LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

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\82X082120W.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	3.148	328	338	346	rBV2	39426	104078	1.23%	0.190%
2	4.867	600	620	639	rBV	2848453	8467901	100.00%	15.427%
3	5.471	707	719	733	rBV	242546	703991	8.31%	1.283%
4	5.629	733	745	759	rBV2	428861	1224745	14.46%	2.231%
5	6.031	802	811	826	rBV	272140	710017	8.38%	1.294%
6	6.830	931	942	958	rBV	623855	1476015	17.43%	2.689%
7	8.696	1241	1248	1256	rBV	1267589	1961116	23.16%	3.573%
8	10.098	1471	1478	1490	rBV	1276469	1697798	20.05%	3.093%
9	11.122	1641	1646	1653	rBV	1033164	1331234	15.72%	2.425%
10	12.061	1795	1800	1808	rBV	1409900	1819151	21.48%	3.314%
11	12.360	1844	1849	1859	rVB4	60464	133260	1.57%	0.243%
12	12.701	1900	1905	1909	rBV2	64112	99006	1.17%	0.180%
13	12.768	1909	1916	1920	rVB4	69396	137865	1.63%	0.251%
14	12.853	1925	1930	1938	rVB2	187798	326862	3.86%	0.596%
15	12.963	1944	1948	1952	rVB	152662	175823	2.08%	0.320%
16	13.079	1963	1967	1970	rVB5	57259	96499	1.14%	0.176%
17	13.201	1981	1987	1990	rBV6	64899	110468	1.30%	0.201%
18	13.286	1997	2001	2005	rBV3	92311	136213	1.61%	0.248%
19	13.335	2005	2009	2014	rVV4	224936	355426	4.20%	0.648%
20	13.445	2023	2027	2036	rBV6	254456	670058	7.91%	1.221%
21	13.567	2041	2047	2052	rBV4	153227	361951	4.27%	0.659%
22	13.622	2053	2056	2061	rVB3	94869	155785	1.84%	0.284%
23	13.670	2061	2064	2068	rBV5	56283	93170	1.10%	0.170%
24	13.713	2068	2071	2075	rBV6	105913	141650	1.67%	0.258%
25	13.811	2079	2087	2090	rBV4	268316	624079	7.37%	1.137%
26	13.841	2090	2092	2095	rVB3	227559	240334	2.84%	0.438%
27	13.890	2096	2100	2105	rBV4	479289	734928	8.68%	1.339%
28	13.969	2107	2113	2118	rBV4	285037	663502	7.84%	1.209%
29	14.012	2118	2120	2124	rBV3	108511	139696	1.65%	0.255%
30	14.109	2132	2136	2140	rBV4	390263	629969	7.44%	1.148%
31	14.213	2148	2153	2156	rBV5	275388	508998	6.01%	0.927%
32	14.262	2157	2161	2167	rVV5	521929	1055354	12.46%	1.923%
33	14.359	2174	2177	2181	rBV3	217834	373457	4.41%	0.680%
34	14.524	2200	2204	2212	rBV6	628650	1373413	16.22%	2.502%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

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\82X082120W.M
Title : SW846 8260

35	14.658	2222	2226	2228	rBV2	1616588	2133484	25.19%	3.887%
36	14.713	2232	2235	2239	rVV	718776	825334	9.75%	1.504%
37	14.798	2246	2249	2250	rBV2	410267	410511	4.85%	0.748%
38	14.823	2250	2253	2257	rVV2	1092131	1495811	17.66%	2.725%
39	14.865	2257	2260	2261	rVV2	361657	404916	4.78%	0.738%
40	14.890	2261	2264	2268	rVB2	868066	1021071	12.06%	1.860%
41	15.225	2315	2319	2322	rBV3	971134	1615315	19.08%	2.943%
42	15.426	2349	2352	2355	rVB2	638052	692027	8.17%	1.261%
43	15.463	2355	2358	2363	rVB2	735433	1051634	12.42%	1.916%
44	15.530	2365	2369	2374	rBV2	1239134	2150106	25.39%	3.917%
45	15.664	2387	2391	2395	rBV	1510306	2197509	25.95%	4.004%
46	15.707	2395	2398	2406	rVV5	925612	1767980	20.88%	3.221%
47	15.792	2408	2412	2418	rVB2	1141581	2309819	27.28%	4.208%
48	16.030	2446	2451	2458	rBV3	3258875	5413997	63.94%	9.864%
49	16.152	2467	2471	2481	rVB2	1407245	2565113	30.29%	4.673%

Sum of corrected areas: 54888439

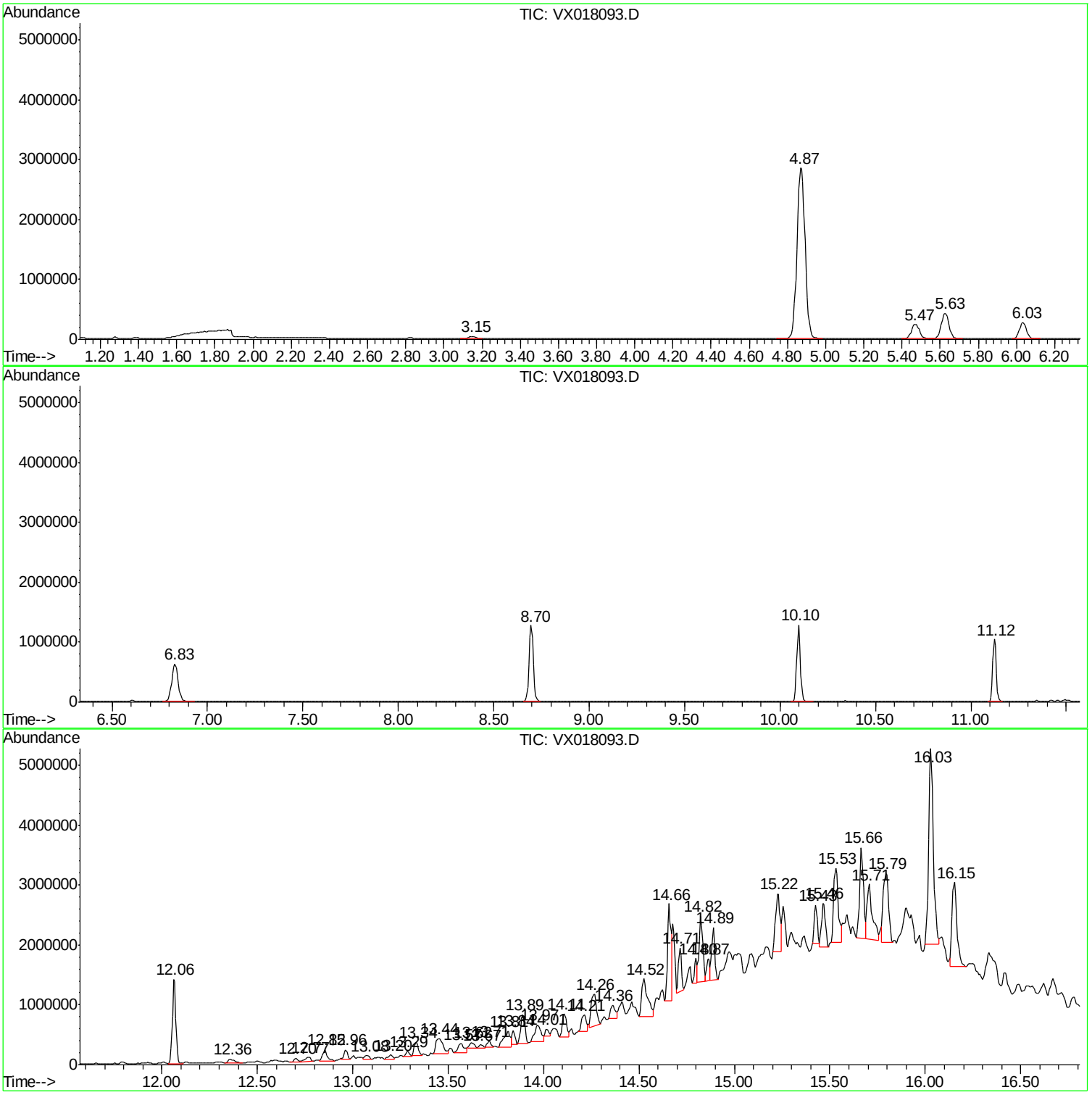
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

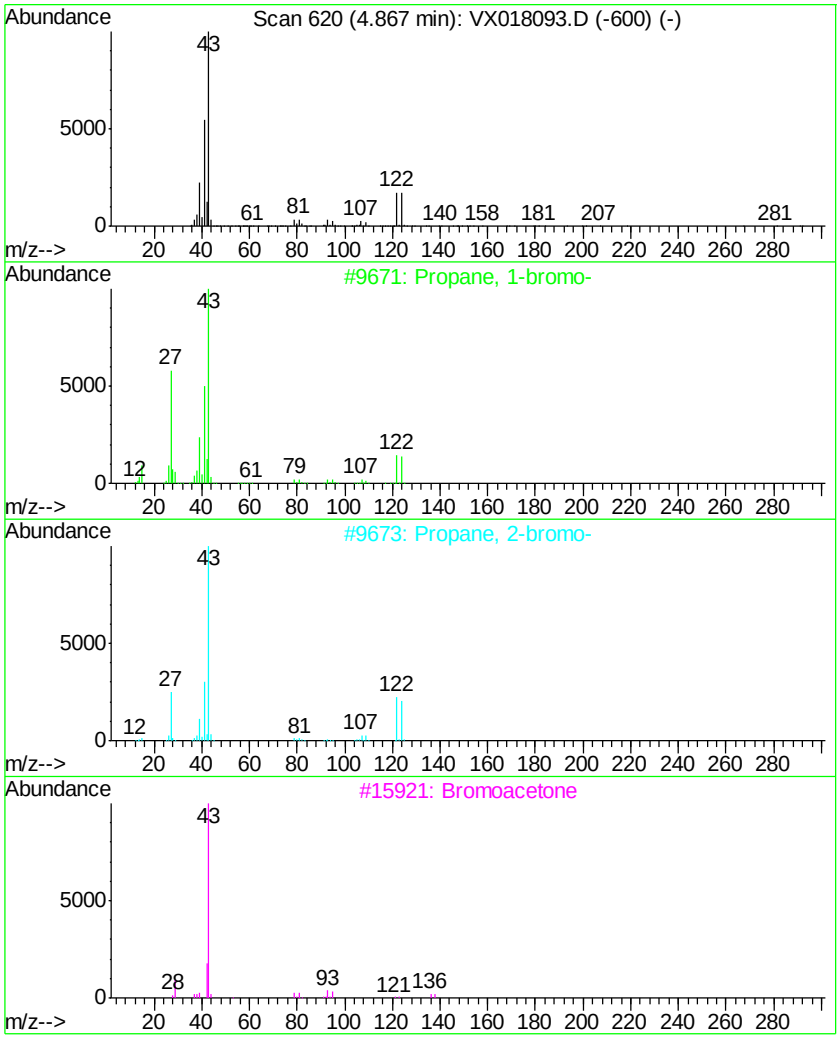
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

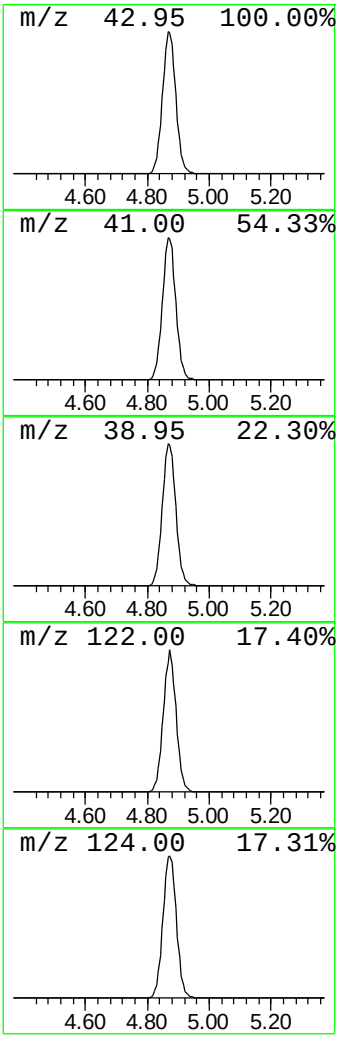
****

Peak Number 1 Propane, 1-bromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	345.70 ug/l	8467900	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-bromo-	122	C3H7Br	000106-94-5	86
2	Propane, 2-bromo-	122	C3H7Br	000075-26-3	50
3	Bromoacetone	136	C3H5BrO	000598-31-2	38
4	Isopropenyl bromide	120	C3H5Br	000557-93-7	22
5	1-Propanesulfonyl chloride	142	C3H7ClO2S	010147-36-1	17





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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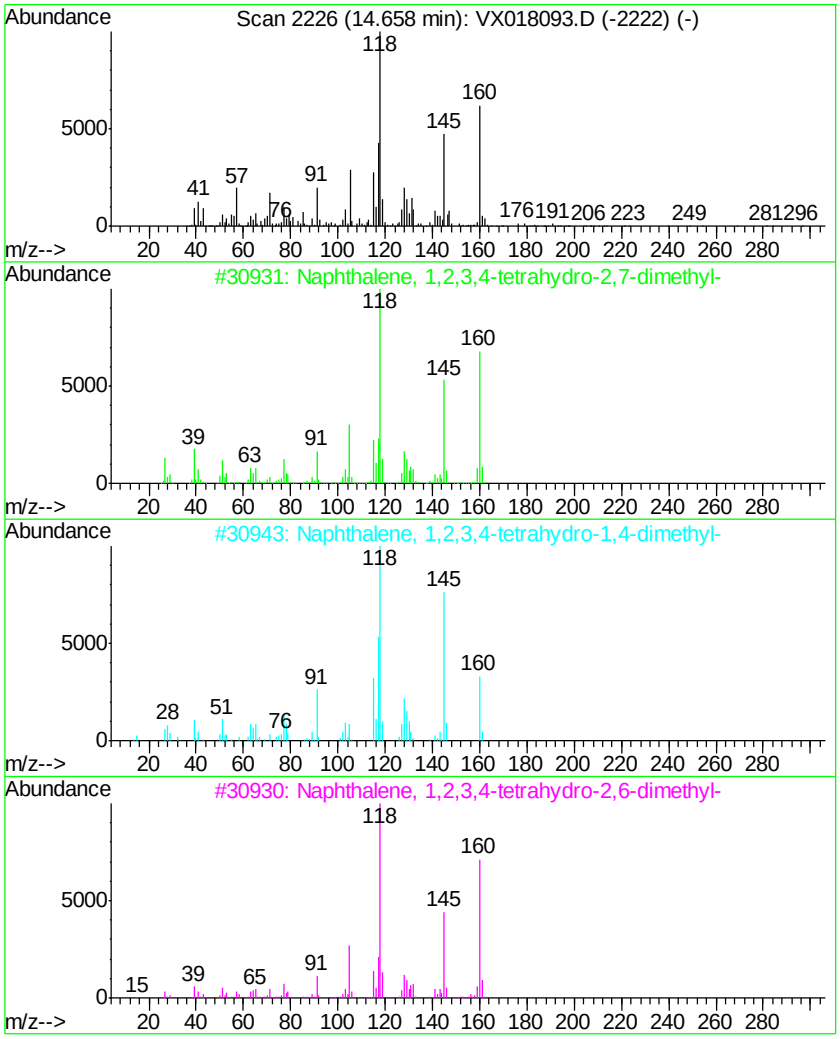
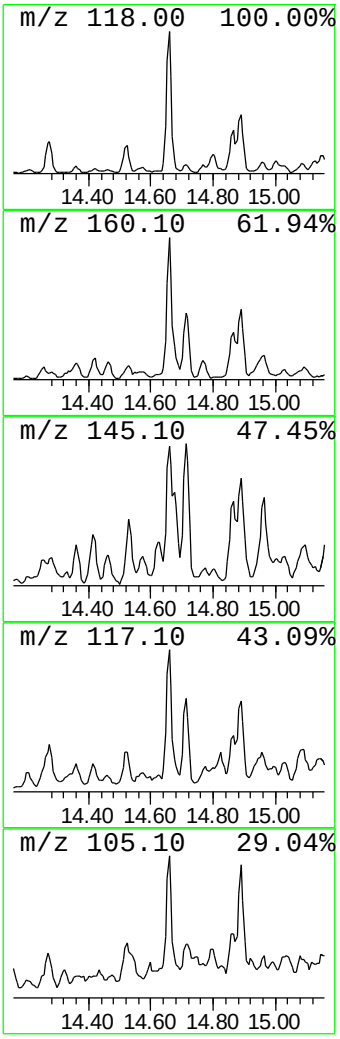
Peak Number 2 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	58.64 ug/l	2133480	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	62
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	58
5	Acetonitrile, 2-[4-(cyanomethyl)...	145	C8H7N3	1000197-65-1	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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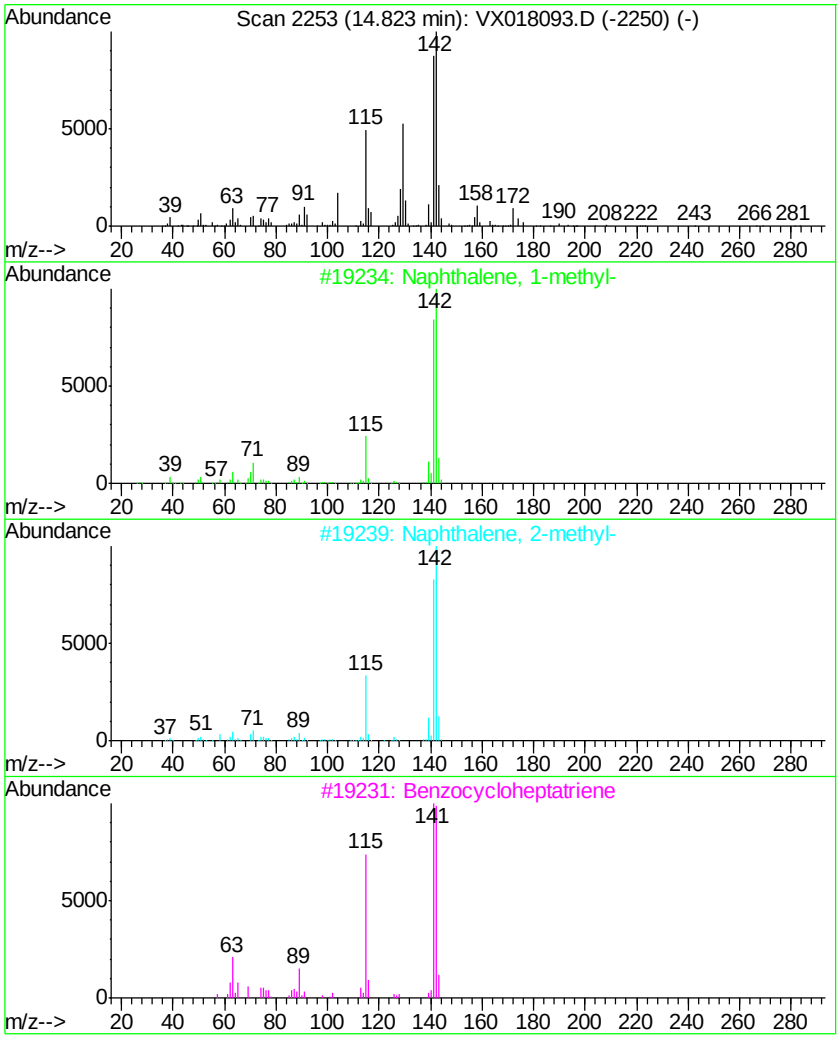
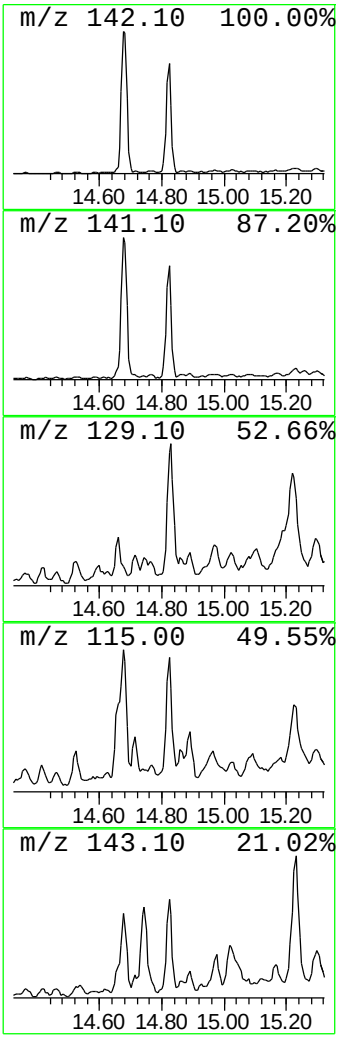
Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	41.11 ug/l	1495810	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	64
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
3	Benzocycloheptatriene	142	C11H10	000264-09-5	64
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	58
5	1-Naphthaleneethanol	172	C12H12O	000773-99-9	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

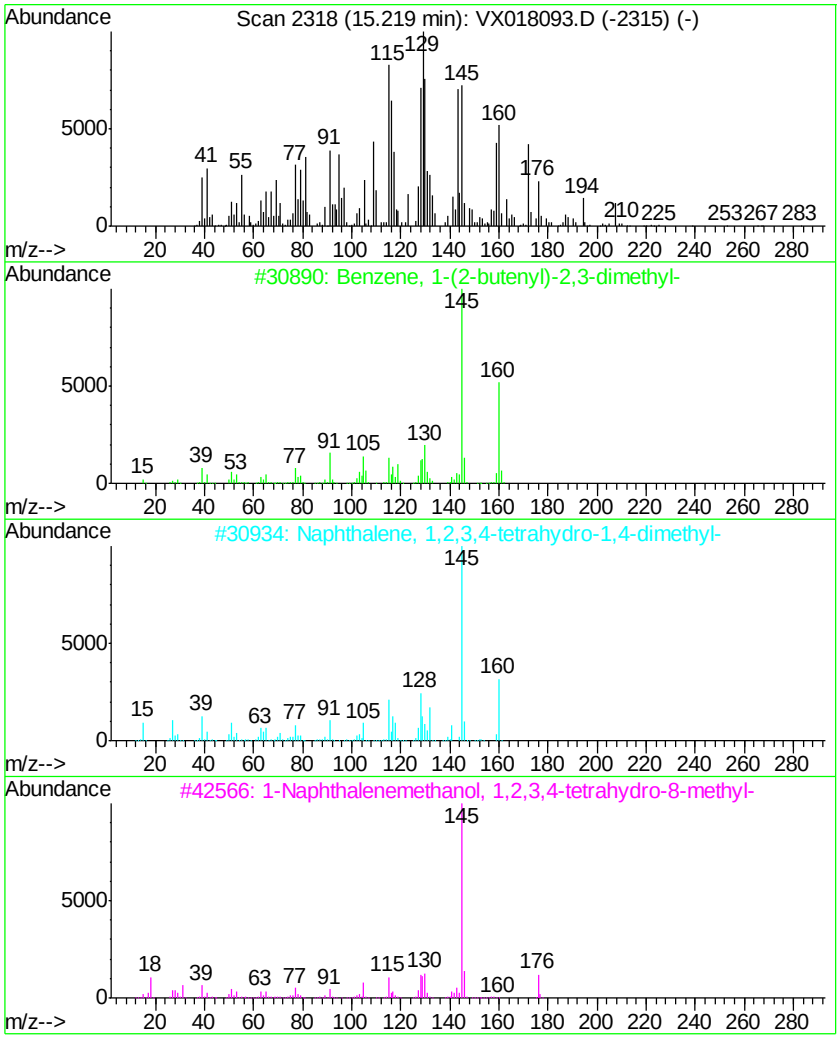
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

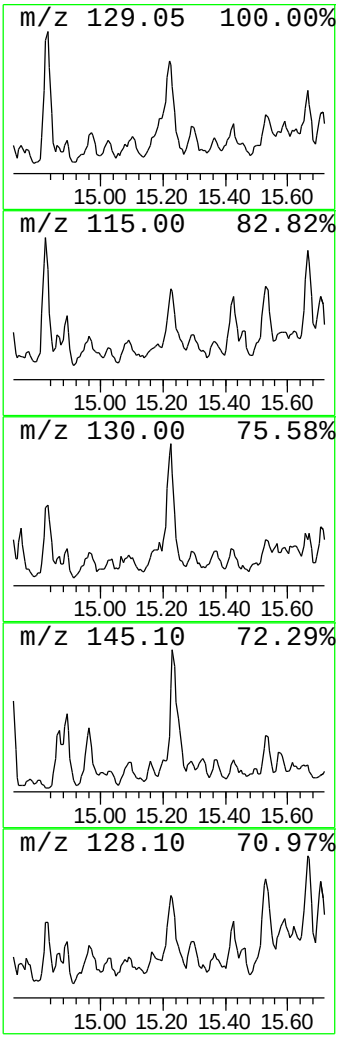
****

Peak Number 4 Benzene, 1-(2-butenyl)-2,3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	44.40 ug/l	1615320	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	70
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64
3	1-Naphthalenemethanol, 1,2,3,4-t...	176	C12H16O	036052-28-5	50
4	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	47
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

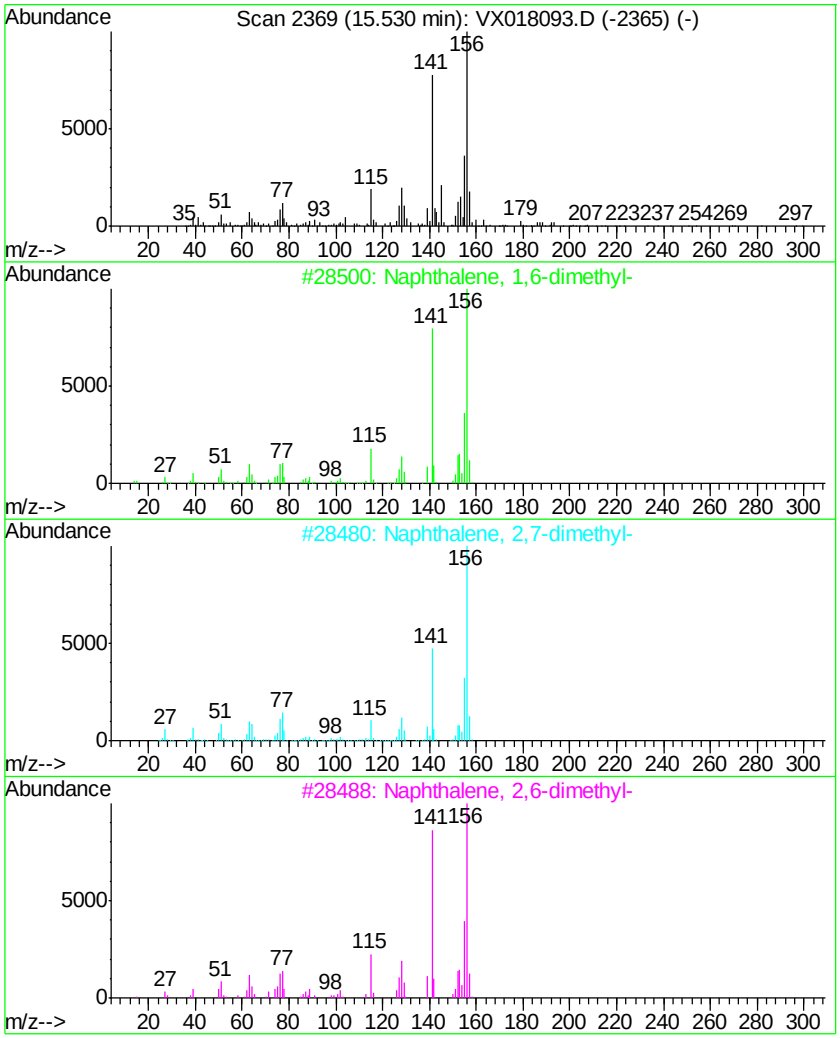
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

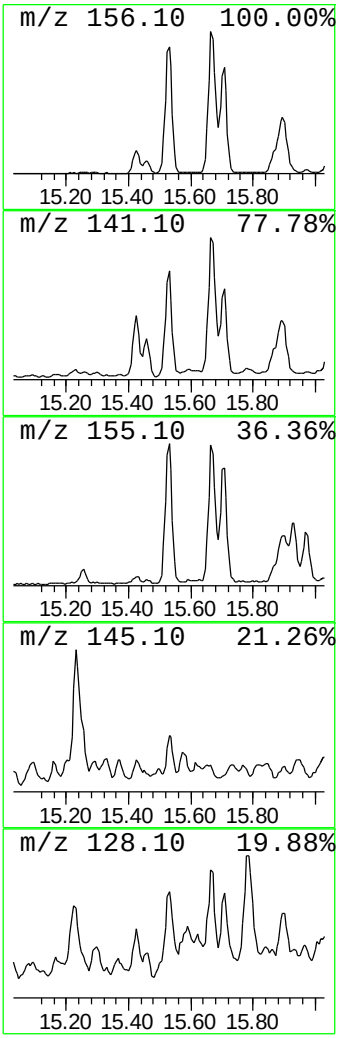
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	59.10 ug/l	2150110	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
3	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

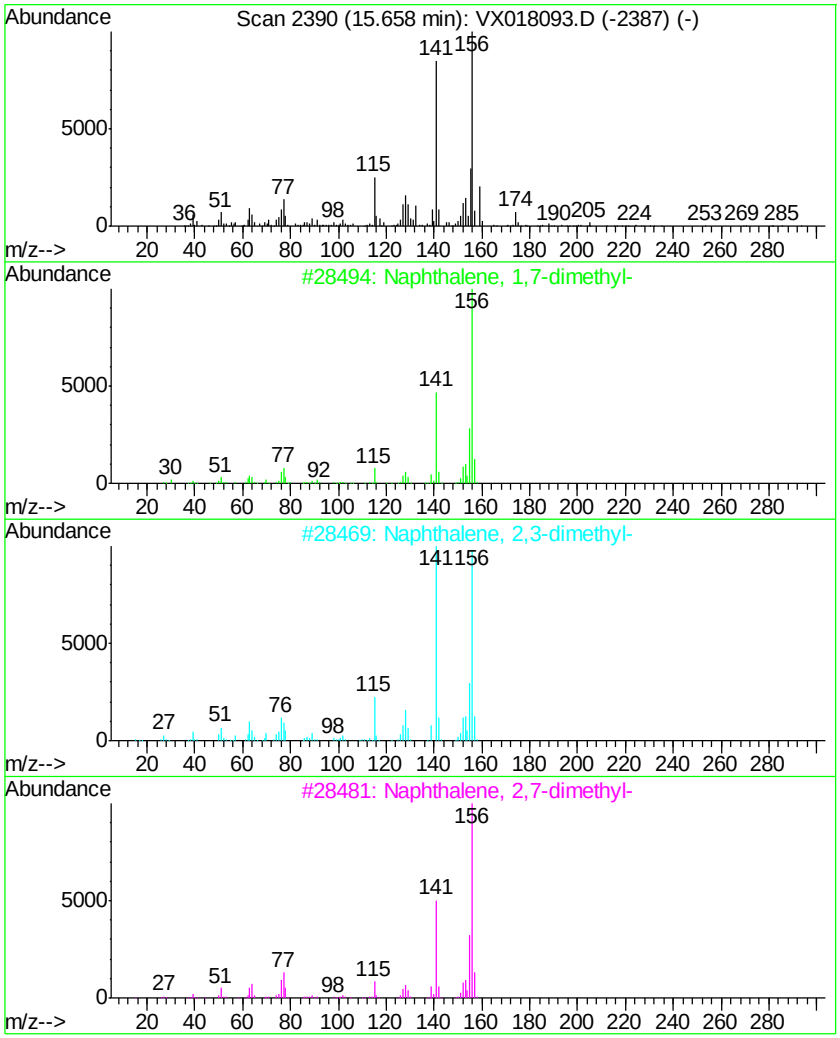
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

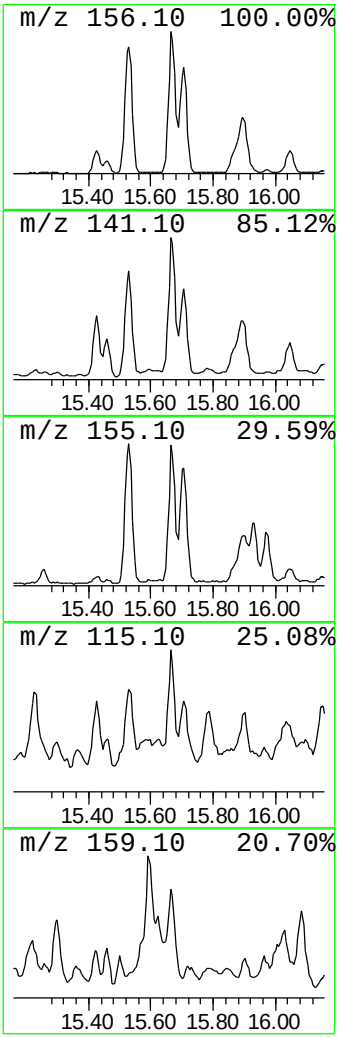
****

Peak Number 6 Naphthalene, 1,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	60.40 ug/l	2197510	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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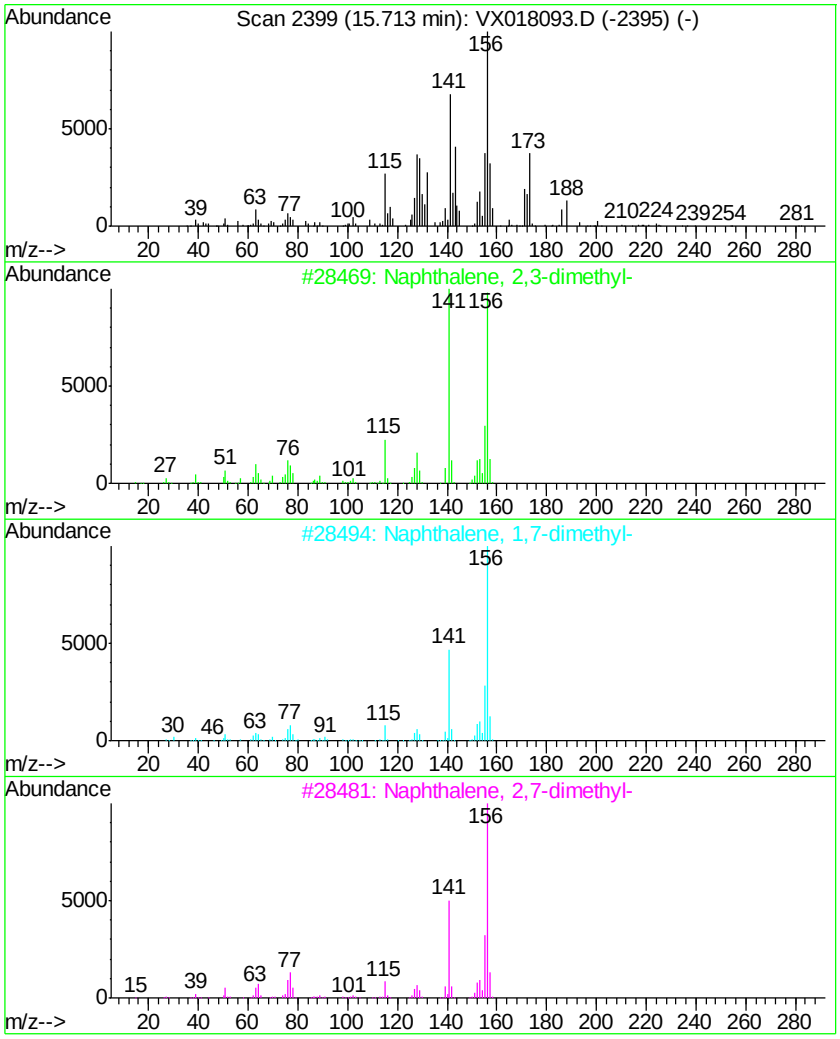
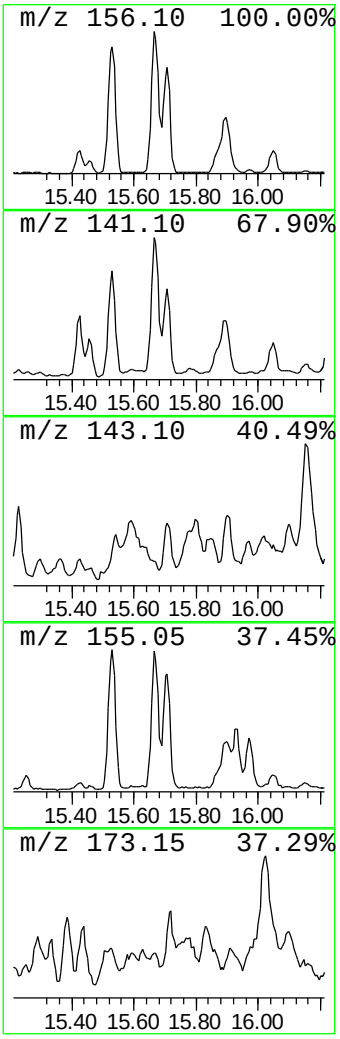
Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	48.59 ug/l	1767980	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	76
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	76
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	76
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	70





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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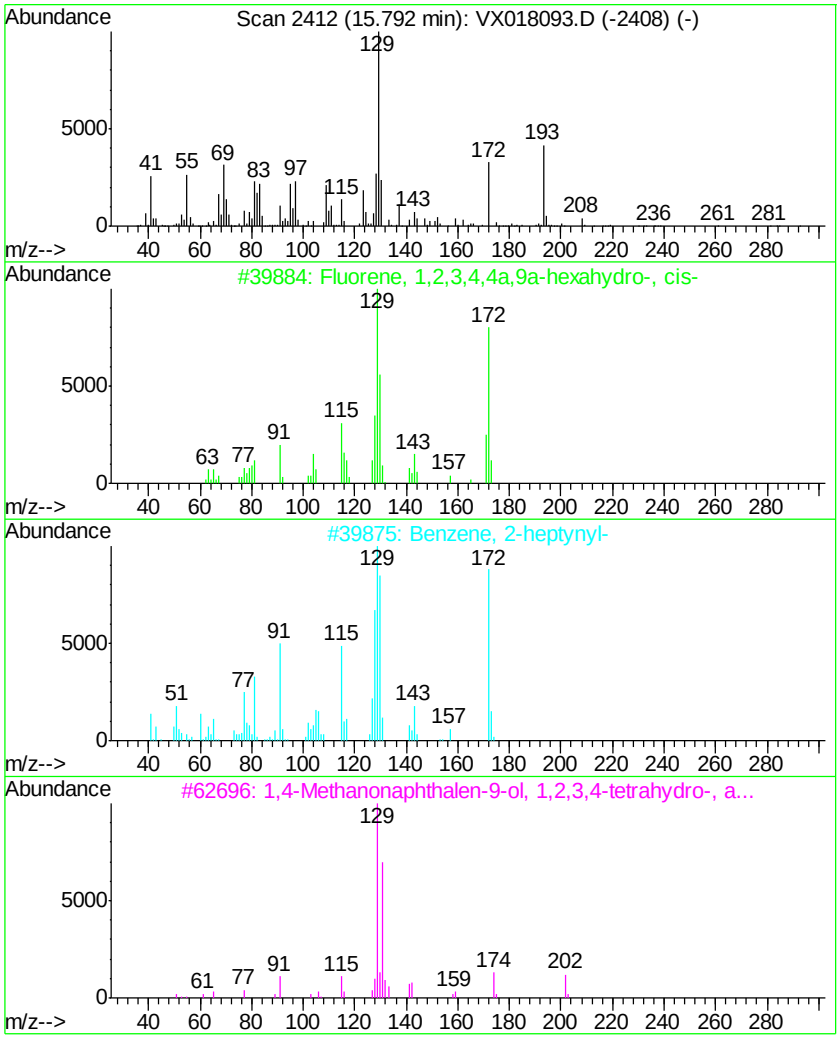
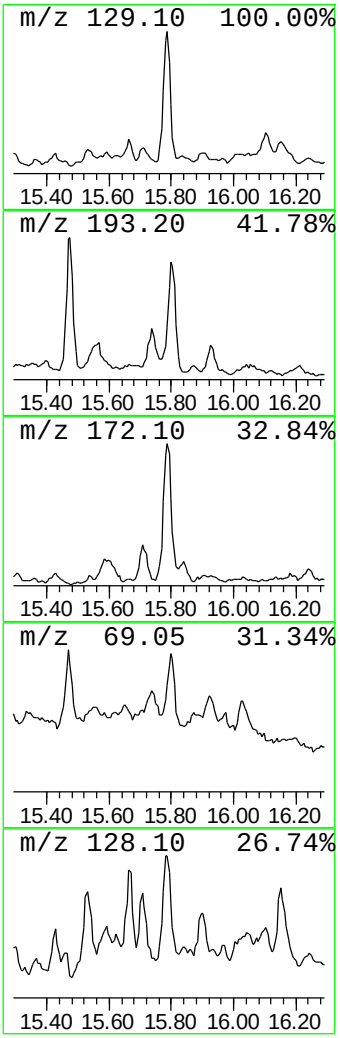
Peak Number 8 unknown15.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	63.49 ug/l	2309820	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene, 1,2,3,4,4a,9a-hexahydr...	172	C13H16	001559-97-3	22
2	Benzene, 2-heptynyl-	172	C13H16	054725-17-6	20
3	1,4-Methanonaphthalen-9-ol, 1,2,...	202	C13H14O2	001207-27-8	16
4	Succinic acid, ethyl 2-norbornyl...	240	C13H20O4	1000330-19-4	16
5	Succinic acid, ethyl tetradec-11...	340	C20H36O4	1000353-35-3	12





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Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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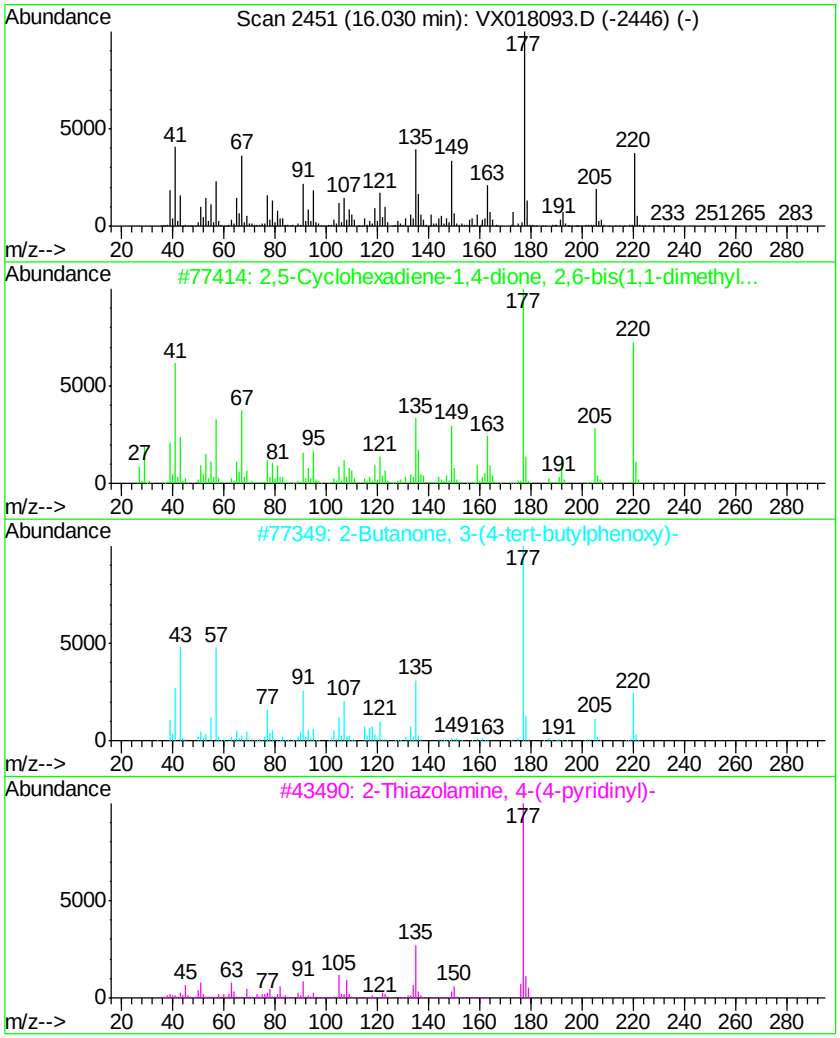
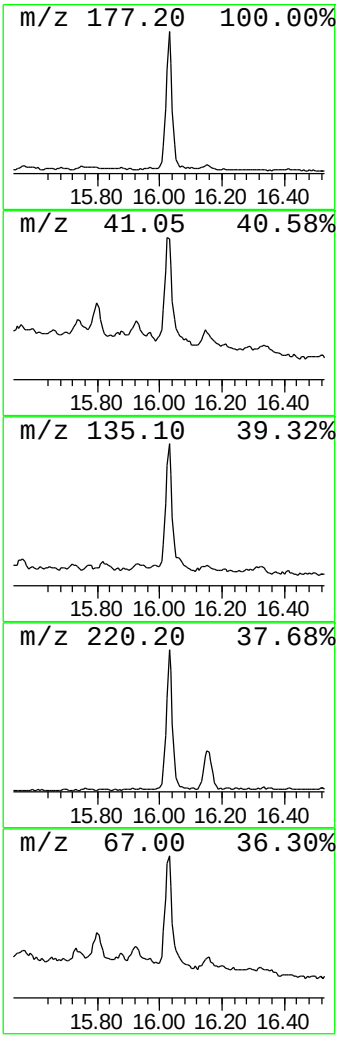
Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	148.81 ug/l	5414000	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	72
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	60
3	2-Thiazolamine, 4-(4-pyridinyl)-	177	C8H7N3S	1000351-69-3	47
4	2H-1-Benzopyran, 3,5,6,8a-tetrah...	192	C13H20O	041678-29-9	46
5	Propanamine, 2-(1-adamantyl)-2-m...	207	C14H25N	079594-24-4	46





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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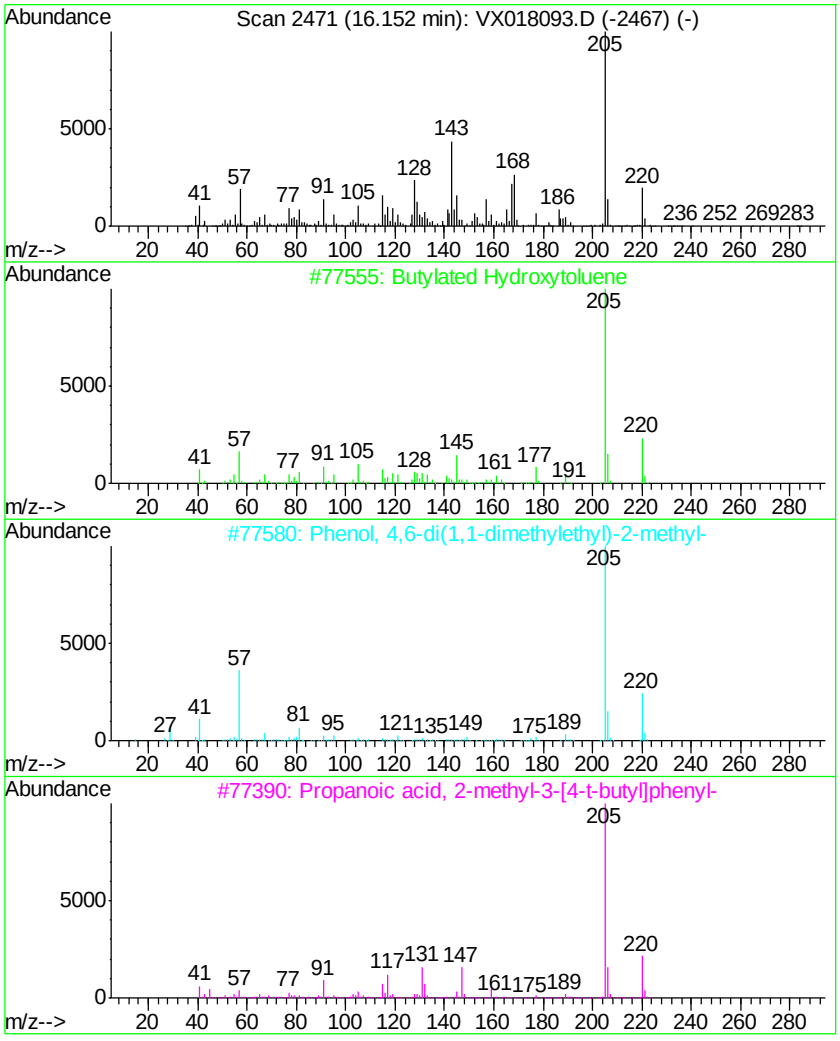
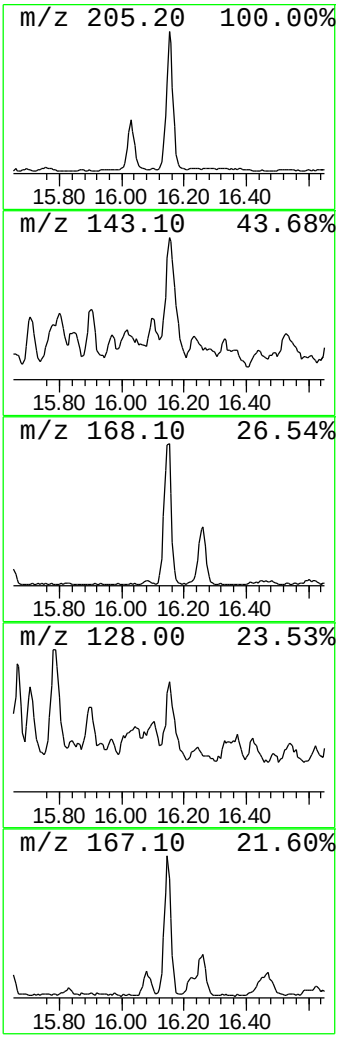
Peak Number 10 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	70.50 ug/l	2565110	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	64
2	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	46
3	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	38
4	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	38
5	2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082720\
Data File : VX018093.D
Acq On : 27 Aug 2020 15:54
Operator : JC/SP
Sample : L3787-01
Misc : 5.05g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20071

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1-bromo-	4.87	345.7	ug/l	8467900	1	5.62	1224750	50.0
Naphthalene, 1,2,...	14.66	58.6	ug/l	2133480	4	12.07	1819150	50.0
Naphthalene, 1-me...	14.82	41.1	ug/l	1495810	4	12.07	1819150	50.0
Benzene, 1-(2-but...	15.22	44.4	ug/l	1615320	4	12.07	1819150	50.0
Naphthalene, 1,6-...	15.53	59.1	ug/l	2150110	4	12.07	1819150	50.0
Naphthalene, 1,7-...	15.66	60.4	ug/l	2197510	4	12.07	1819150	50.0
Naphthalene, 2,3-...	15.71	48.6	ug/l	1767980	4	12.07	1819150	50.0
unknown15.79	15.79	63.5	ug/l	2309820	4	12.07	1819150	50.0
2,5-Cyclohexadien...	16.03	148.8	ug/l	5414000	4	12.07	1819150	50.0
Butylated Hydroxy...	16.15	70.5	ug/l	2565110	4	12.07	1819150	50.0