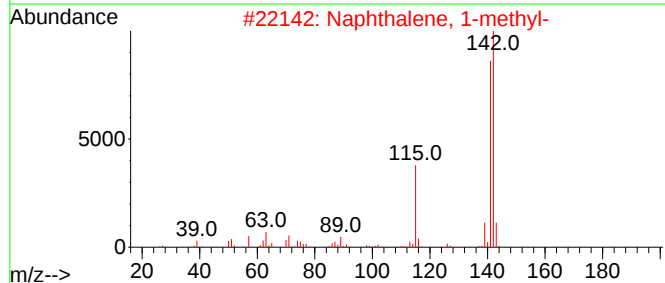
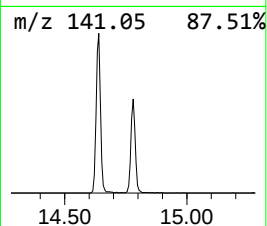
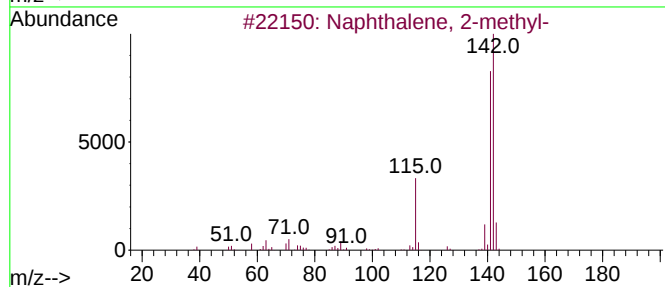
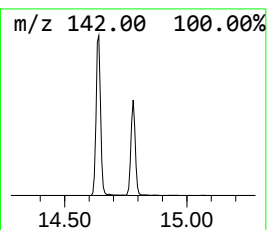
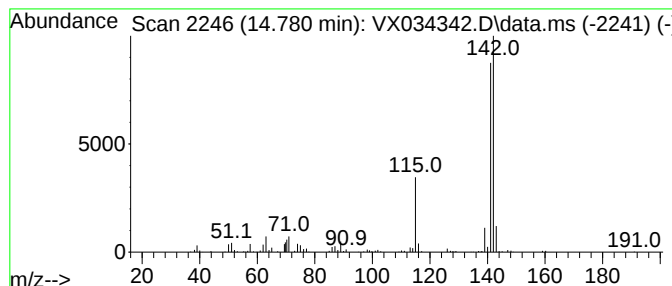
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	8.66 ug/l	180007	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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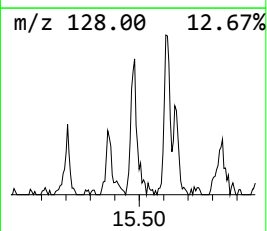
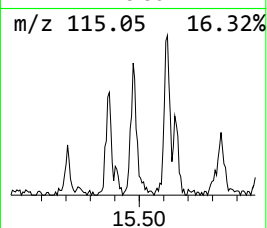
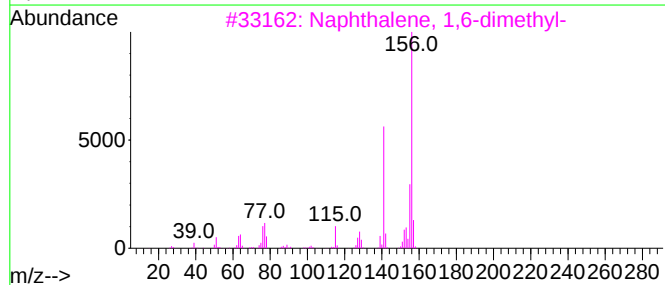
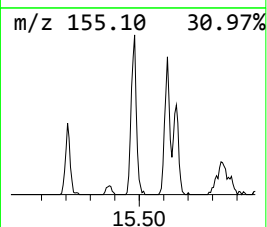
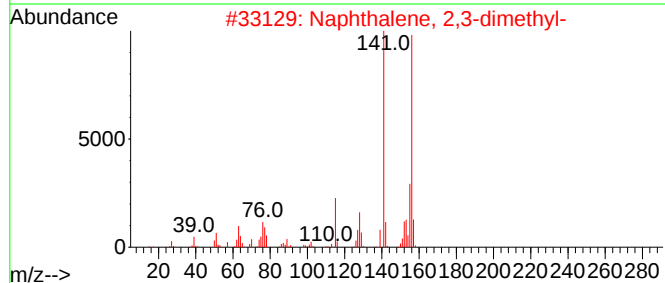
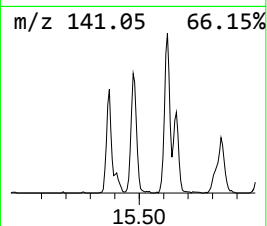
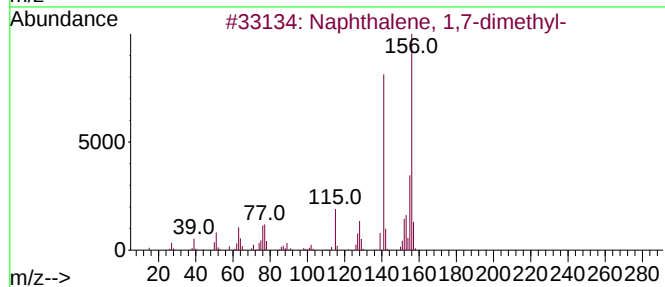
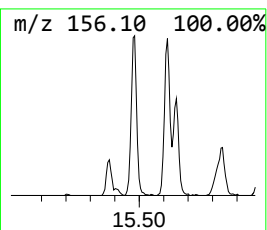
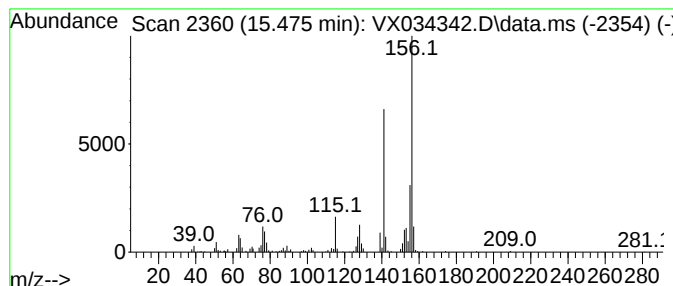
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,7-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	5.36 ug/l	111378	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96



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72-11939

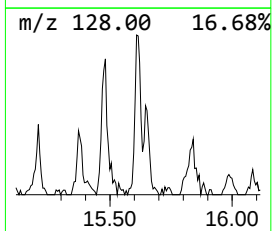
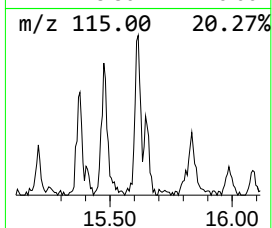
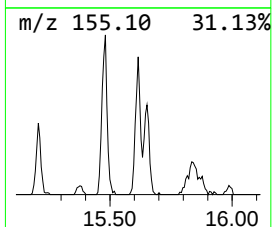
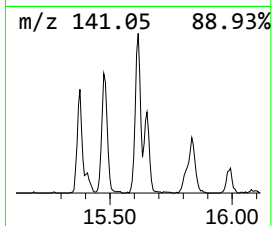
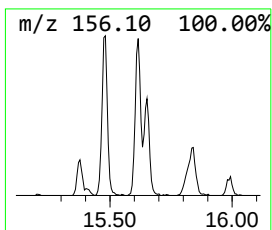
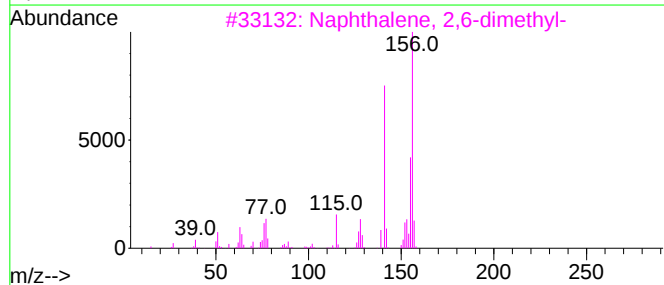
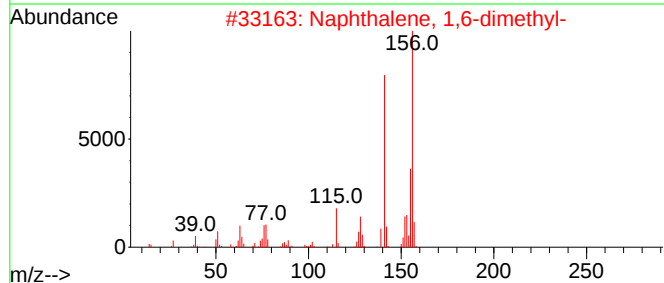
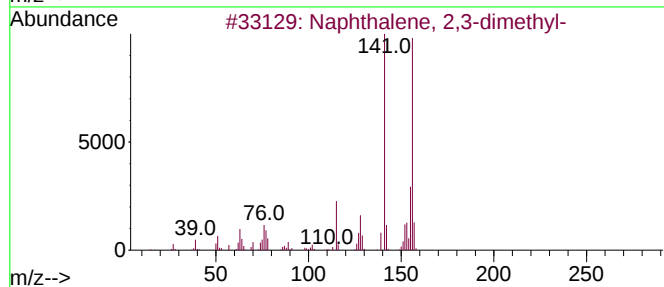
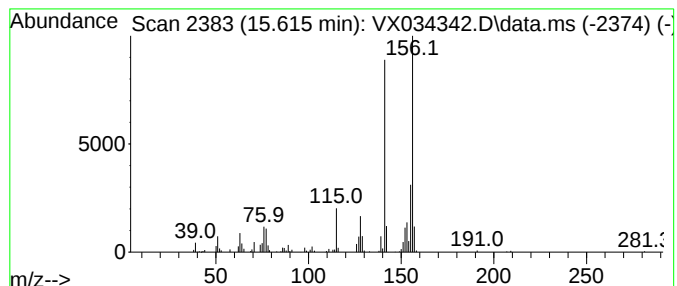
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.60 ug/l	116335	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034342.D
Acq On : 06 Mar 2023 12:12
Operator : JC/MD
Sample : 01744-01
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-11939

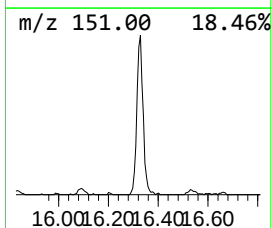
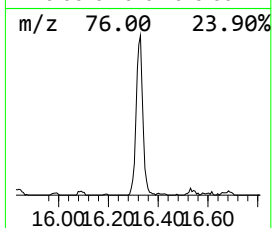
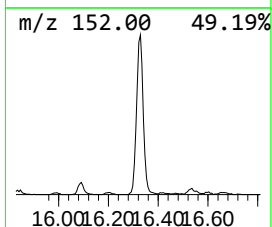
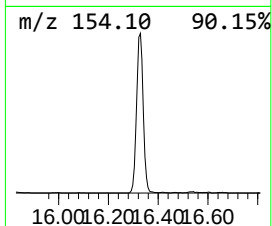
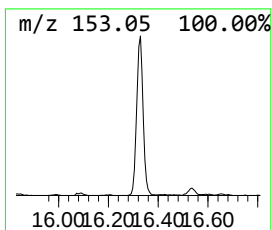
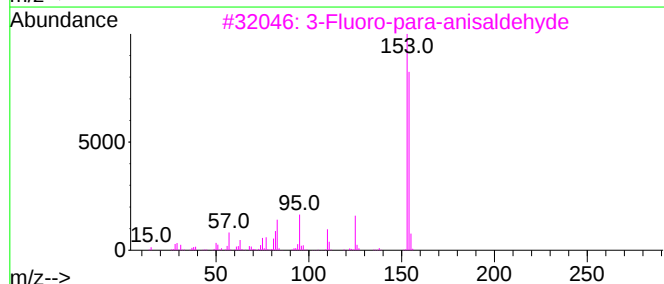
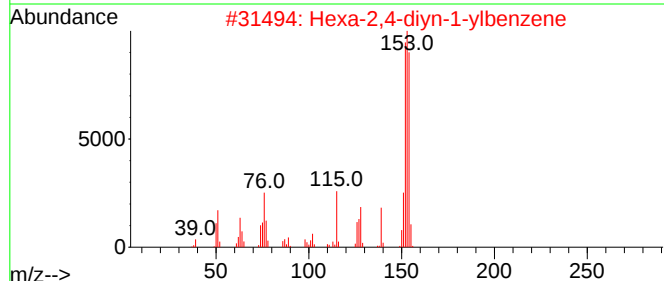
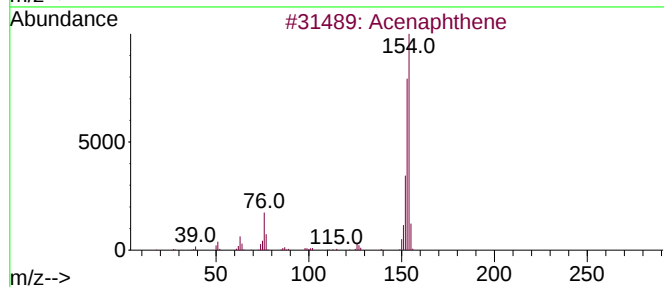
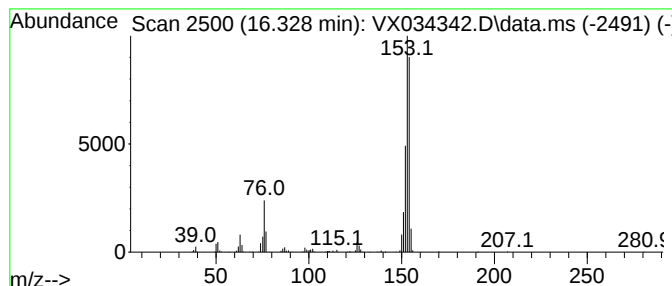
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Quant Title : SW846 8260

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

Peak Number 7 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	20.28 ug/l	421412	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
4			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	47
5			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034342.D
Acq On : 06 Mar 2023 12:12
Operator : JC/MD
Sample : 01744-01
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-11939

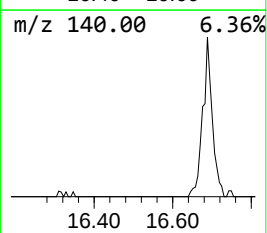
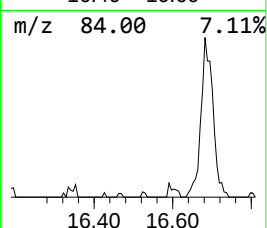
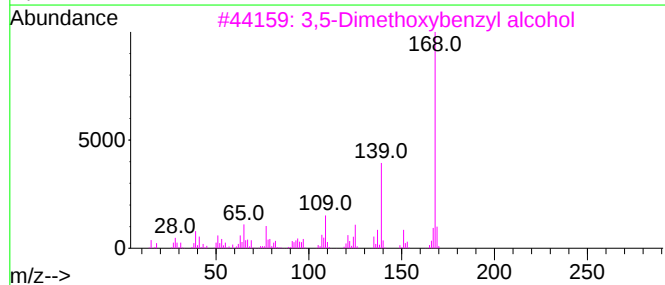
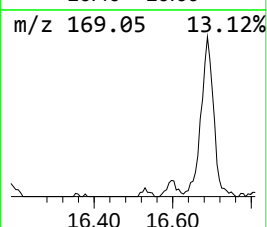
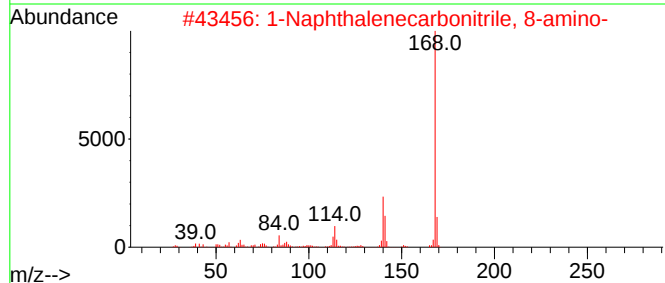
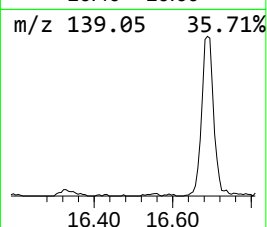
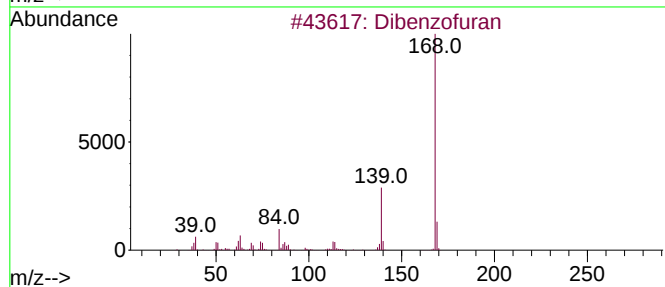
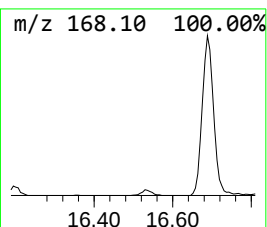
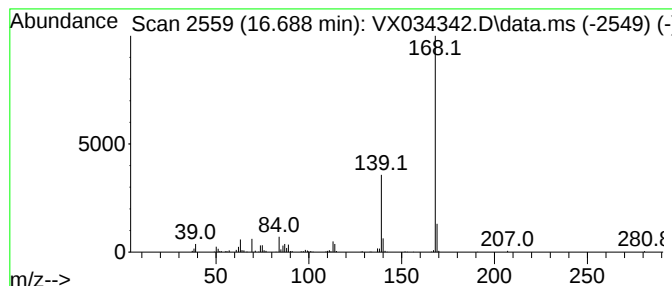
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Naphthalenecarbonitrile, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.688	8.14 ug/l	169101	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzofuran	168	C12H8O	000132-64-9	91
2			1-Naphthalenecarbonitrile, 8-amino-	168	C11H8N2	038515-13-8	59
3			3,5-Dimethoxybenzyl alcohol	168	C9H12O3	000705-76-0	50
4			3,6-Diazahomoadamantan-9-ol	168	C9H16N2O	138023-21-9	47
5			1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034342.D
Acq On : 06 Mar 2023 12:12
Operator : JC/MD
Sample : 01744-01
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-11939

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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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1H-Indene, 1-me...	13.774	12.0	ug/l	248674	4	12.024	1039150	50.0
Benzocyclohepta...	14.640	14.4	ug/l	299513	4	12.024	1039150	50.0
1,4-Methanonaph...	14.780	8.7	ug/l	180007	4	12.024	1039150	50.0
Naphthalene, 1,...	15.475	5.4	ug/l	111378	4	12.024	1039150	50.0
Naphthalene, 2,...	15.615	5.6	ug/l	116335	4	12.024	1039150	50.0
Hexa-2,4-diyne-1...	16.328	20.3	ug/l	421412	4	12.024	1039150	50.0
1-Naphthaleneca...	16.688	8.1	ug/l	169101	4	12.024	1039150	50.0