LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011421\
Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1717-1718

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\82X011121W.M
Title : SW846 8260

Signal : TIC: VX020626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.636	75	90	91	rBV7	9120	30357	3.22%	0.350%
2	2.770	268	276	280	rBV	5961	15121	1.60%	0.174%
3	5.465	706	718	732	rBV2	105936	323974	34.34%	3.738%
4	5.623	732	744	760	rVB	192556	548200	58.10%	6.325%
5	6.032	800	811	826	rBV	110439	308835	32.73%	3.564%
6	6.824	931	941	956	rBV	280904	689072	73.03%	7.951%
7	8.696	1240	1248	1257	rBV	584837	943485	100.00%	10.886%
8	10.098	1471	1478	1488	rBV	563248	835046	88.51%	9.635%
9	11.122	1640	1646	1658	rBV	460605	634653	67.27%	7.323%
10	11.348	1673	1683	1688	rBV	49035	66079	7.00%	0.762%
11	12.061	1795	1800	1808	rVB	598484	816062	86.49%	9.416%
12	12.146	1808	1814	1823	rVB	61515	85183	9.03%	0.983%
13	12.256	1827	1832	1845	rBV	39583	71483	7.58%	0.825%
14	12.908	1934	1939	1949	rVB2	10547	17348	1.84%	0.200%
15	13.012	1951	1956	1965	rBV	26096	47300	5.01%	0.546%
16	13.110	1968	1972	1975	rVV2	14436	22703	2.41%	0.262%
17	13.140	1975	1977	1984	rVV6	10432	19015	2.02%	0.219%
18	13.555	2039	2045	2053	rBV	46442	70802	7.50%	0.817%
19	13.634	2054	2058	2067	rVB	4793	10247	1.09%	0.118%
20	13.744	2068	2076	2081	rBV	278372	380143	40.29%	4.386%
21	13.786	2081	2083	2096	rVV2	49166	112170	11.89%	1.294%
22	13.896	2096	2101	2103	rVV2	30147	47079	4.99%	0.543%
23	13.926	2104	2106	2118	rVB5	30708	71791	7.61%	0.828%
24	14.146	2138	2142	2149	rVB	83093	101213	10.73%	1.168%
25	14.268	2157	2162	2167	rBV5	9688	18693	1.98%	0.216%
26	14.402	2181	2184	2187	rBV4	10759	15384	1.63%	0.178%
27	14.445	2187	2191	2195	rVV	297885	353181	37.43%	4.075%
28	14.481	2195	2197	2201	rVV	41114	65971	6.99%	0.761%
29	14.524	2201	2204	2212	rVB5	55026	99521	10.55%	1.148%
30	14.591	2212	2215	2218	rBV4	9844	16768	1.78%	0.193%
31	14.658	2219	2226	2232	rVV4	68314	157201	16.66%	1.814%
32	14.713	2232	2235	2239	rVB2	53952	64772	6.87%	0.747%
33	14.817	2246	2252	2257	rBV6	29870	71460	7.57%	0.825%
34	14.865	2257	2260	2261	rVV2	11554	14685	1.56%	0.169%
35	14.890	2261	2264	2267	rVB2	34302	43824	4.64%	0.506%
36	15.085	2291	2296	2300	rBV4	36888	73597	7.80%	0.849%

LSC Area Percent Report

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Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1717-1718

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Title : SW846 8260

37	15.231	2315	2320	2322	rBV	70921	115872	12.28%	1.337%
38	15.292	2327	2330	2333	rBV3	27952	45794	4.85%	0.528%
39	15.365	2338	2342	2347	rVB6	36363	69359	7.35%	0.800%
40	15.426	2348	2352	2355	rBV4	53684	80802	8.56%	0.932%
41	15.469	2355	2359	2362	rBV4	37330	57710	6.12%	0.666%
42	15.536	2365	2370	2372	rBV3	71630	116242	12.32%	1.341%
43	15.591	2376	2379	2381	rVV2	43542	60206	6.38%	0.695%
44	15.621	2381	2384	2386	rVV3	59237	86369	9.15%	0.997%
45	15.658	2386	2390	2395	rVB2	111741	202946	21.51%	2.342%
46	15.902	2426	2430	2442	rBV6	70945	227593	24.12%	2.626%
47	16.030	2447	2451	2456	rVV3	131032	236253	25.04%	2.726%
48	16.152	2467	2471	2476	rBV7	52275	105013	11.13%	1.212%

Sum of corrected areas: 8666577

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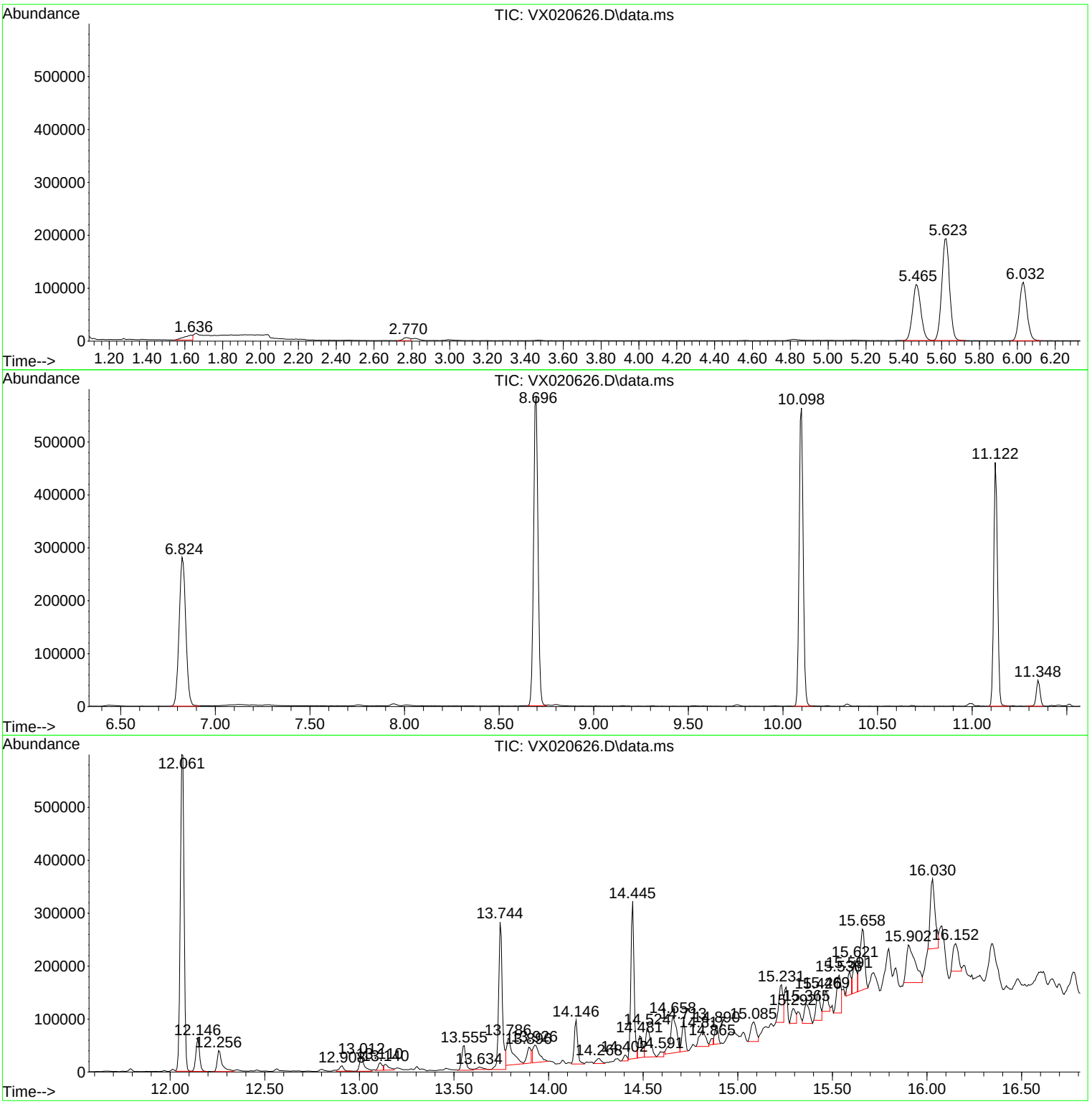
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011421\
Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
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Instrument :
MSVOA_X
ClientSampleId :
1717-1718

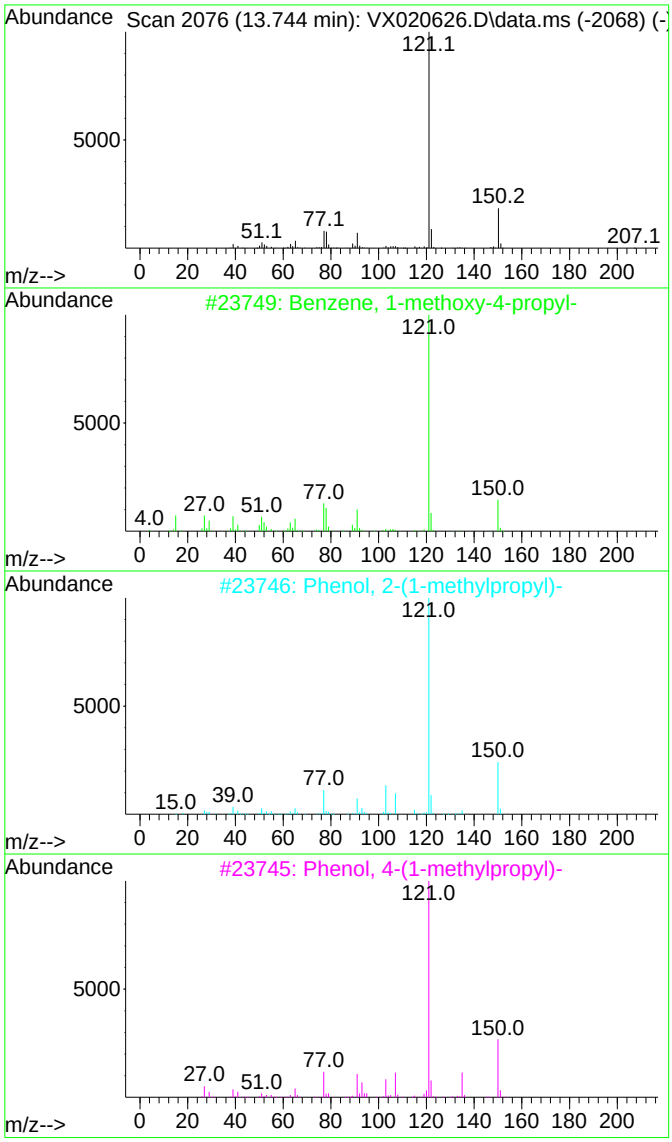
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

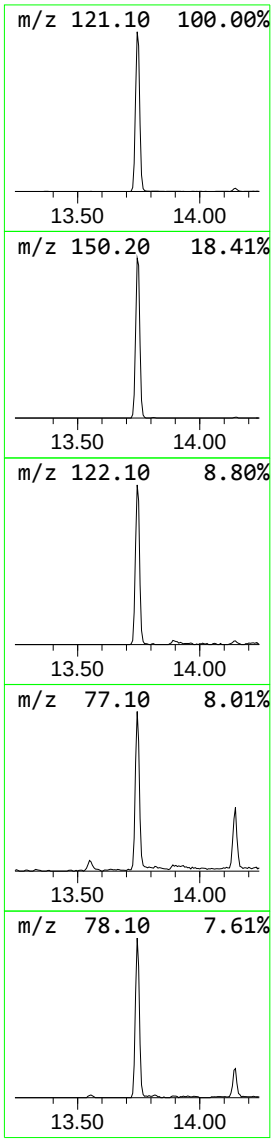
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-methoxy-4-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.744	23.29 ug/l	380143	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	72
4	Paroxypropione	150	C9H10O2	000070-70-2	72
5	ortho-Hydroxypropiophenone	150	C9H10O2	000610-99-1	72





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Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

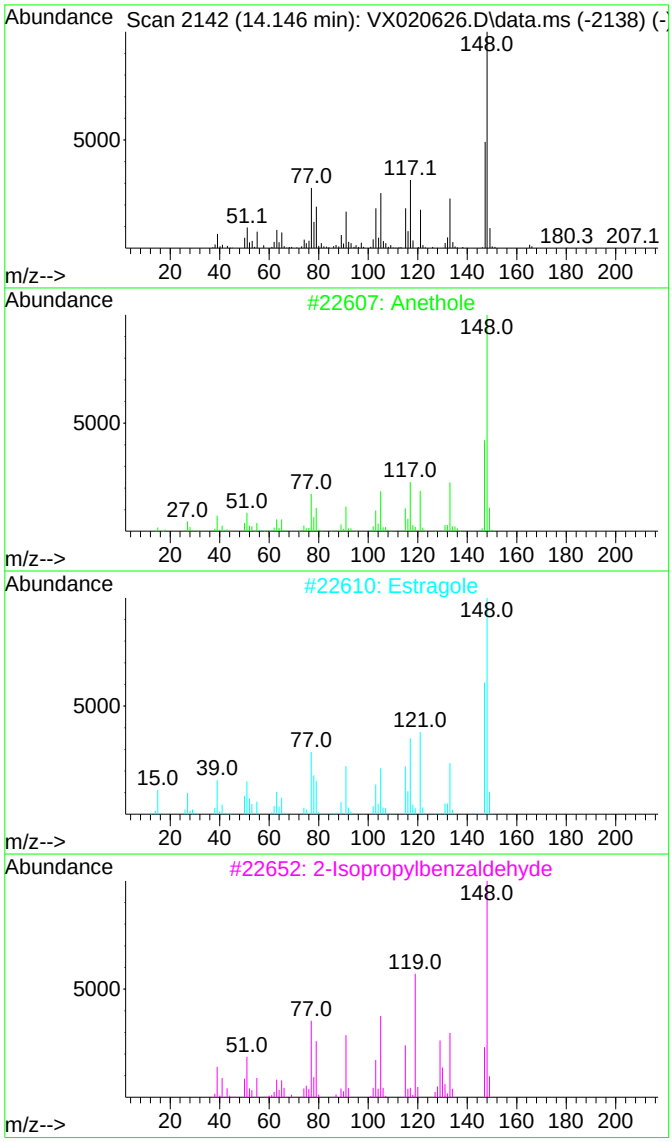
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

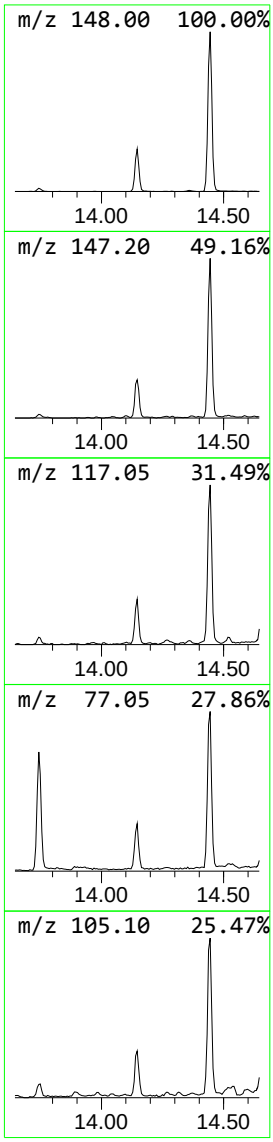
****

Peak Number 2 Anethole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.146	6.20 ug/l	101213	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole	148	C10H12O	000104-46-1	95
2	Estragole	148	C10H12O	000140-67-0	90
3	2-Isopropylbenzaldehyde	148	C10H12O	006502-22-3	68
4	Methanimidamide, N,N-dimethyl-N'...	148	C9H12N2	001783-25-1	58
5	3H-Indazol-3-one, 1,2-dihydro-1-...	148	C8H8N2O	001006-19-5	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011421\
Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

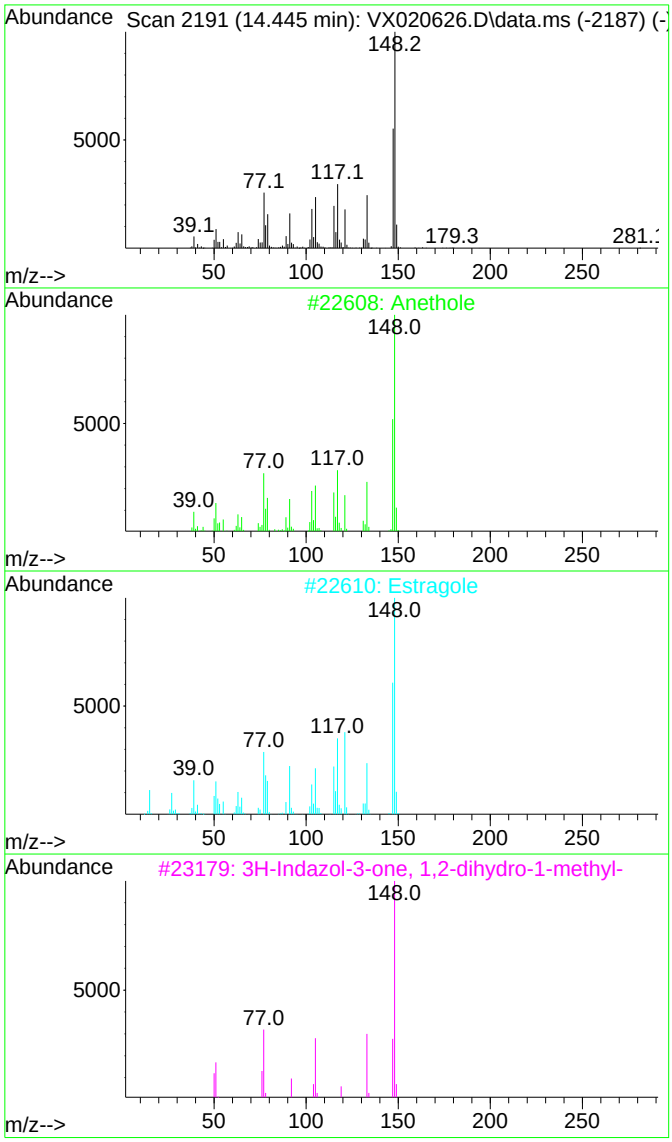
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

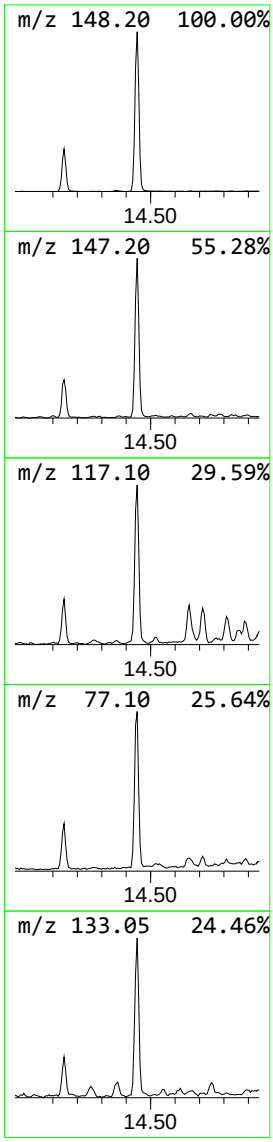
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Estragole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	21.64 ug/l	353181	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole	148	C10H12O	000104-46-1	98
2	Estragole	148	C10H12O	000140-67-0	94
3	3H-Indazol-3-one, 1,2-dihydro-1-...	148	C8H8N2O	001006-19-5	52
4	2-(1-Propenyl)-6-methylphenol	148	C10H12O	1000306-52-9	52
5	Benzene, (1-propynylthio)-	148	C9H8S	006212-77-7	50





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Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

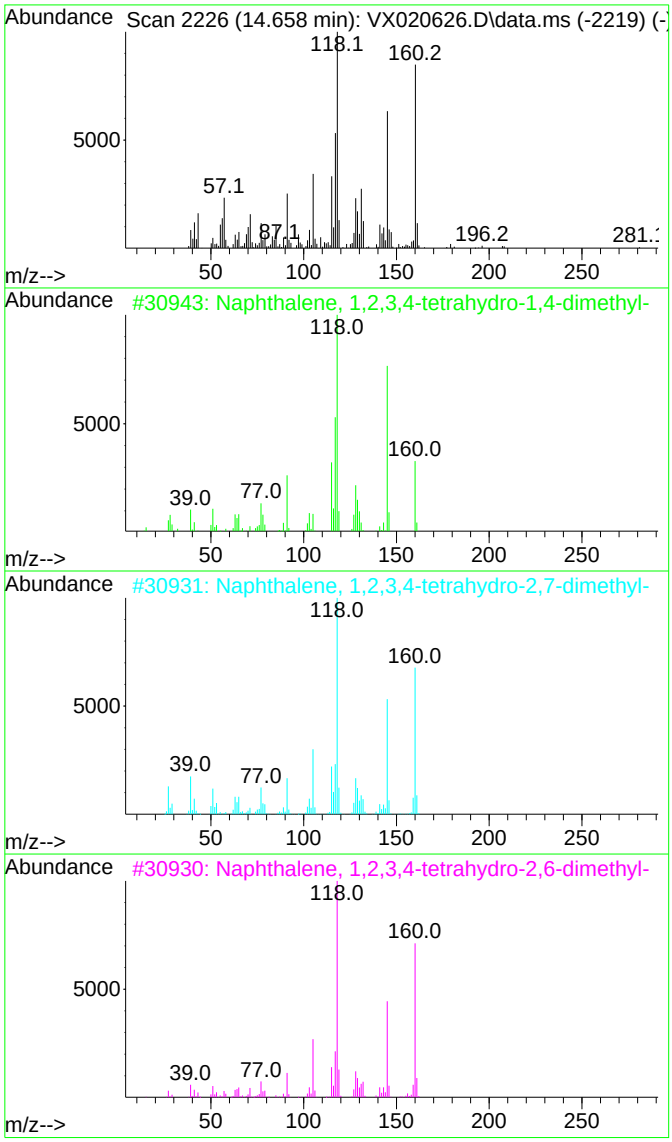
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

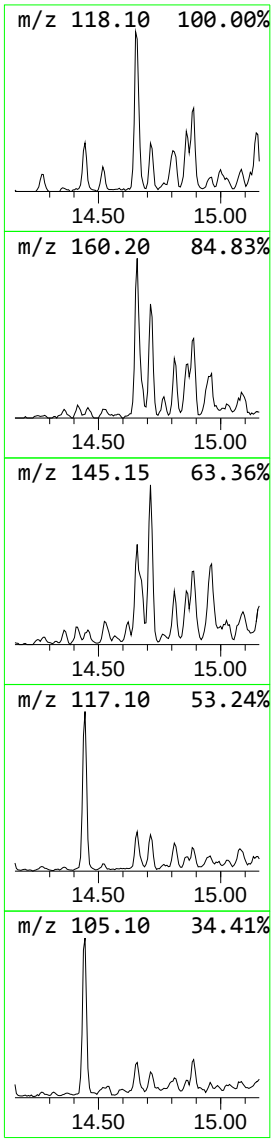
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.658	9.63 ug/l	157201	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	87
4	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	62
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	55





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Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

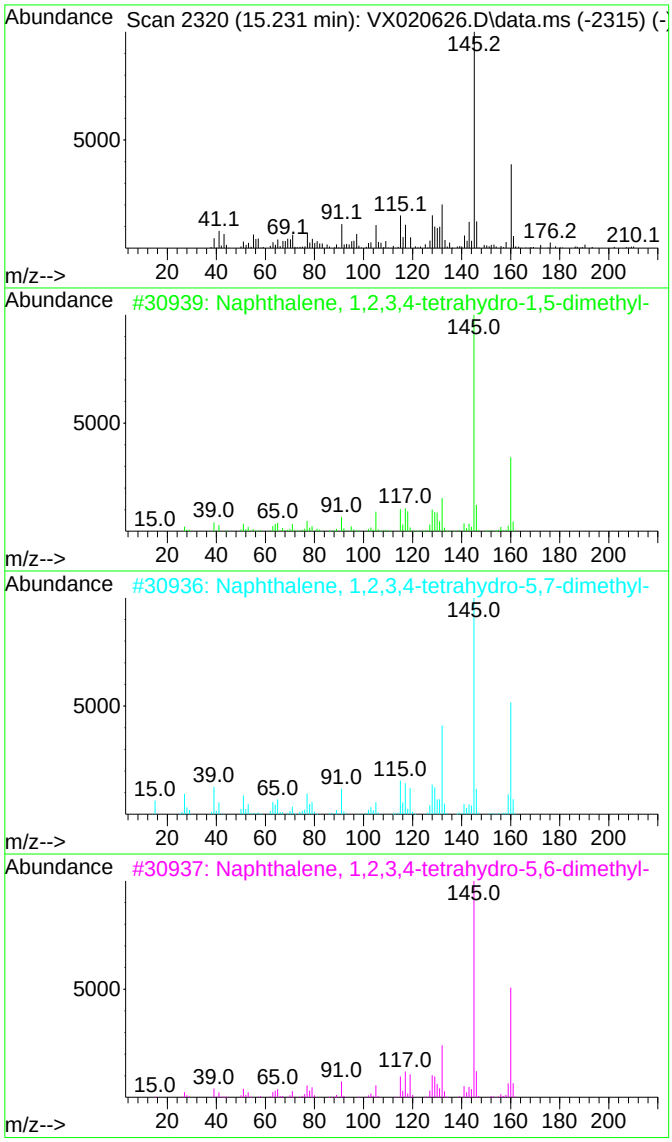
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

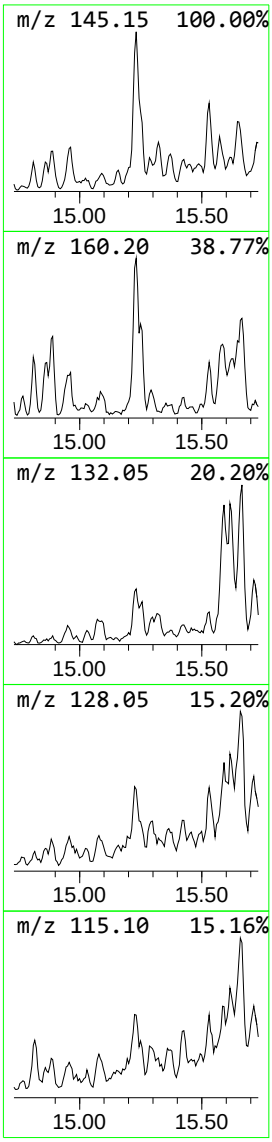
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.231	7.10 ug/l	115872	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	94
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	90
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	87
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	81





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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

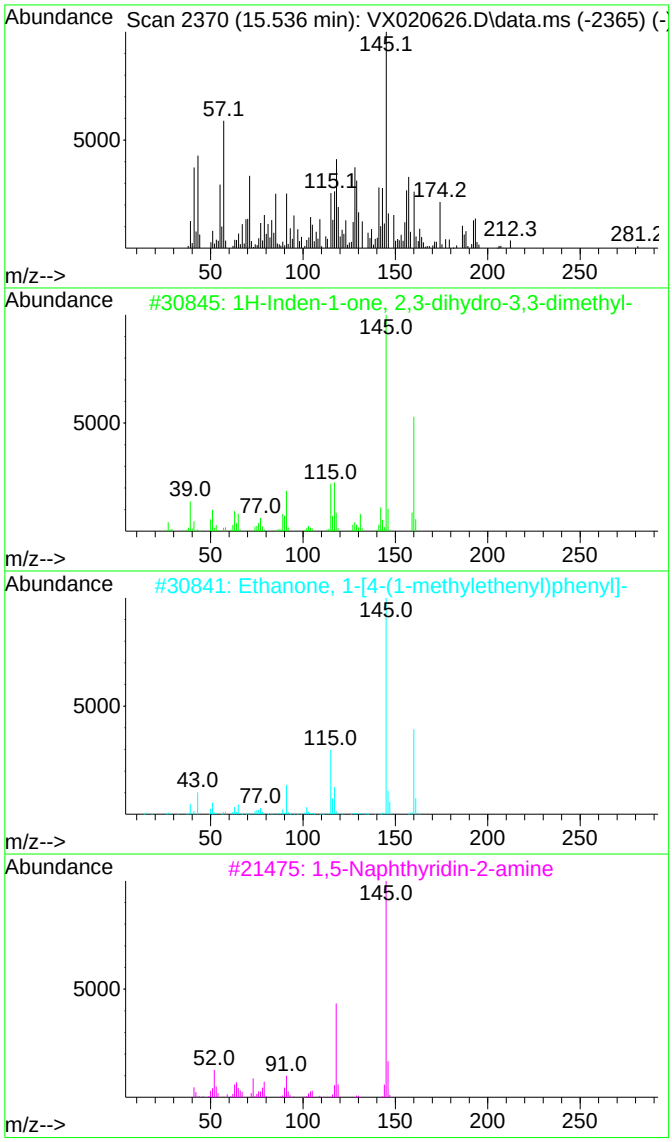
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

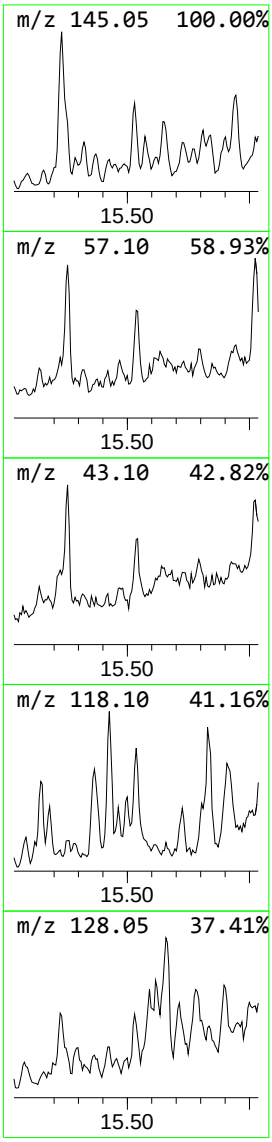
****

Peak Number 6 unknown15.536 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	7.12 ug/l	116242	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	38
2	Ethanone, 1-[4-(1-methylethenyl)...	160	C11H12O	005359-04-6	38
3	1,5-Naphthyridin-2-amine	145	C8H7N3	017965-80-9	35
4	3-(1H-Pyrazol-4-yl)pyridine	145	C8H7N3	1000311-62-5	35
5	Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	30





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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

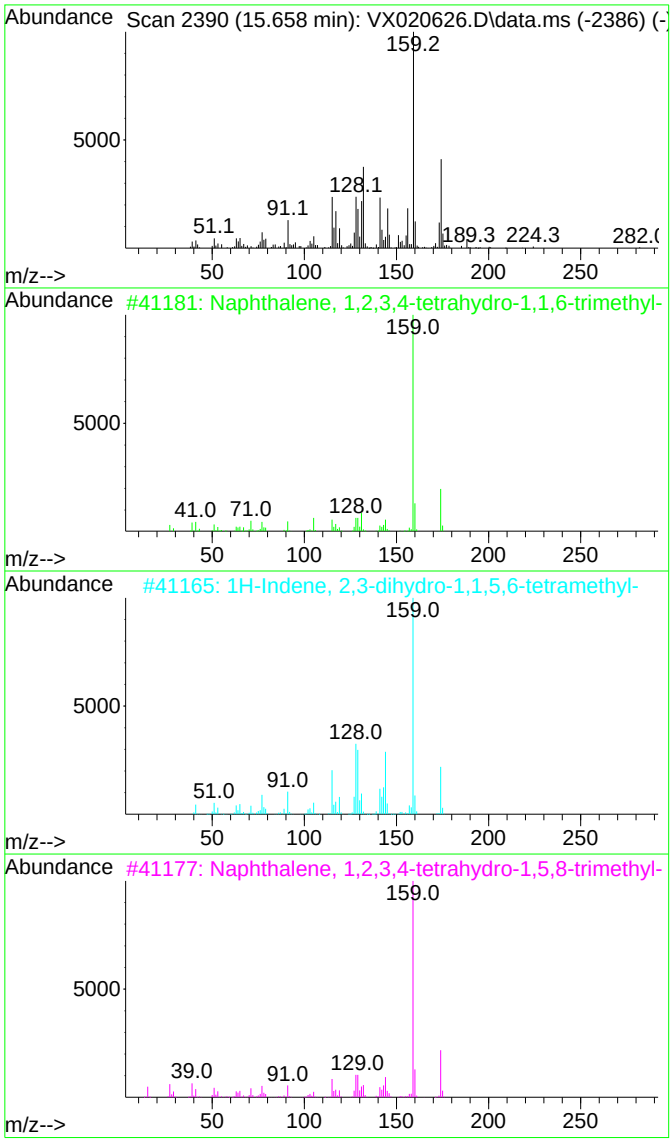
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

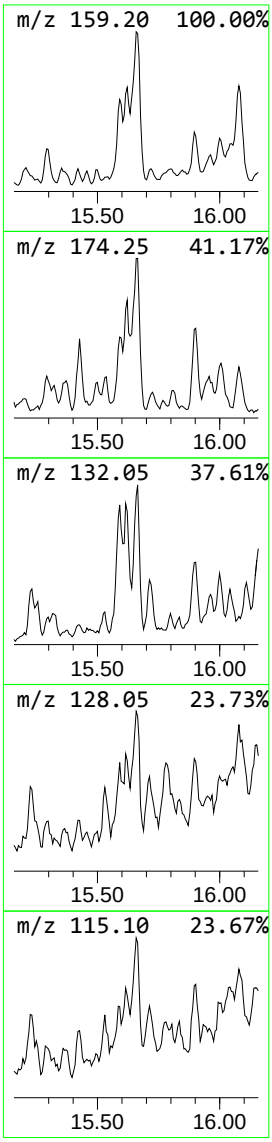
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.658	12.43 ug/l	202946	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	89
2	1H-Indene, 2,3-dihydro-1,1,5,6-t...	174	C13H18	000942-43-8	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	64
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	62
5	1H-Indene, 2,3-dihydro-1,1,4,5-t...	174	C13H18	016204-57-2	60





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Instrument :
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ClientSampleId :
1717-1718

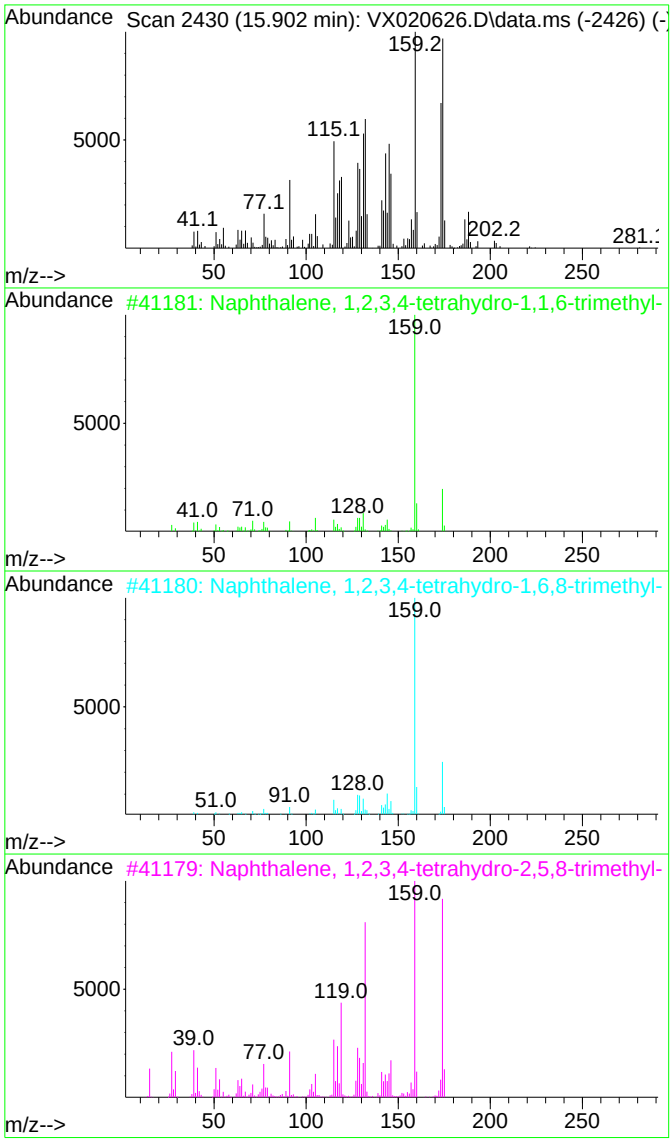
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

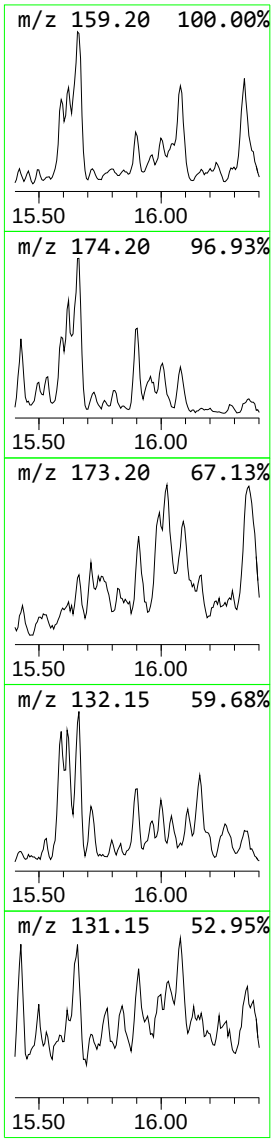
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.902	13.94 ug/l	227593	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	60
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	55
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-17-7	55
4	Benzene, 1,2,3,4-tetramethyl-4-(...	174	C13H18	061142-76-5	50
5	7-Methoxy-8-aminoisoquinoline	174	C10H10N2O	055766-74-0	43





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Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

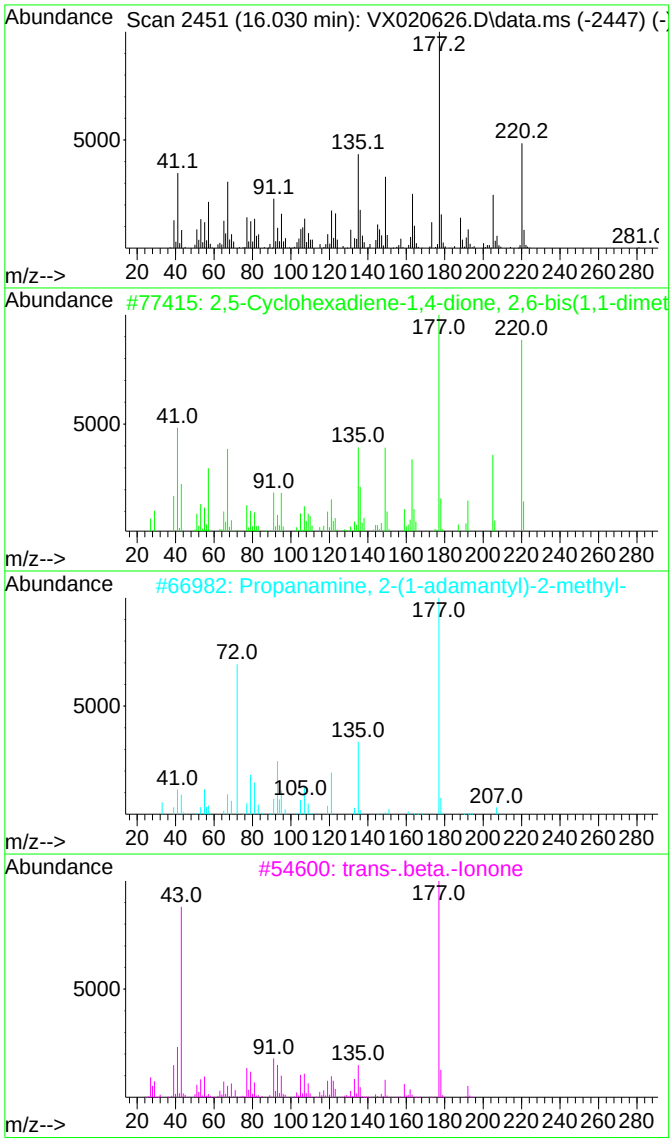
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

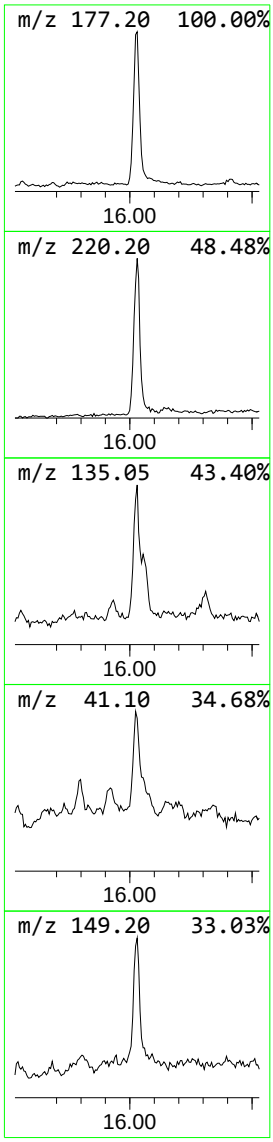
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.030	14.48 ug/l	236253	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2	Propanamine, 2-(1-adamantyl)-2-m...	207	C14H25N	079594-24-4	45
3	trans-.beta.-Ionone	192	C13H20O	000079-77-6	42
4	1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	35
5	Benzofuran-2-one, 4-amino-2,3-di...	177	C10H11NO2	1000129-51-7	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011421\
Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1717-1718

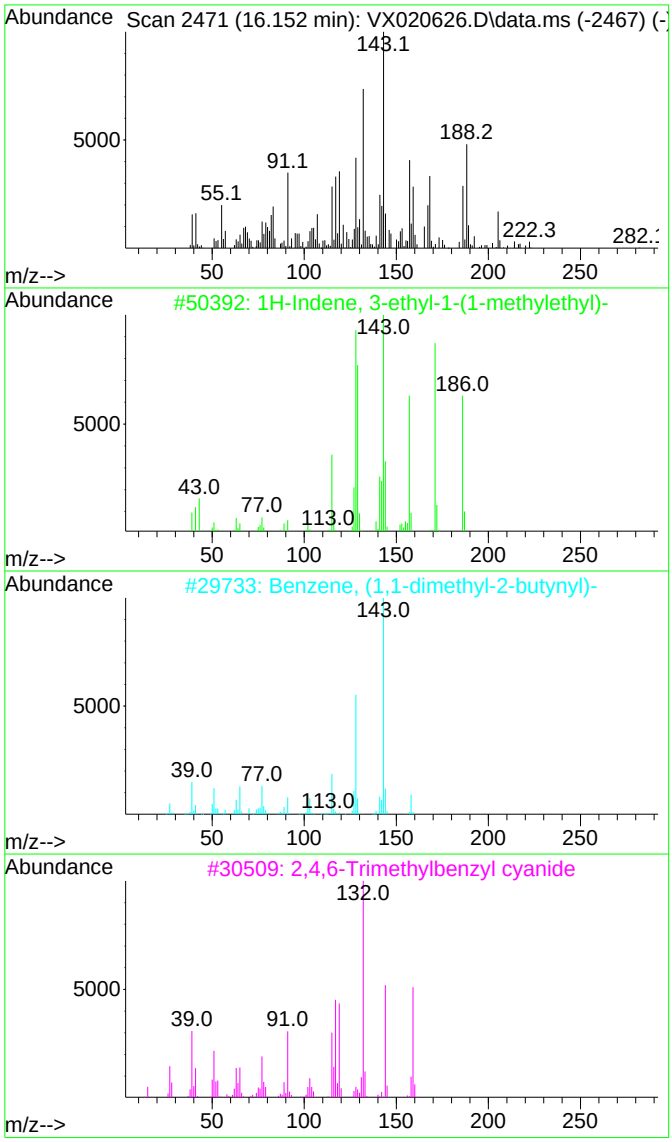
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.M
Quant Title : SW846 8260

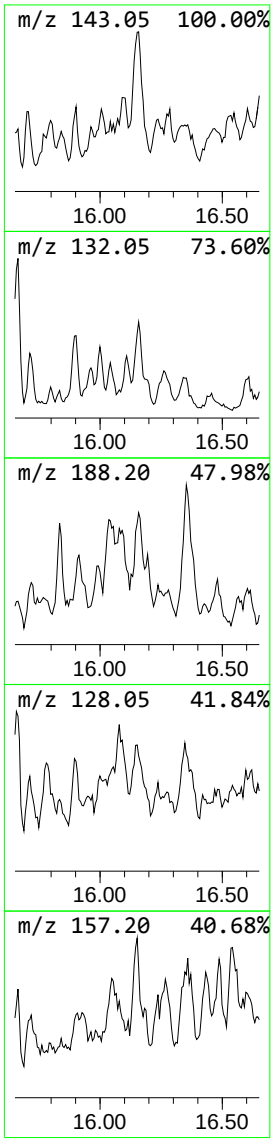
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.152 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.152	6.43 ug/l	105013	1,4-Dichlorobenzene-d4	12.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 3-ethyl-1-(1-methylet...	186	C14H18	111400-85-2	25
2	Benzene, (1,1-dimethyl-2-butynyl)-	158	C12H14	001007-91-6	20
3	2,4,6-Trimethylbenzyl cyanide	159	C11H13N	034688-71-6	15
4	2-Butanone, 4-(2,3-dihydro-1H-in...	189	C12H15NO	040135-92-0	11
5	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011421\
Data File : VX020626.D
Acq On : 14 Jan 2021 20:26
Operator : JC/MD
Sample : M1125-01
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1717-1718

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011121W.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
Benzene, 1-meth...	13.744	23.3	ug/l	380143	4	12.067	816062	50.0
Anethole	14.146	6.2	ug/l	101213	4	12.067	816062	50.0
Estragole	14.445	21.6	ug/l	353181	4	12.067	816062	50.0
Naphthalene, 1,...	14.658	9.6	ug/l	157201	4	12.067	816062	50.0
Naphthalene, 1,...	15.231	7.1	ug/l	115872	4	12.067	816062	50.0
unknown15.536	15.536	7.1	ug/l	116242	4	12.067	816062	50.0
Naphthalene, 1,...	15.658	12.4	ug/l	202946	4	12.067	816062	50.0
Naphthalene, 1,...	15.902	13.9	ug/l	227593	4	12.067	816062	50.0
2,5-Cyclohexadi...	16.030	14.5	ug/l	236253	4	12.067	816062	50.0
unknown16.152	16.152	6.4	ug/l	105013	4	12.067	816062	50.0