LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

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\82X061518W.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	1.075	76	80	94	rBV	1437626	1765092	100.00%	11.771%
2	1.270	108	112	123	rBV	55173	79873	4.53%	0.533%
3	2.355	285	290	295	rBV	11170	17950	1.02%	0.120%
4	2.447	300	305	312	rVB	32790	54364	3.08%	0.363%
5	5.507	797	807	822	rBV	150791	428145	24.26%	2.855%
6	5.666	822	833	848	rVV	228967	639009	36.20%	4.261%
7	6.074	888	900	911	rBV	166245	436737	24.74%	2.912%
8	6.867	1020	1030	1049	rBV	329818	766100	43.40%	5.109%
9	8.659	1318	1324	1327	rBV2	16012	25822	1.46%	0.172%
10	8.720	1327	1334	1343	rVV	806648	1225041	69.40%	8.169%
11	9.604	1472	1479	1484	rBV	17912	30632	1.74%	0.204%
12	10.116	1553	1563	1575	rBV	695570	943623	53.46%	6.293%
13	10.957	1695	1701	1705	rVB3	10425	21644	1.23%	0.144%
14	11.140	1726	1731	1737	rBV	718702	908031	51.44%	6.055%
15	11.366	1761	1768	1771	rBV7	9351	17987	1.02%	0.120%
16	11.634	1807	1812	1815	rVB5	16037	29864	1.69%	0.199%
17	11.677	1815	1819	1821	rBV2	17751	24547	1.39%	0.164%
18	11.744	1827	1830	1834	rVB4	17976	24222	1.37%	0.162%
19	11.805	1834	1840	1843	rBV4	31012	57368	3.25%	0.383%
20	11.945	1859	1863	1866	rBV2	29725	42142	2.39%	0.281%
21	11.975	1866	1868	1872	rVB3	21666	24537	1.39%	0.164%
22	12.042	1874	1879	1880	rBV5	12454	18720	1.06%	0.125%
23	12.079	1880	1885	1891	rVV	820306	1080632	61.22%	7.206%
24	12.134	1891	1894	1900	rVV7	21527	49786	2.82%	0.332%
25	12.207	1903	1906	1911	rVB5	27516	41897	2.37%	0.279%
26	12.262	1911	1915	1917	rBV3	12809	18122	1.03%	0.121%
27	12.347	1926	1929	1934	rVB2	25330	33198	1.88%	0.221%
28	12.396	1934	1937	1940	rBV4	25428	29521	1.67%	0.197%
29	12.555	1957	1963	1965	rBV6	19907	37142	2.10%	0.248%
30	12.609	1965	1972	1975	rVV	69771	109701	6.22%	0.732%
31	12.670	1980	1982	1987	rVB3	23497	31111	1.76%	0.207%
32	12.725	1987	1991	1996	rBV5	54199	102204	5.79%	0.682%
33	12.786	1996	2001	2005	rBV6	27785	49858	2.82%	0.332%
34	12.981	2028	2033	2036	rBV2	173333	243901	13.82%	1.627%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

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\82X061518W.M
Title : SW846 8260

35	13.012	2036	2038	2046	rVB2	137468	197851	11.21%	1.319%
36	13.085	2046	2050	2056	rBV4	40723	80525	4.56%	0.537%
37	13.146	2056	2060	2064	rBV4	43478	68489	3.88%	0.457%
38	13.256	2074	2078	2079	rBV	53975	59792	3.39%	0.399%
39	13.353	2087	2094	2100	rVB6	88482	215978	12.24%	1.440%
40	13.542	2122	2125	2126	rBV3	19617	19668	1.11%	0.131%
41	13.567	2126	2129	2132	rBV3	39342	59400	3.37%	0.396%
42	13.658	2138	2144	2148	rBV5	70713	143047	8.10%	0.954%
43	13.707	2149	2152	2155	rBV4	41068	64737	3.67%	0.432%
44	13.810	2165	2169	2173	rBV2	161092	227621	12.90%	1.518%
45	13.865	2174	2178	2181	rVB4	37633	53519	3.03%	0.357%
46	13.908	2181	2185	2188	rBV4	70462	112888	6.40%	0.753%
47	13.945	2188	2191	2193	rVB3	43091	45279	2.57%	0.302%
48	13.987	2194	2198	2200	rBV3	48239	83271	4.72%	0.555%
49	14.079	2211	2213	2214	rBV	33864	27615	1.56%	0.184%
50	14.170	2225	2228	2231	rVB4	78874	97232	5.51%	0.648%
51	14.304	2246	2250	2253	rBV4	92862	151406	8.58%	1.010%
52	14.377	2258	2262	2267	rVV5	137790	288944	16.37%	1.927%
53	14.432	2268	2271	2278	rVB2	238654	344717	19.53%	2.299%
54	14.548	2287	2290	2293	rVB2	110460	141058	7.99%	0.941%
55	14.585	2293	2296	2302	rVB7	62193	115470	6.54%	0.770%
56	14.646	2303	2306	2309	rBV3	53928	77783	4.41%	0.519%
57	14.774	2323	2327	2329	rBV2	108416	155928	8.83%	1.040%
58	14.835	2334	2337	2343	rVB2	226664	326525	18.50%	2.178%
59	14.969	2351	2359	2367	rVB5	239120	638251	36.16%	4.256%
60	15.121	2379	2384	2388	rBV3	224411	402176	22.78%	2.682%
61	15.243	2400	2404	2412	rBV6	68667	133077	7.54%	0.887%
62	15.402	2425	2430	2443	rVB	557204	917437	51.98%	6.118%
63	15.591	2458	2461	2472	rVB3	123297	269363	15.26%	1.796%
64	16.182	2555	2558	2568	rVB4	36044	67822	3.84%	0.452%

Sum of corrected areas: 14995392

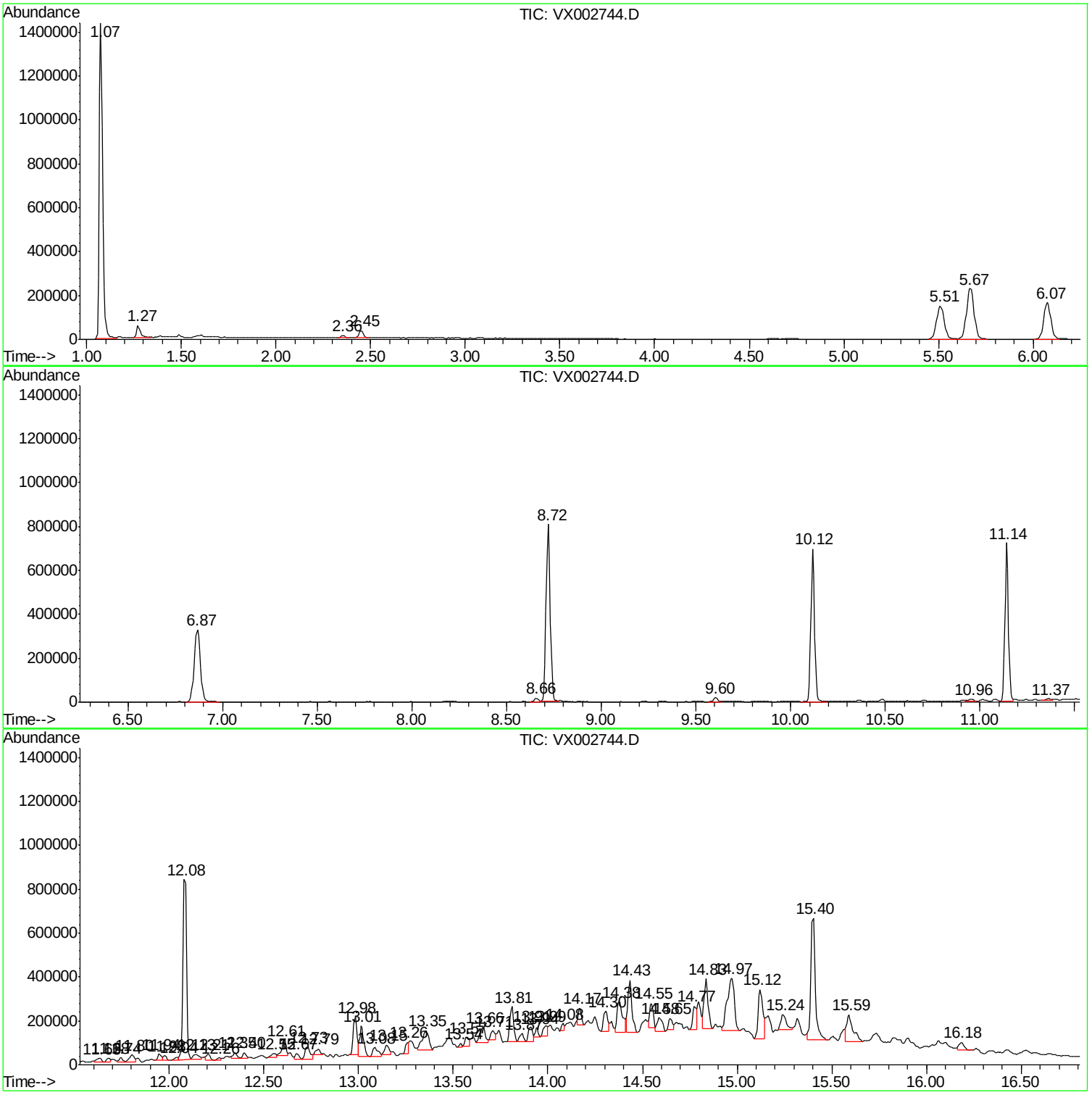
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

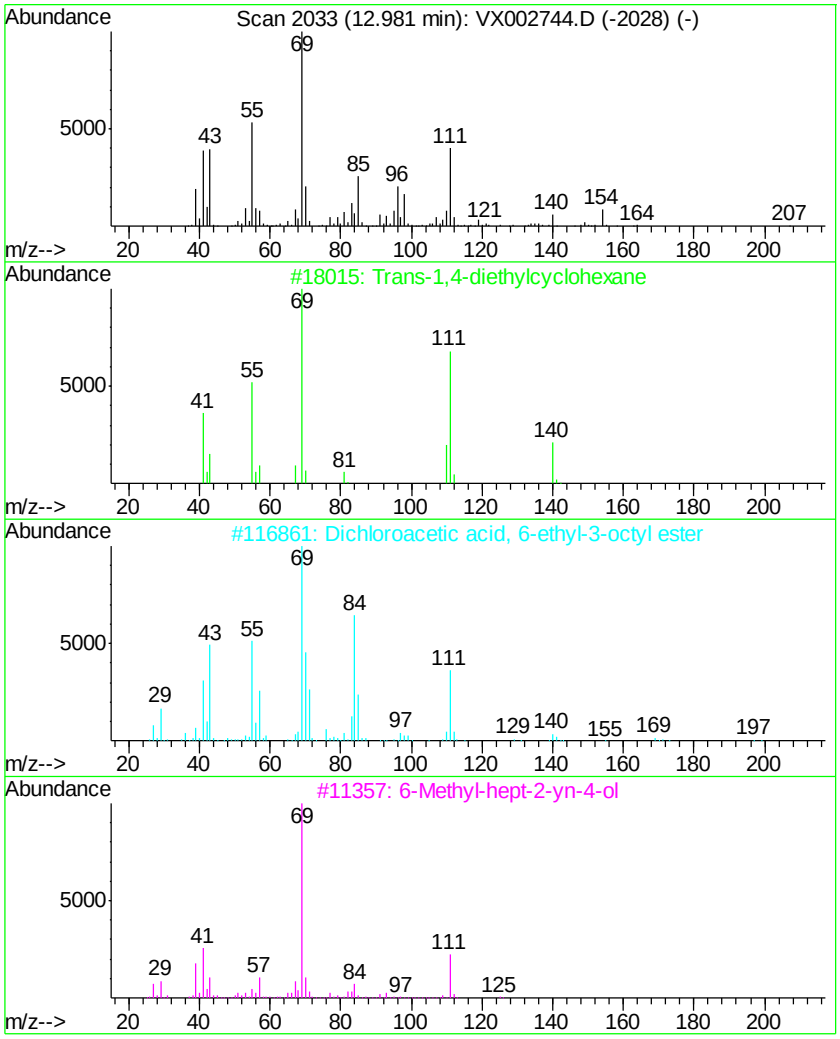
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

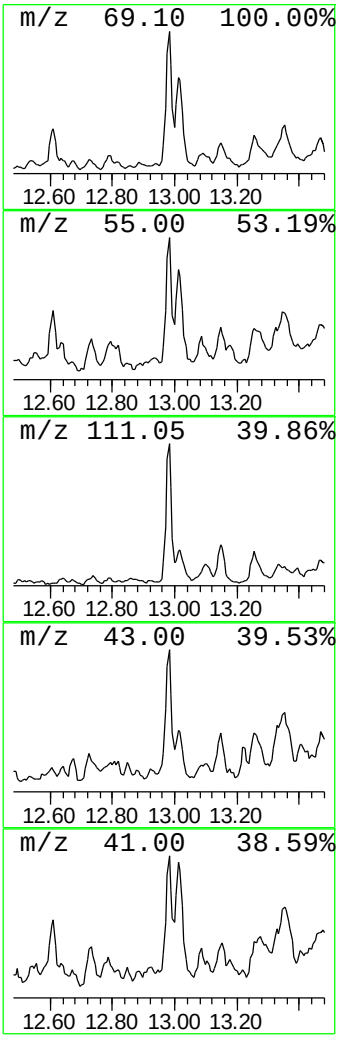
****

Peak Number 2 Trans-1,4-diethylcyclohexane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	11.29 ug/l	243901	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trans-1,4-diethylcyclohexane	140	C10H20	013990-93-7	64
2	Dichloroacetic acid, 6-ethyl-3-o...	268	C12H22Cl2O2	1000282-56-6	53
3	6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	50
4	Cyclohexane, 1,2-diethyl-, cis-	140	C10H20	000824-43-1	50
5	Cyclooctane, ethyl-	140	C10H20	013152-02-8	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

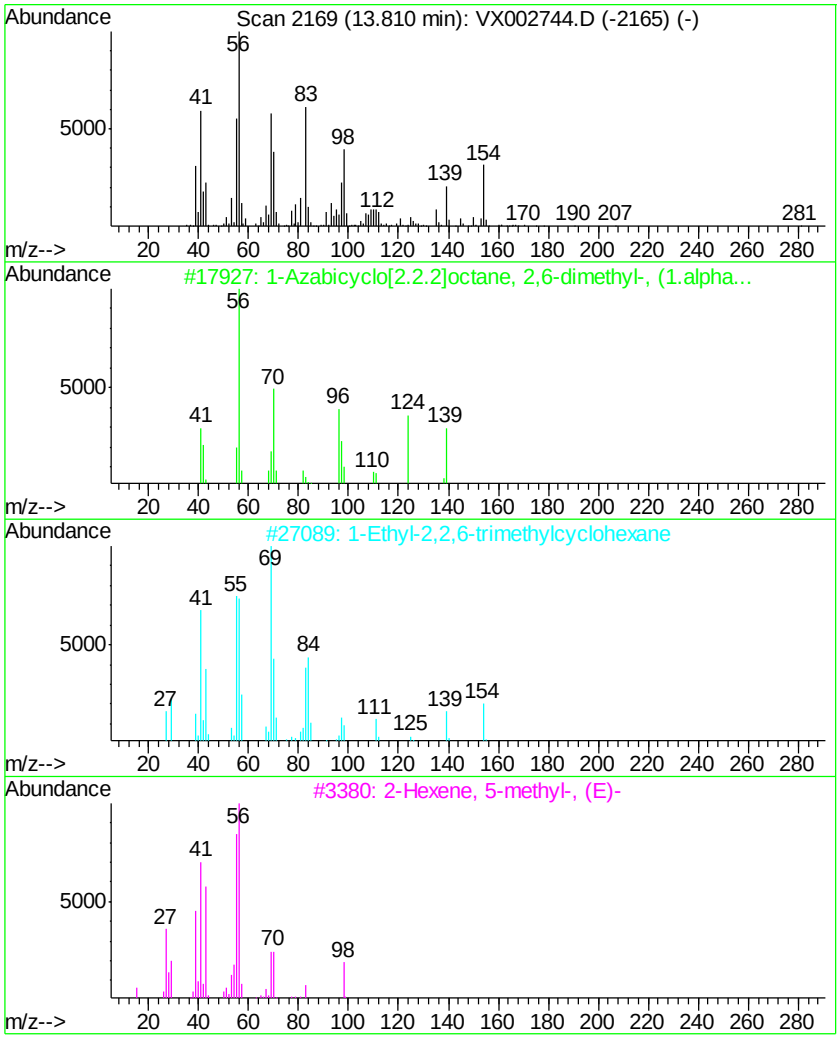
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

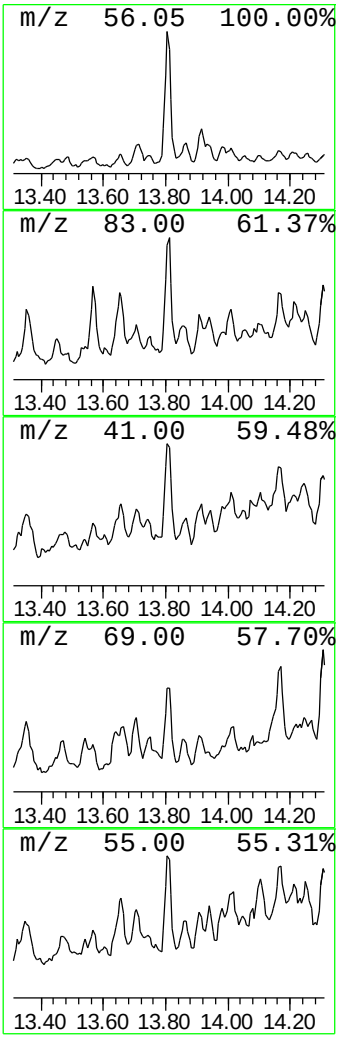
****

Peak Number 3 1-Azabicyclo[2.2.2]octane, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	10.53 ug/l	227621	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Azabicyclo[2.2.2]octane, 2,6-d...	139	C9H17N	013218-10-5	53
2	1-Ethyl-2,2,6-trimethylcyclohexane	154	C11H22	071186-27-1	52
3	2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	49
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46
5	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

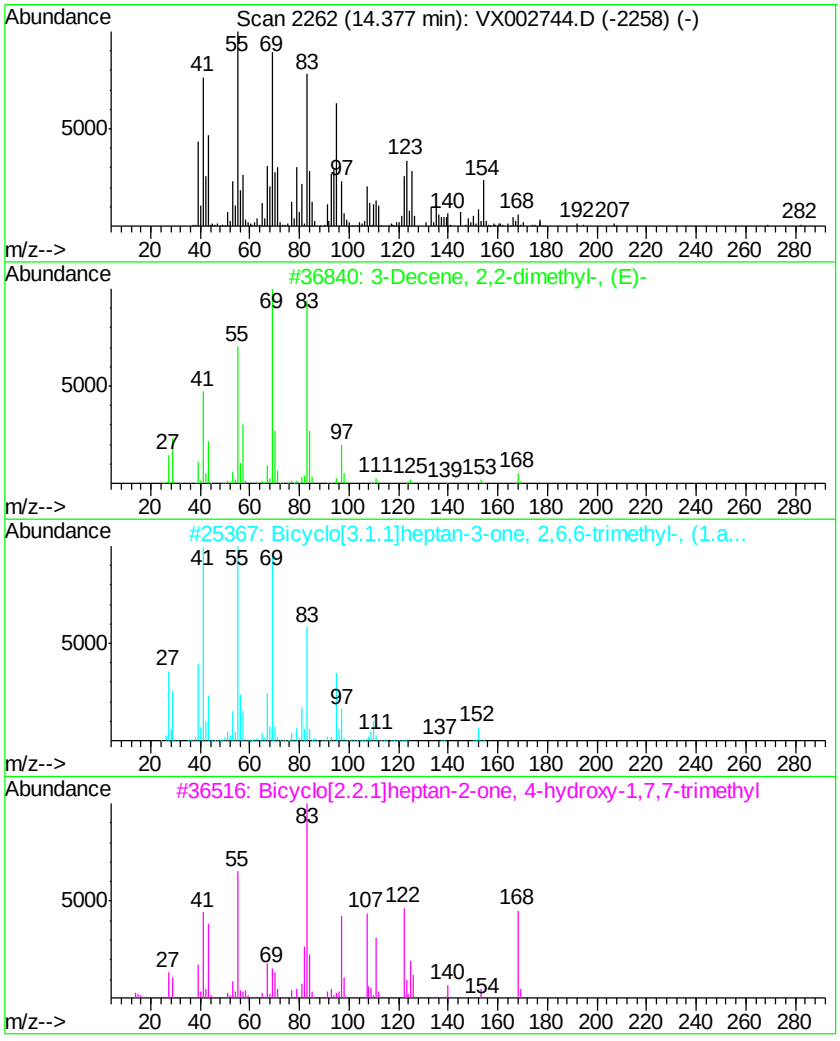
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

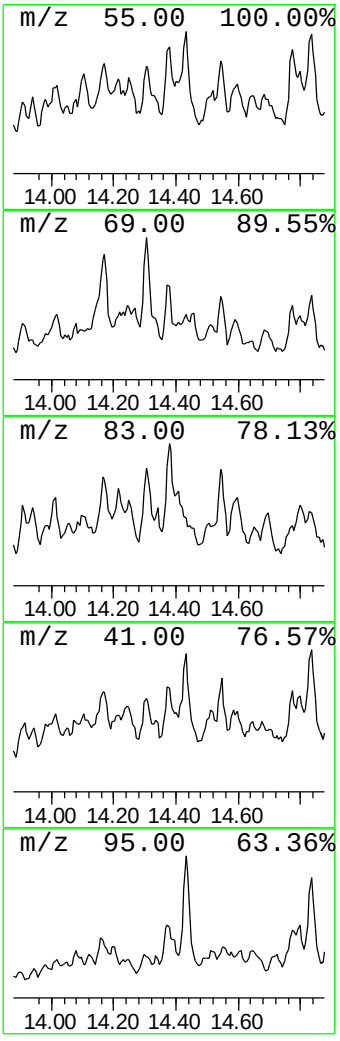
****

Peak Number 4 3-Decene, 2,2-dimethyl-, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	13.37 ug/l	288944	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	50
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	49
3	Bicyclo[2.2.1]heptan-2-one, 4-hy...	168	C10H16O2	055784-66-2	46
4	2-sec-Butyl-3-methyl-1-pentene	140	C10H20	075144-24-0	46
5	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	46





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

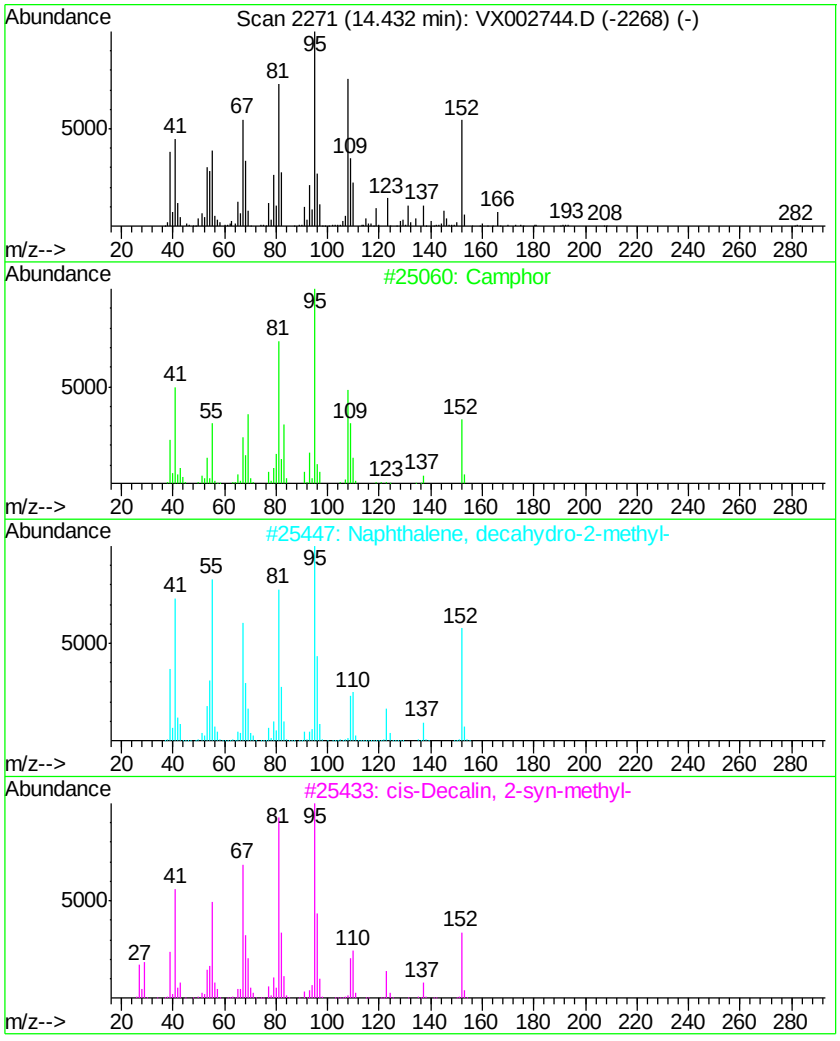
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

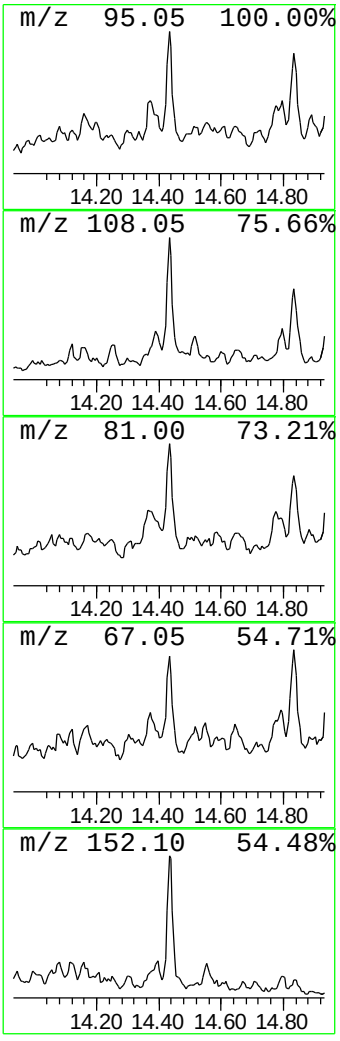
****

Peak Number 5 Camphor Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	15.95 ug/l	344717	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphor	152	C10H16O	000076-22-2	87
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	86
3	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
4	Pulegone	152	C10H16O	000089-82-7	45
5	1,3,3-Trimethylcyclohex-1-ene-4-...	152	C10H16O	127128-60-3	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

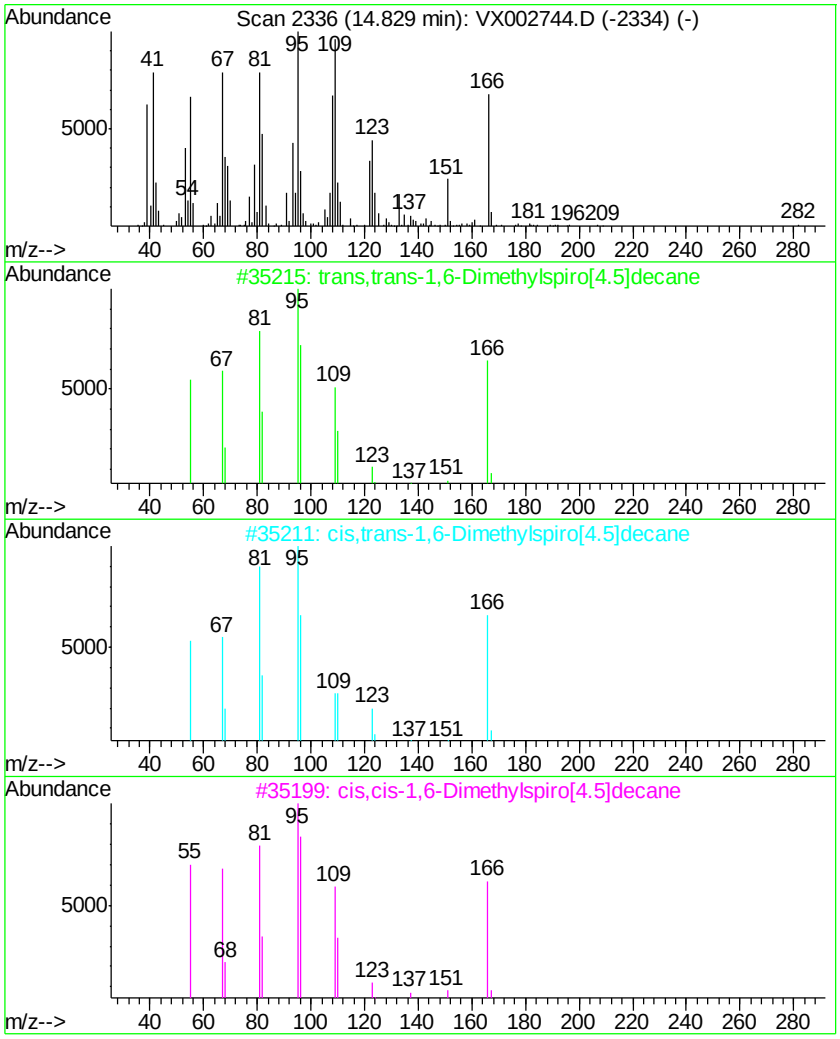
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

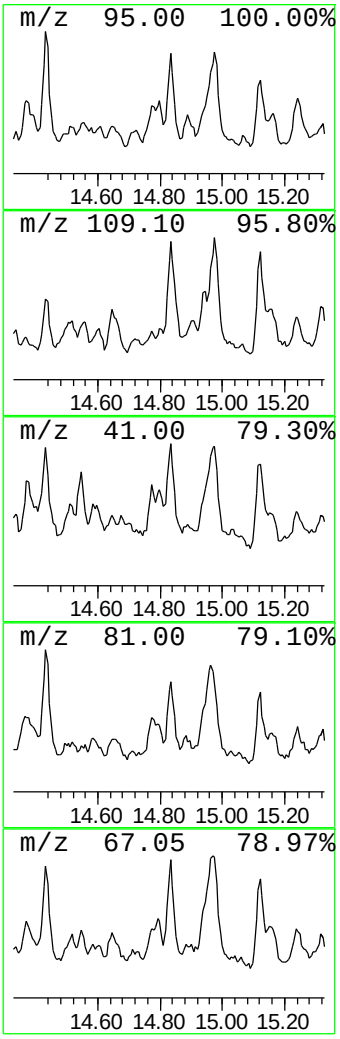
****

Peak Number 6 trans,trans-1,6-Dimethylspi... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	15.11 ug/l	326525	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	64
2	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	64
3	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	58
4	cis-p-mentha-1(7),8-dien-2-ol	152	C10H16O	1000374-16-8	49
5	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	46





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

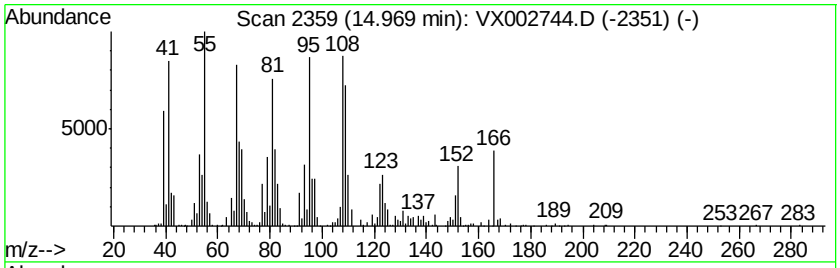
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

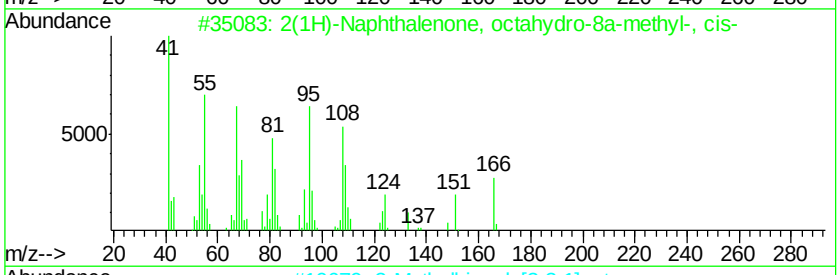
****

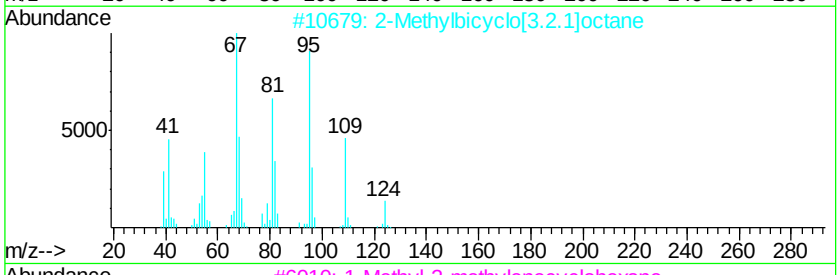
Peak Number 7 2(1H)-Naphthalenone, octahy... Concentration Rank 3

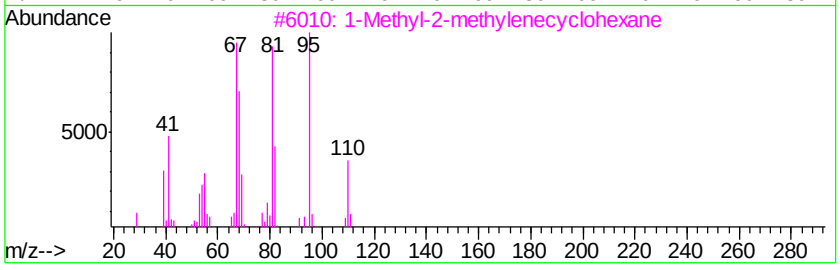
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	29.53 ug/l	638251	1,4-Dichlorobenzene-d4	12.09

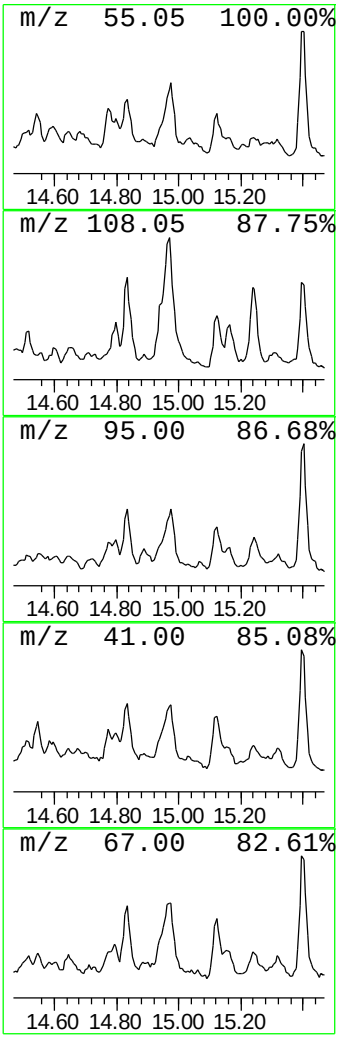
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-8...	166	C11H18O	002530-17-8	70
2	2-Methylbicyclo[3.2.1]octane	124	C9H16	1000215-28-0	55
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	55
4	Hexen-1-ylcyclohexane	166	C12H22	067975-92-2	53
5	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	53











Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
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Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

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

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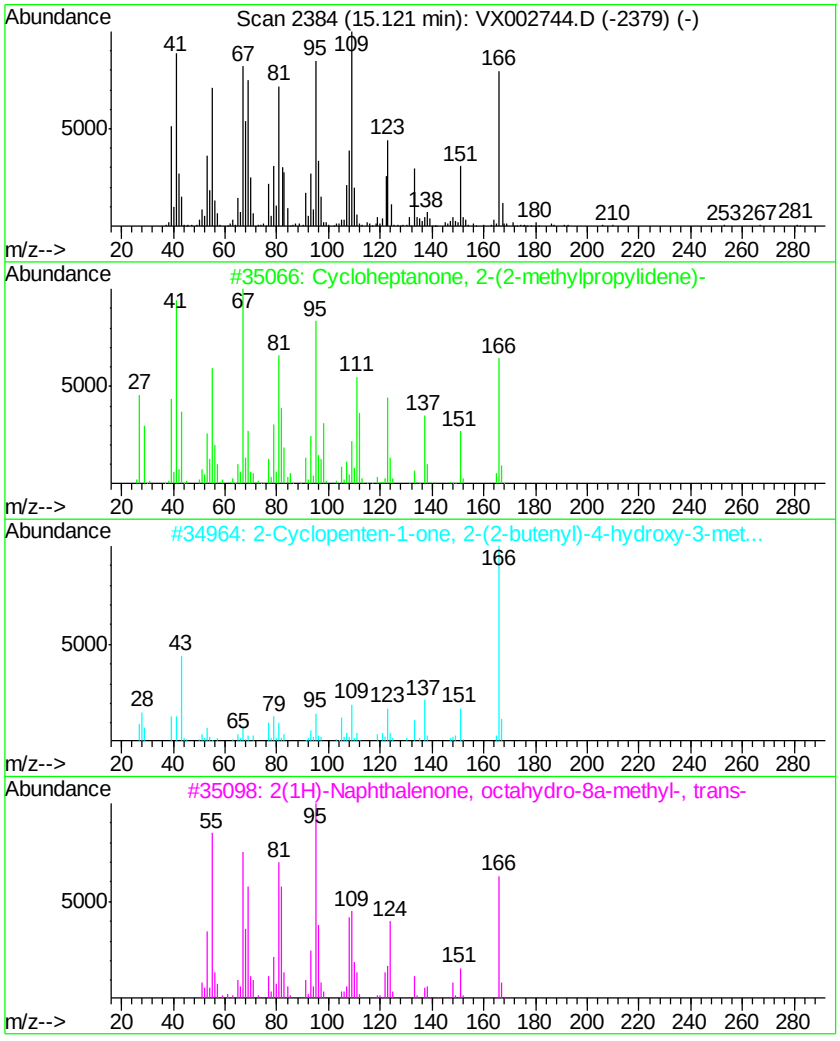
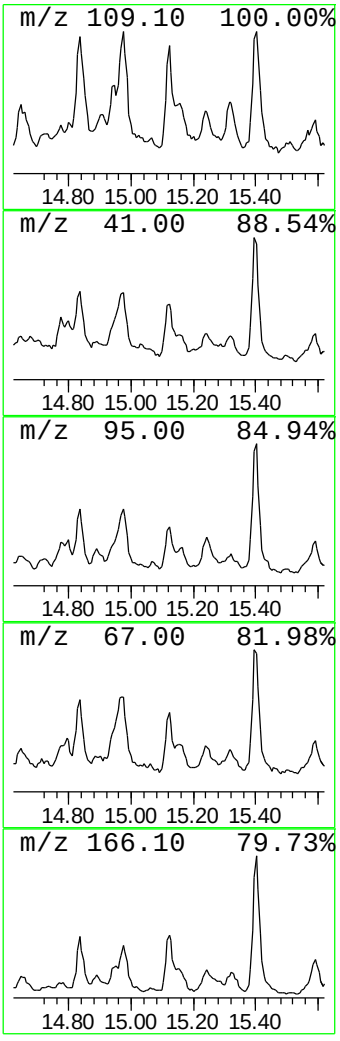
Peak Number 8 Cycloheptanone, 2-(2-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	18.61 ug/l	402176	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptanone, 2-(2-methylpropy...	166	C11H18O	120694-89-5	55
2	2-Cyclopenten-1-one, 2-(2-butenyl...	166	C10H14O2	017190-74-8	55
3	2(1H)-Naphthalenone, octahydro-8...	166	C11H18O	001197-95-1	52
4	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	49
5	3-Tridecene	180	C13H24	060186-78-9	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

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

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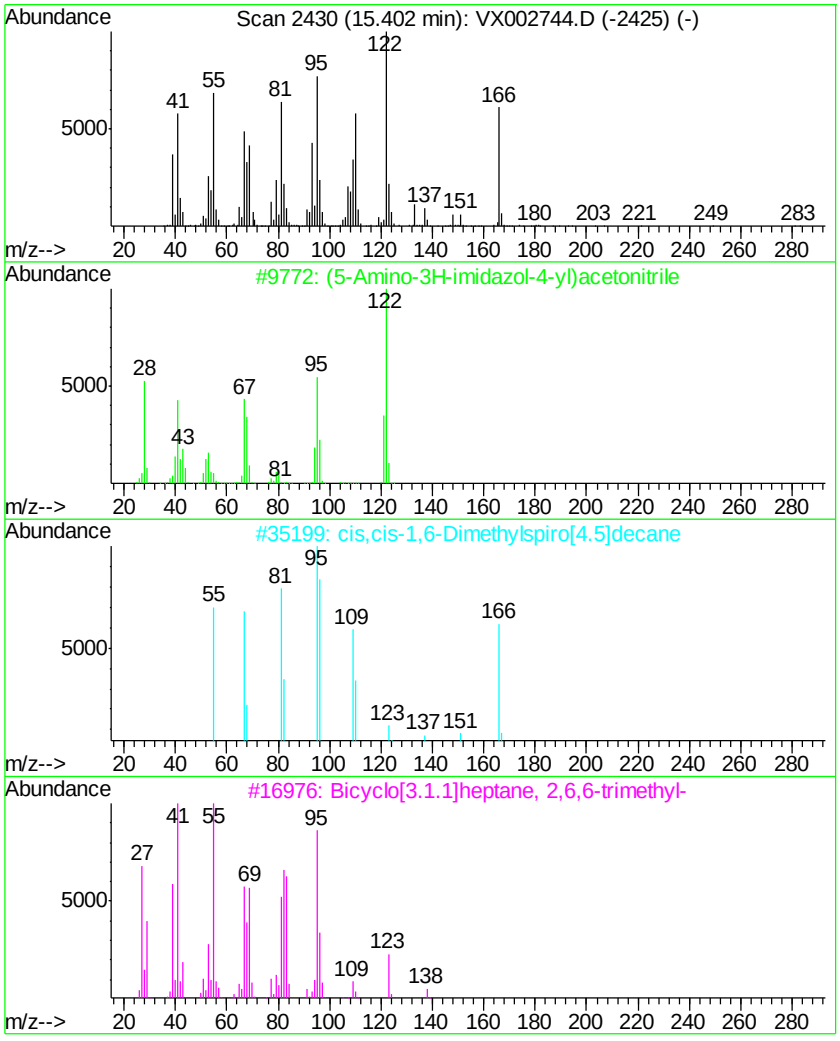
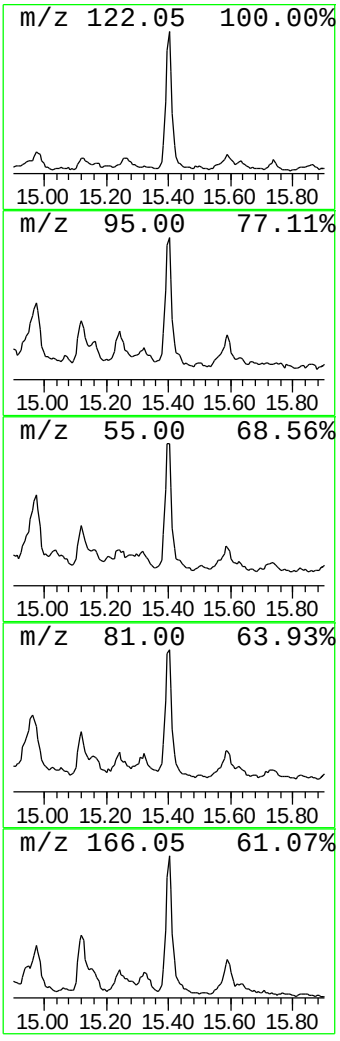
Peak Number 9 (5-Amino-3H-imidazol-4-yl)a... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	42.45 ug/l	917437	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(5-Amino-3H-imidazol-4-yl)aceton...	122	C5H6N4	1000191-16-3	55
2	cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	50
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	42
4	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	42
5	1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX062018\
Data File : VX002744.D
Acq On : 20 Jun 2018 16:20
Operator : JC/MD
Sample : J3596-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.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
Trans-1,4-diethyl...	12.98	11.3	ug/l	243901	4	12.09	1080630	50.0
1-Azabicyclo[2.2....	13.81	10.5	ug/l	227621	4	12.09	1080630	50.0
3-Decene, 2,2-dim...	14.38	13.4	ug/l	288944	4	12.09	1080630	50.0
Camphor	14.43	15.9	ug/l	344717	4	12.09	1080630	50.0
trans,trans-1,6-D...	14.83	15.1	ug/l	326525	4	12.09	1080630	50.0
2(1H)-Naphthaleno...	14.97	29.5	ug/l	638251	4	12.09	1080630	50.0
Cycloheptanone, 2...	15.12	18.6	ug/l	402176	4	12.09	1080630	50.0
(5-Amino-3H-imida...	15.40	42.5	ug/l	917437	4	12.09	1080630	50.0