

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101818\
 Data File : VX005423.D
 Acq On : 18 Oct 2018 12:10
 Operator : JC/MD
 Sample : J5573-01
 Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 0689-KM-CA-COMP

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.666	63	84	87	rBV4	34722	160025	11.84%	1.338%
2	5.501	699	713	727	rBV	141735	418963	30.99%	3.504%
3	5.659	727	739	756	rBV	269273	774894	57.32%	6.480%
4	6.068	793	806	819	rBV	160660	435350	32.21%	3.641%
5	6.860	925	936	964	rBV	376947	962329	71.19%	8.048%
6	8.714	1234	1240	1255	rBV	817409	1351773	100.00%	11.304%
7	10.116	1464	1470	1483	rBV	814809	1160887	85.88%	9.708%
8	11.140	1633	1638	1652	rVB	741384	981597	72.62%	8.209%
9	11.628	1714	1718	1720	rBV	27682	42360	3.13%	0.354%
10	12.079	1788	1792	1801	rVB	1030639	1275749	94.38%	10.669%
11	12.816	1909	1913	1919	rVB	51035	69728	5.16%	0.583%
12	13.115	1958	1962	1965	rBV5	28971	52014	3.85%	0.435%
13	13.353	1998	2001	2002	rBV3	17951	19266	1.43%	0.161%
14	13.408	2003	2010	2011	rBV2	59104	111100	8.22%	0.929%
15	13.902	2087	2091	2097	rVB3	37233	61263	4.53%	0.512%
16	14.542	2193	2196	2199	rBV3	17173	22705	1.68%	0.190%
17	14.670	2214	2217	2220	rBV2	64987	86996	6.44%	0.728%
18	14.841	2242	2245	2250	rVB	72036	91269	6.75%	0.763%
19	14.908	2253	2256	2263	rVB9	24791	36549	2.70%	0.306%
20	15.023	2272	2275	2284	rVB6	36877	63077	4.67%	0.527%
21	15.249	2308	2312	2313	rBV2	35463	42167	3.12%	0.353%
22	15.279	2313	2317	2320	rVB	88827	118446	8.76%	0.991%
23	15.444	2340	2344	2347	rBV	71740	98096	7.26%	0.820%
24	15.487	2347	2351	2356	rVB3	49049	81361	6.02%	0.680%
25	15.548	2356	2361	2368	rBV	298821	465724	34.45%	3.895%
26	15.688	2379	2384	2387	rBV	313389	464227	34.34%	3.882%
27	15.724	2387	2390	2399	rVB	180302	288099	21.31%	2.409%
28	15.822	2403	2406	2412	rVB5	36769	52816	3.91%	0.442%
29	15.913	2414	2421	2432	rVB	100567	261341	19.33%	2.186%
30	16.072	2443	2447	2451	rVB	54092	79182	5.86%	0.662%
31	16.170	2458	2463	2469	rBV	65907	111699	8.26%	0.934%
32	16.279	2478	2481	2487	rVB2	61066	94657	7.00%	0.792%
33	16.352	2489	2493	2495	rBV	39041	65048	4.81%	0.544%
34	16.444	2503	2508	2516	rVB	203042	360049	26.64%	3.011%

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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

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Title : SW846 8260

35	16.511	2516	2519	2524	rVB	39736	59697	4.42%	0.499%
36	16.566	2524	2528	2534	rVB	60077	103003	7.62%	0.861%
37	16.657	2538	2543	2544	rBV4	70899	114937	8.50%	0.961%
38	16.694	2544	2549	2554	rVV	247410	450086	33.30%	3.764%
39	16.749	2554	2558	2564	rVV	269648	469360	34.72%	3.925%

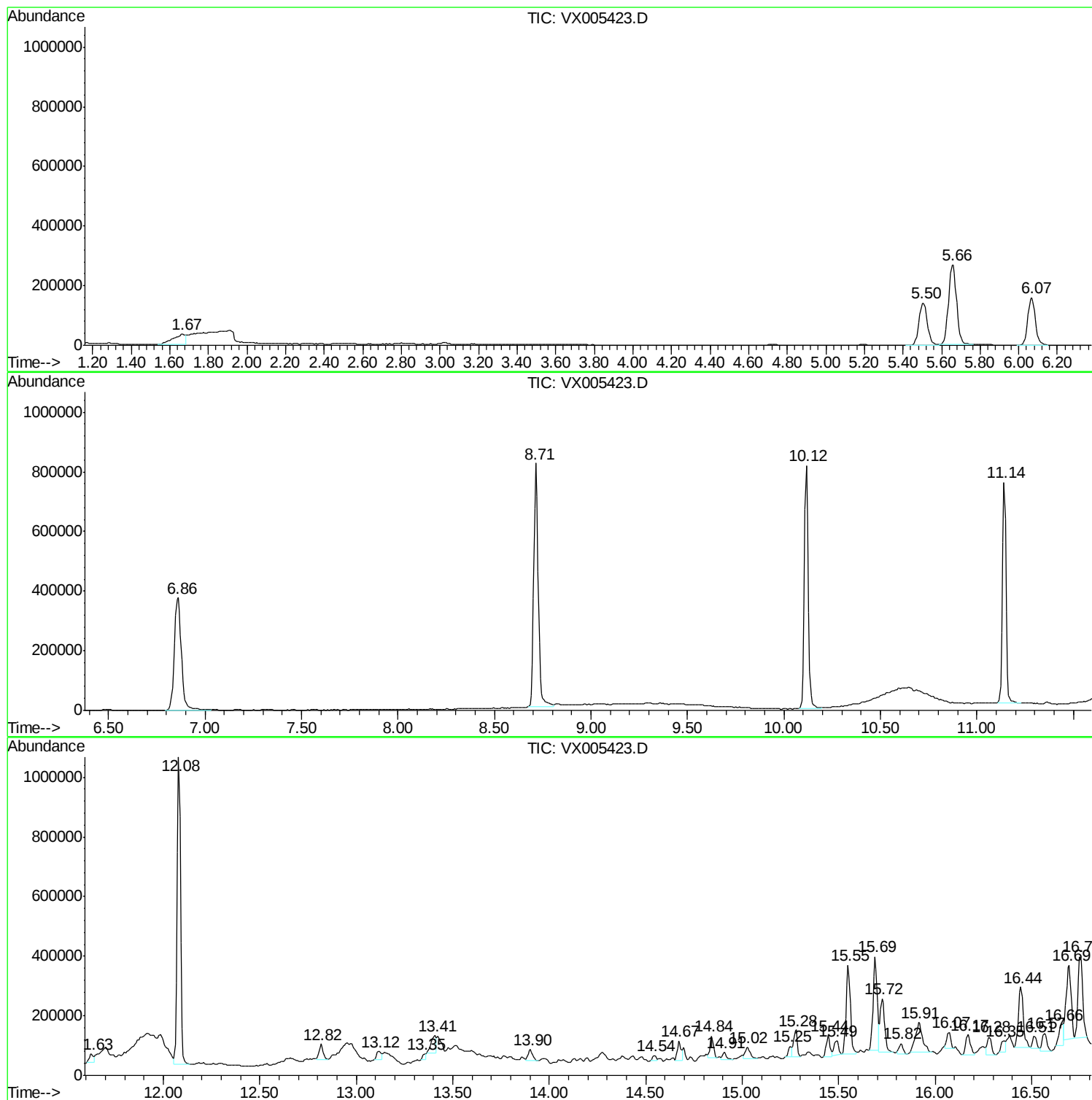
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Quant Title : SW846 8260

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



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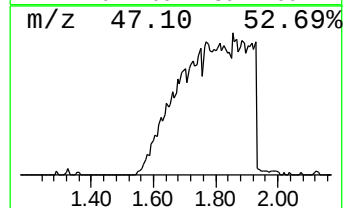
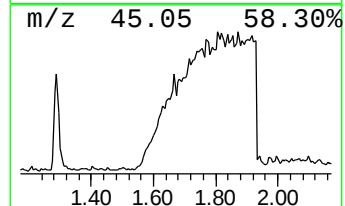
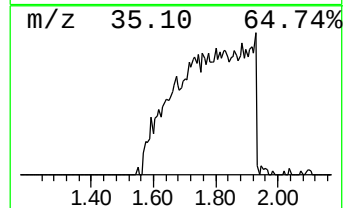
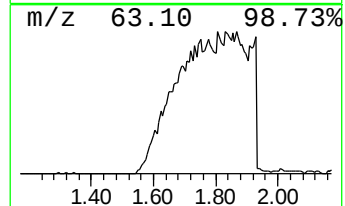
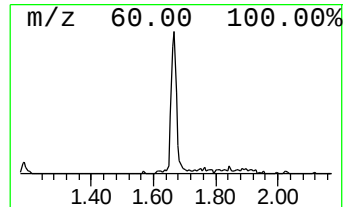
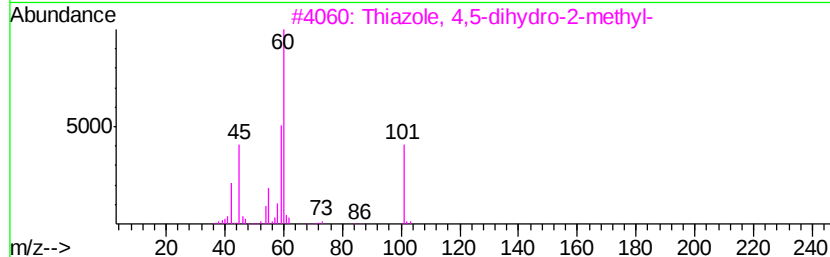
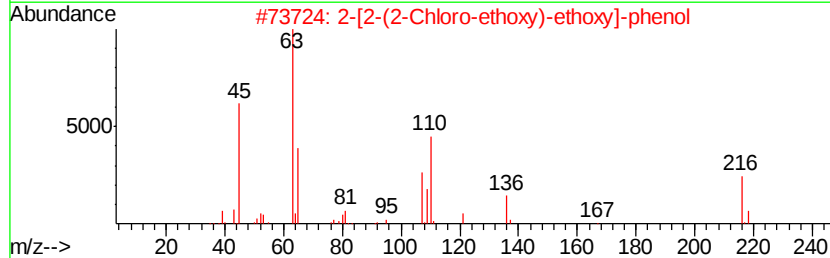
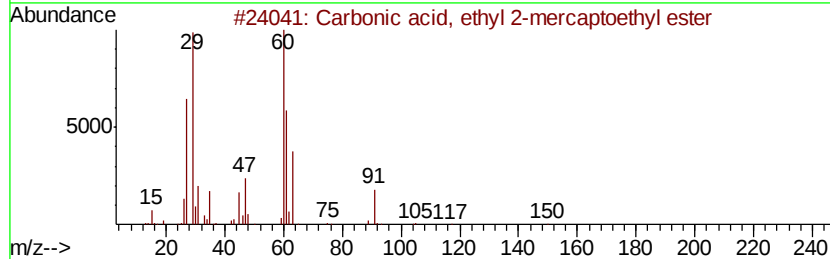
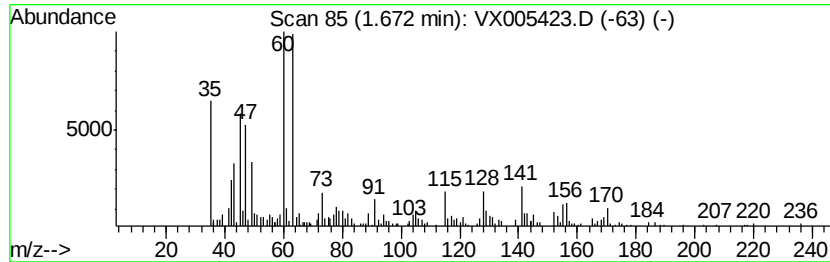
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.67 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	10.33 ug/l	160025	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, ethyl 2-mercaptoe...	150	C5H10O3S	005628-96-6	37
2		2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	12
3		Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	10
4		Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	10
5		2-(p-Nitrophenyl)-1,3-propanediol	197	C9H11NO4	091748-03-7	9



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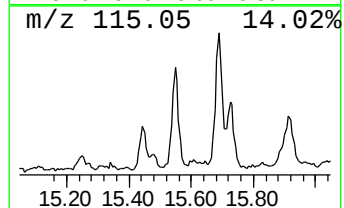
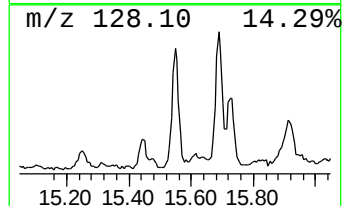
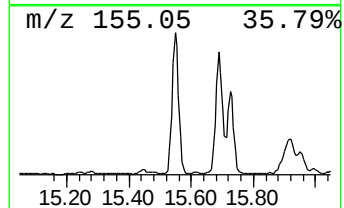
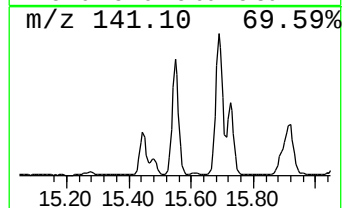
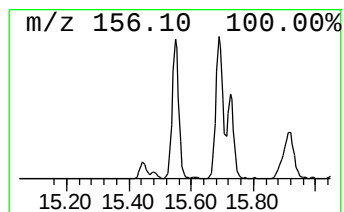
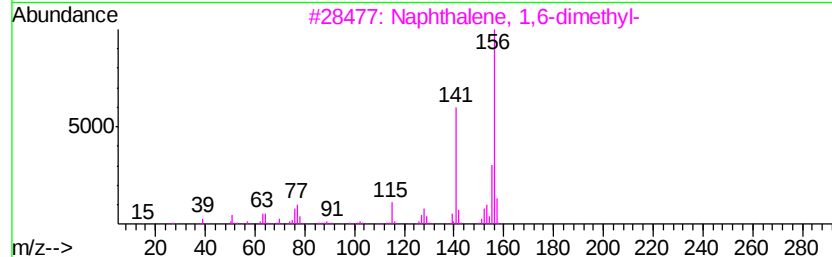
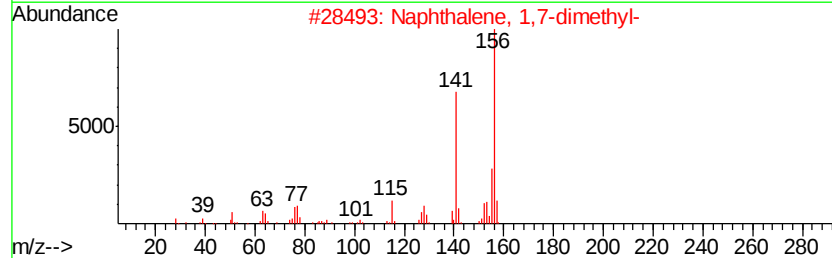
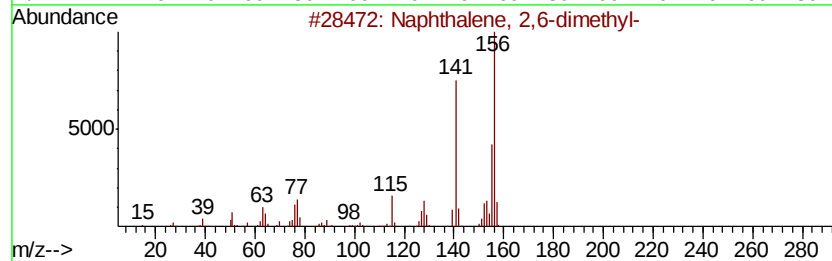
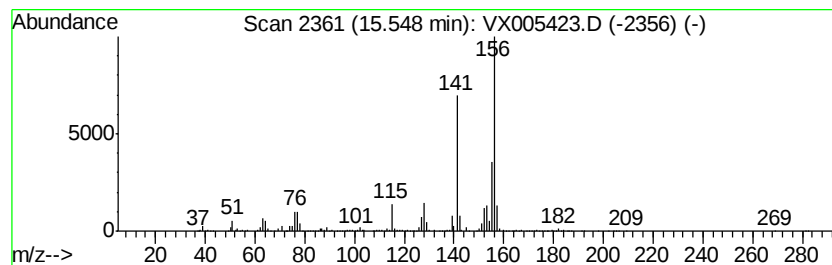
Instrument :
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	18.25 ug/l	465724	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 98
2		Naphthalene, 1,7-dimethyl-	156 C12H12	000575-37-1 97
3		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 97
4		Naphthalene, 2,7-dimethyl-	156 C12H12	000582-16-1 97
5		Naphthalene, 2,3-dimethyl-	156 C12H12	000581-40-8 97



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ALS Vial : 7 Sample Multiplier: 1

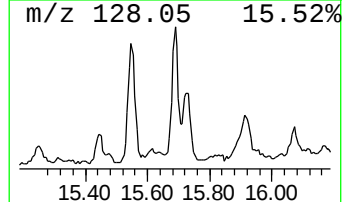
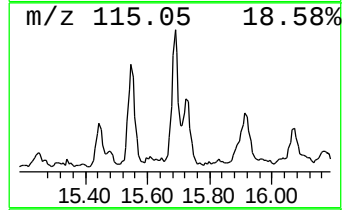
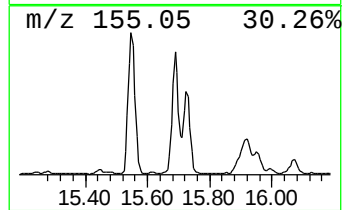
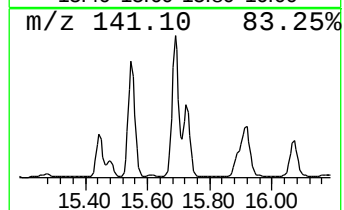
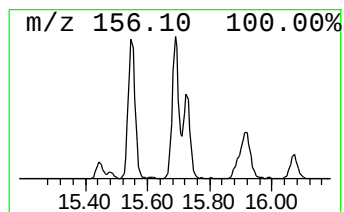
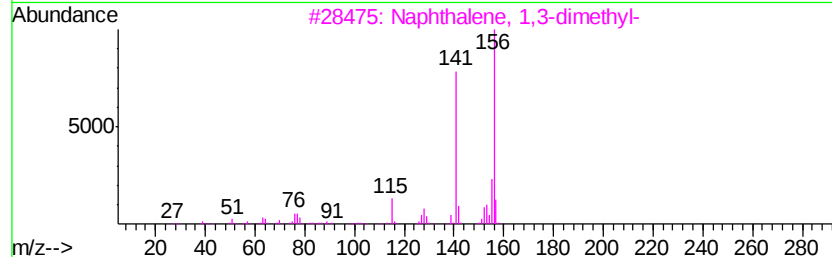
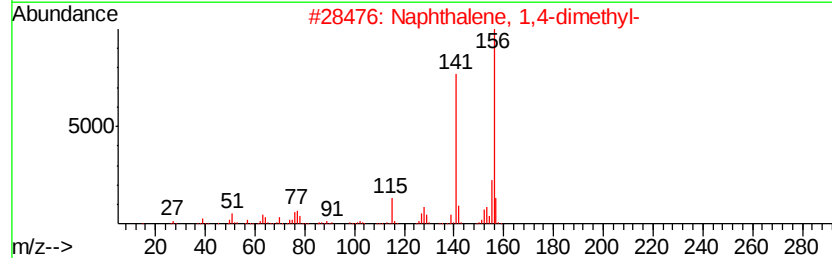
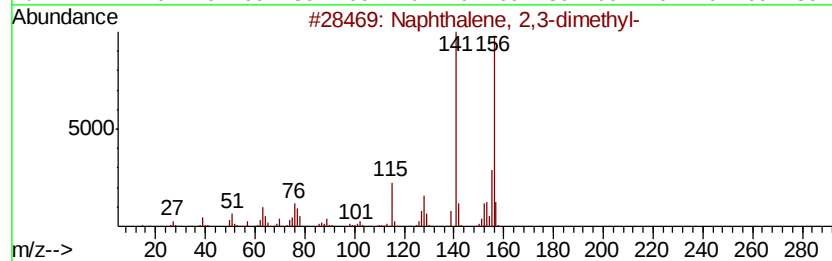
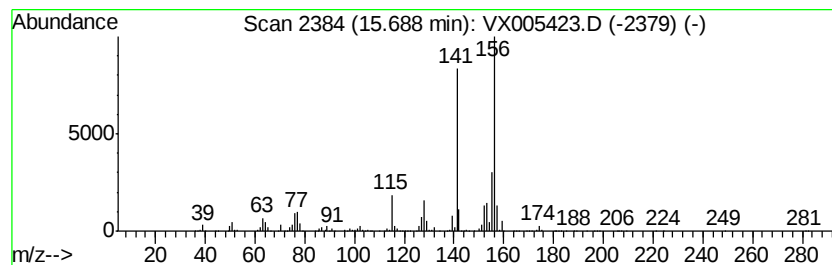
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.69	18.19 ug/l	464227	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97



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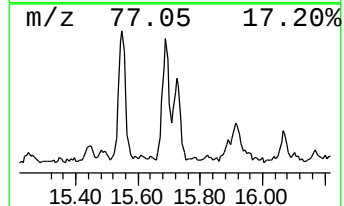
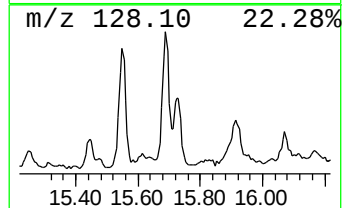
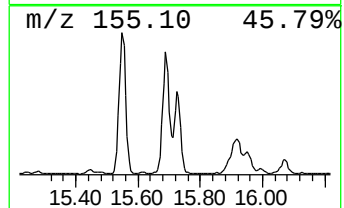
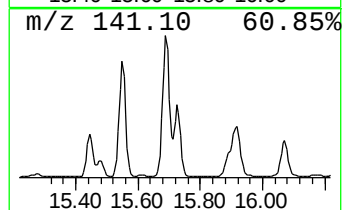
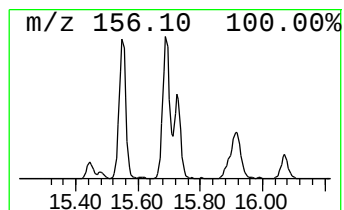
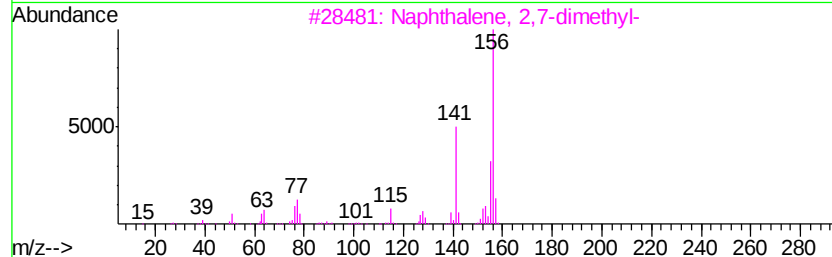
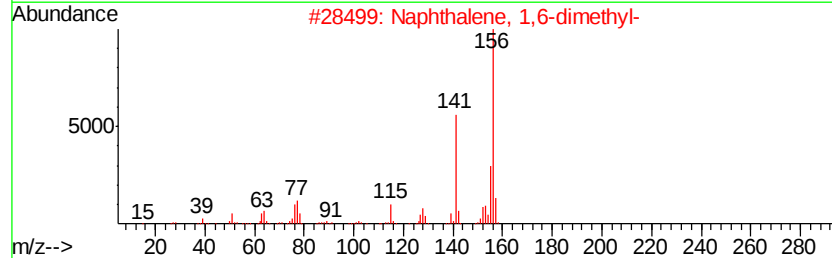
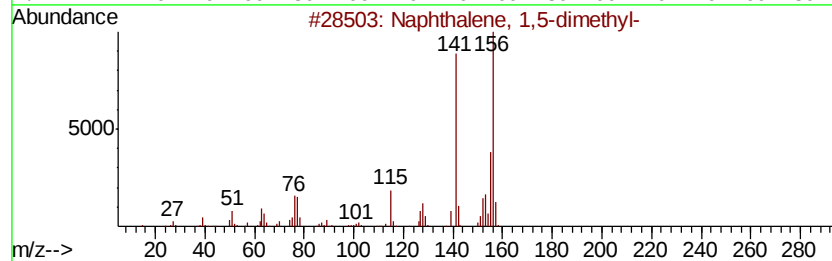
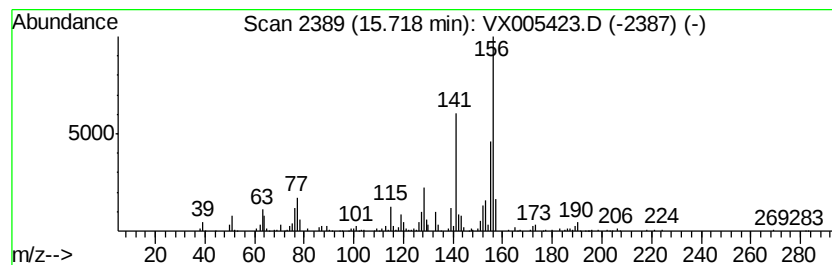
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	11.29 ug/l	288099	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
2		Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4		Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
5		Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



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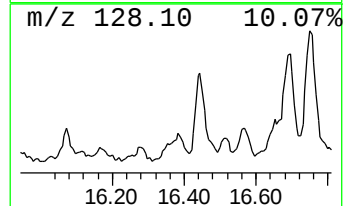
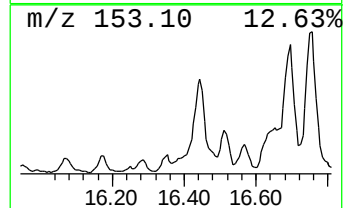
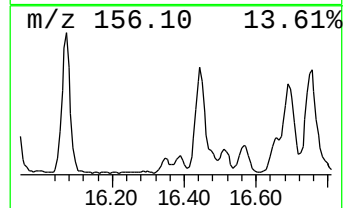
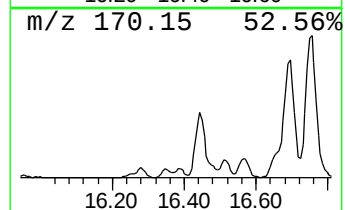
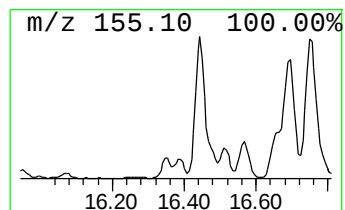
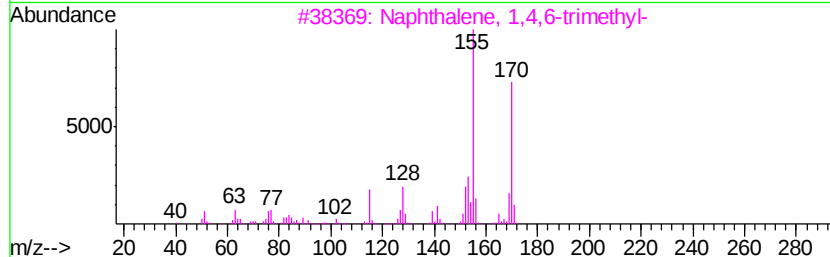
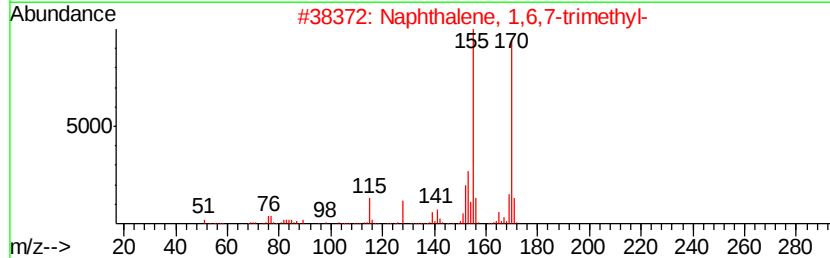
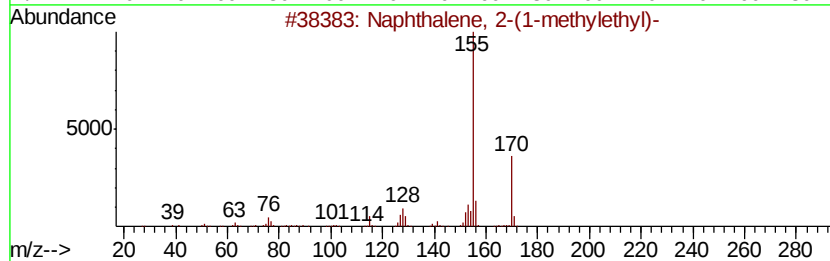
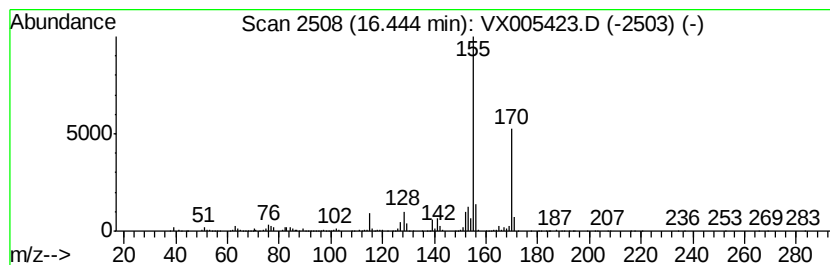
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 2-(1-methylethyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.44	14.11 ug/l	360049	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-(1-methylethyl)-	170	C13H14	002027-17-0	91
2	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	76
3	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	72
4	Ethanone, 1-(1-Naphthalenyl)-	170	C12H10O	000941-98-0	64
5	Naphthalene, 2-methyl-1-propyl-	184	C14H16	054774-89-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101818\
Data File : VX005423.D
Acq On : 18 Oct 2018 12:10
Operator : JC/MD
Sample : J5573-01
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

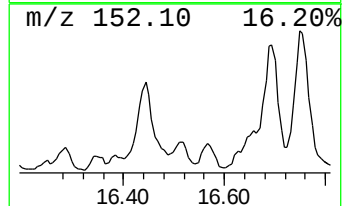
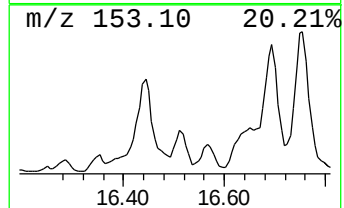
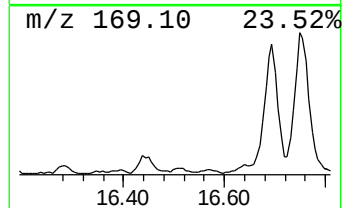
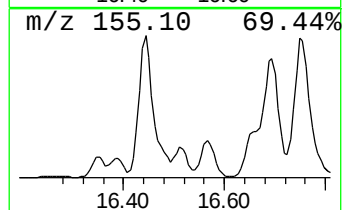
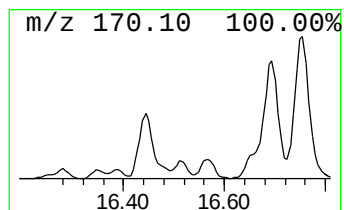
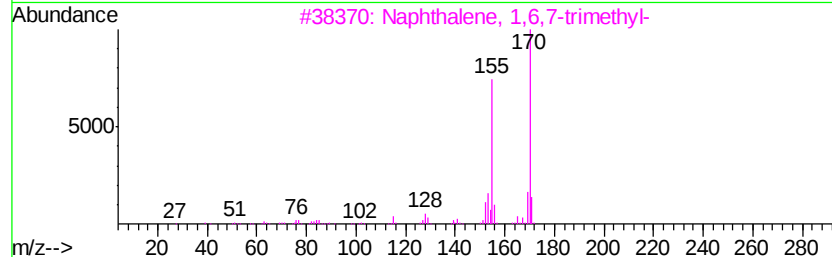
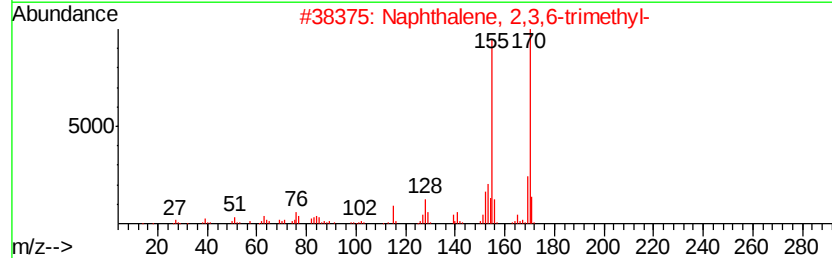
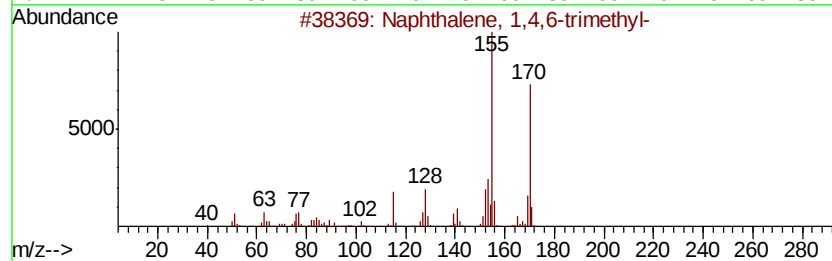
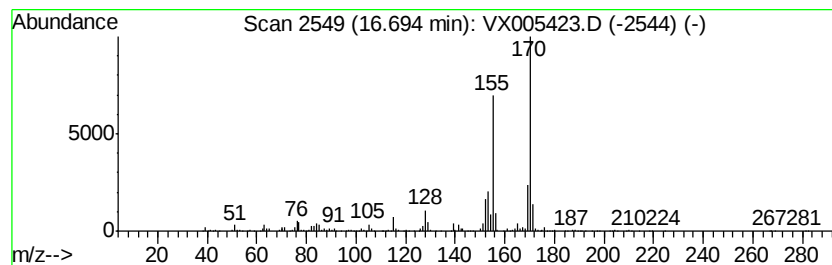
Instrument :
MSVOA_X
ClientSampleId :
0689-KM-CA-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,4,6-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.69	17.64 ug/l	450086	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	94
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	93
3	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	93
4	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	91
5	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	86



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101818\
Data File : VX005423.D
Acq On : 18 Oct 2018 12:10
Operator : JC/MD
Sample : J5573-01
Misc : 5.09µL/10µL/100µL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

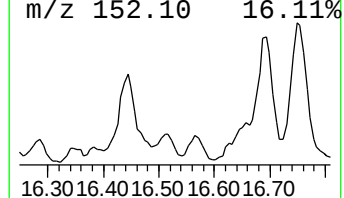
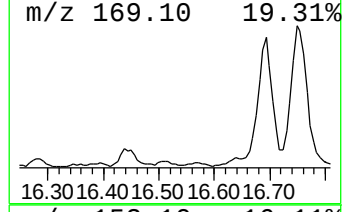
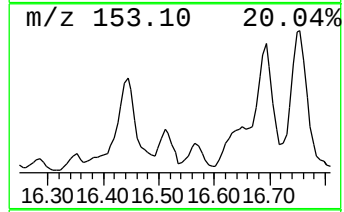
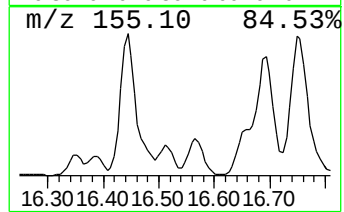
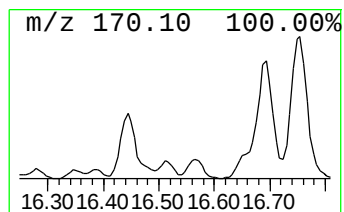
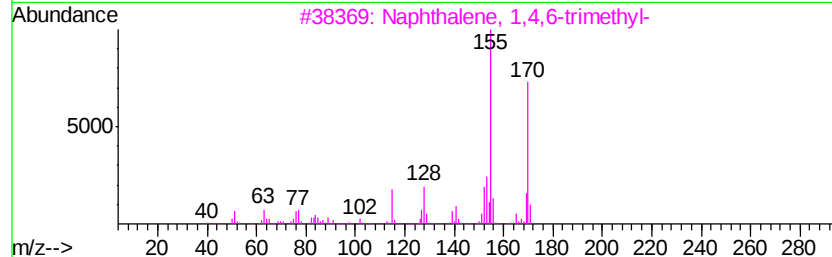
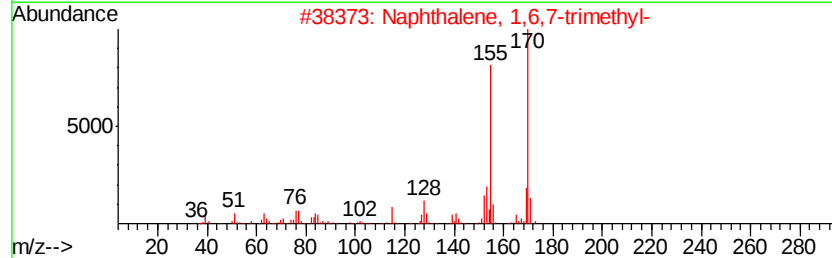
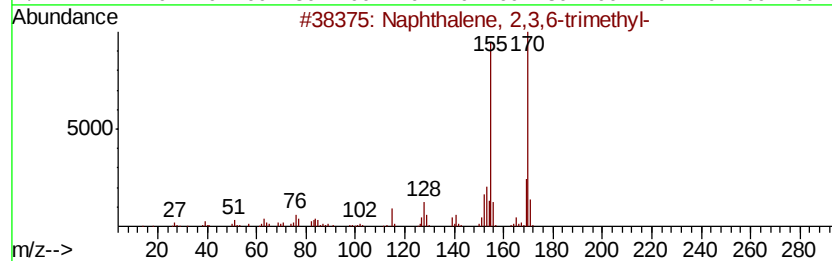
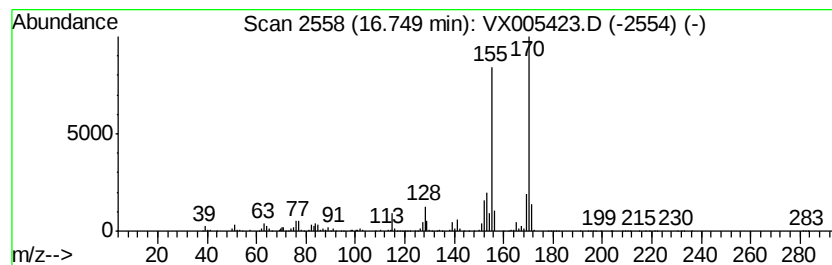
Instrument :
MSVOA_X
ClientSampleId :
0689-KM-CA-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.75	18.40 ug/l	469360	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	98
2		Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	97
3		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	96
4		4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94
5		Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101818\
Data File : VX005423.D
Acq On : 18 Oct 2018 12:10
Operator : JC/MD
Sample : J5573-01
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0689-KM-CA-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.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
unknown1.67	1.67	10.3	ug/l	160025	1	5.66	774894	50.0
Naphthalene, 2,6-...	15.55	18.3	ug/l	465724	4	12.08	1275750	50.0
Naphthalene, 2,3-...	15.69	18.2	ug/l	464227	4	12.08	1275750	50.0
Naphthalene, 1,5-...	15.72	11.3	ug/l	288099	4	12.08	1275750	50.0
Naphthalene, 2-(1...	16.44	14.1	ug/l	360049	4	12.08	1275750	50.0
Naphthalene, 1,4,...	16.69	17.6	ug/l	450086	4	12.08	1275750	50.0
Naphthalene, 2,3,...	16.75	18.4	ug/l	469360	4	12.08	1275750	50.0