LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

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\82X032923W.M
Title : SW846 8260

Signal : TIC: VX035082.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	210	219	264	rBV	1680915	5115429	16.34%	8.044%
2	5.385	695	705	710	rBV	151691	445535	1.42%	0.701%
3	5.489	710	722	736	rVV4	1323659	5536187	17.68%	8.706%
4	5.605	736	741	760	rVB	359421	1070797	3.42%	1.684%
5	5.812	760	775	789	rBV	1482941	4314081	13.78%	6.784%
6	5.952	789	798	811	rBV	186162	497596	1.59%	0.782%
7	6.165	819	833	841	rBV6	146861	617386	1.97%	0.971%
8	6.342	854	862	881	rVB2	130216	378946	1.21%	0.596%
9	6.598	891	904	916	rBV	1414710	3410288	10.89%	5.363%
10	6.757	920	930	949	rVB	473613	1140220	3.64%	1.793%
11	7.372	1020	1031	1043	rBV	773125	1747001	5.58%	2.747%
12	8.647	1235	1240	1245	rBV	943382	1481985	4.73%	2.330%
13	8.720	1245	1252	1265	rVB	18952654	31313798	100.00%	49.241%
14	10.055	1466	1471	1480	rVB	912943	1244790	3.98%	1.957%
15	11.085	1634	1640	1647	rBV	709775	1019871	3.26%	1.604%
16	12.024	1789	1794	1800	rBV	948304	1234058	3.94%	1.941%
17	14.639	2216	2223	2226	rBV	733165	1072028	3.42%	1.686%
18	14.780	2240	2246	2250	rVB	378847	490207	1.57%	0.771%
19	15.188	2307	2313	2320	rBV4	188013	398649	1.27%	0.627%
20	15.560	2369	2374	2379	rBV	759421	1064690	3.40%	1.674%

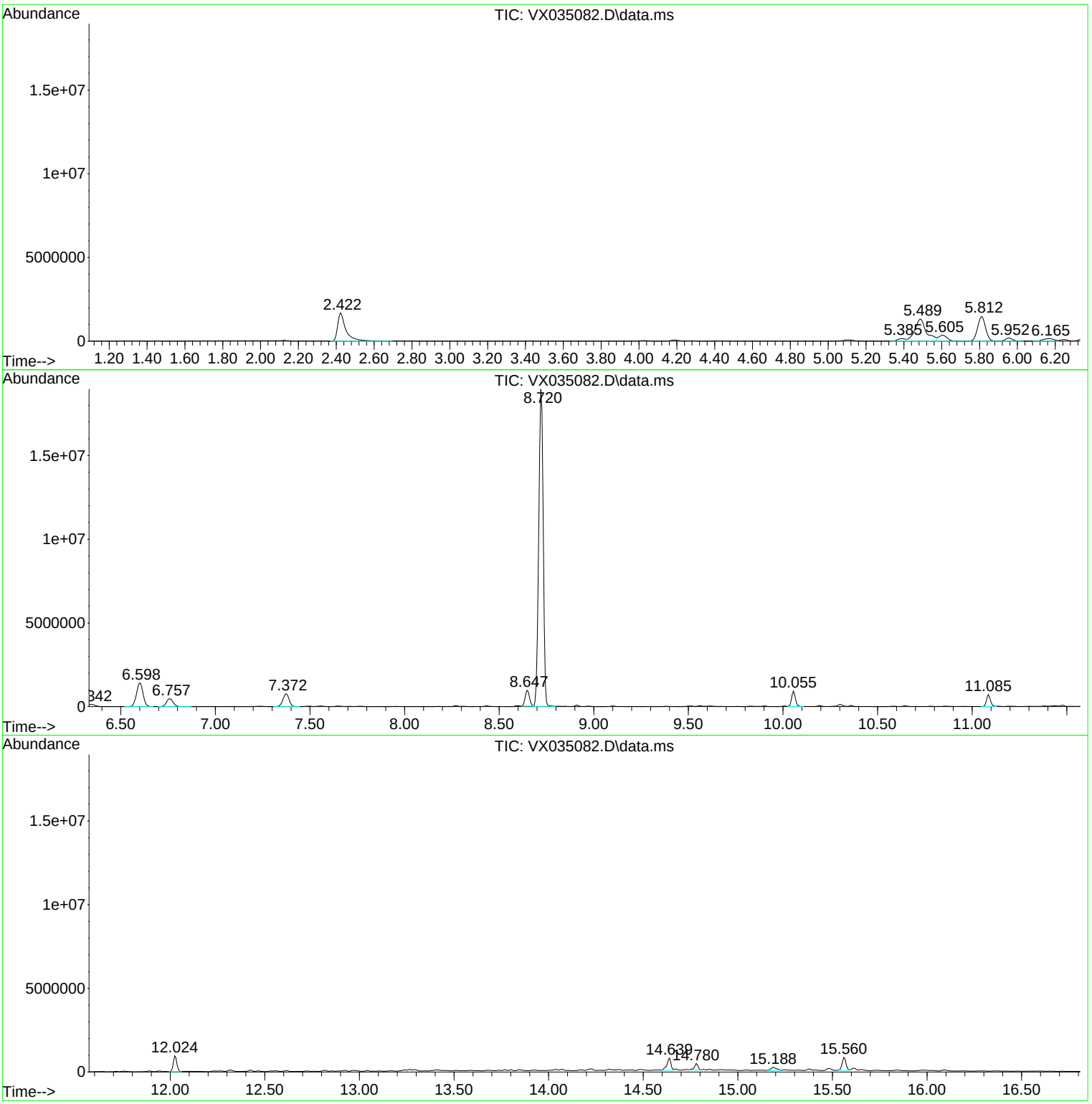
Sum of corrected areas: 63593542

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

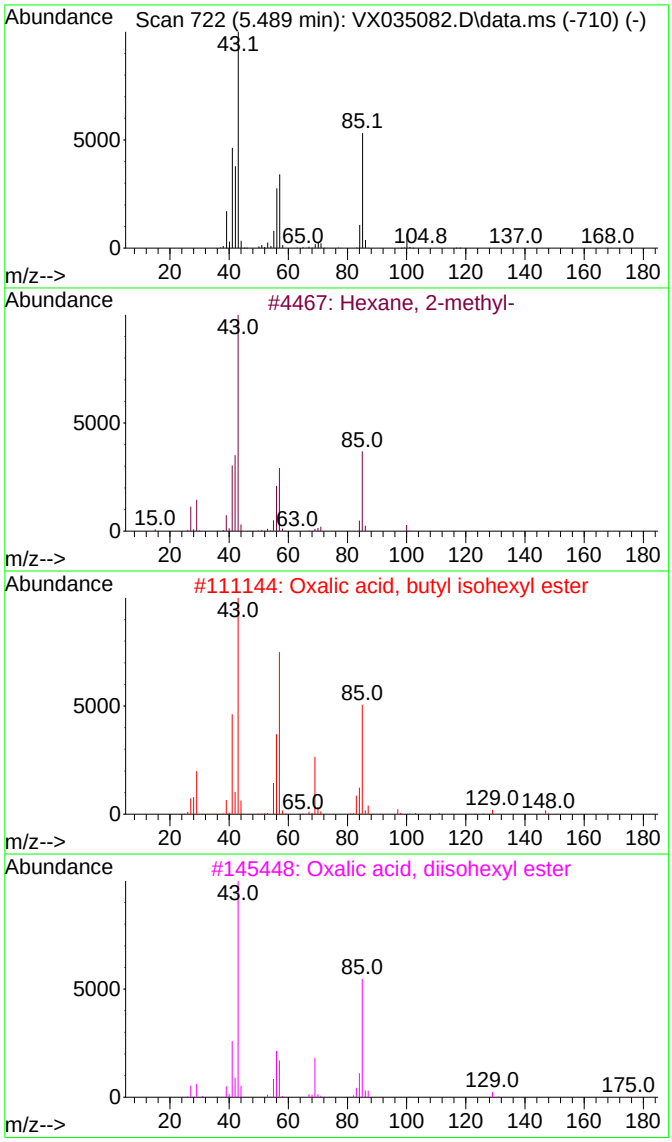
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

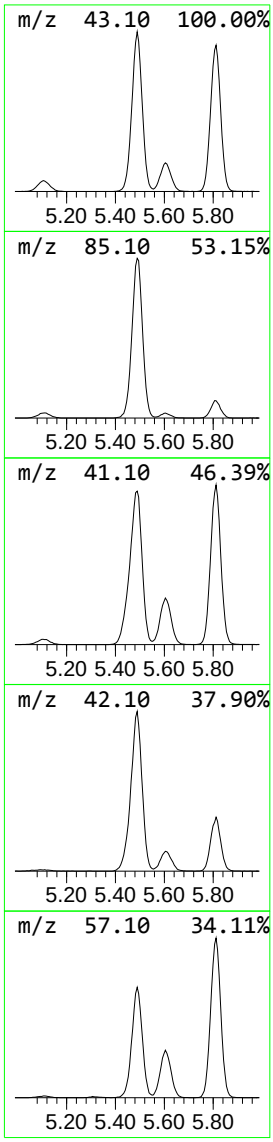
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.489	258.51 ug/l	5536190	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2-methyl-	100	C7H16	000591-76-4	90
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	56
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
5	Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

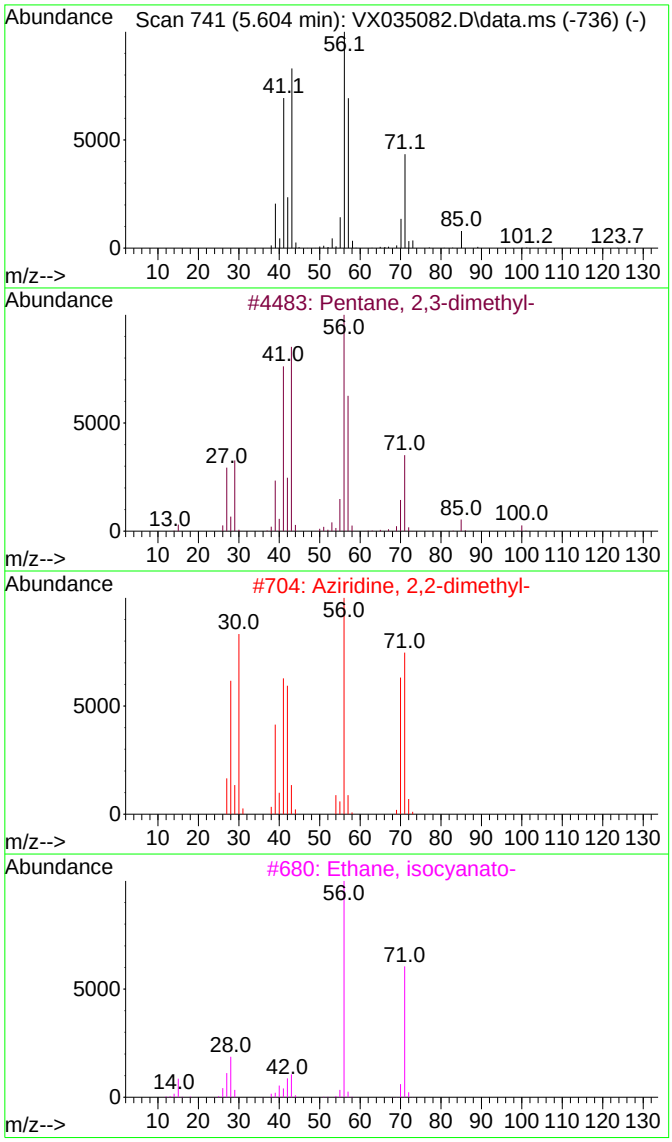
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

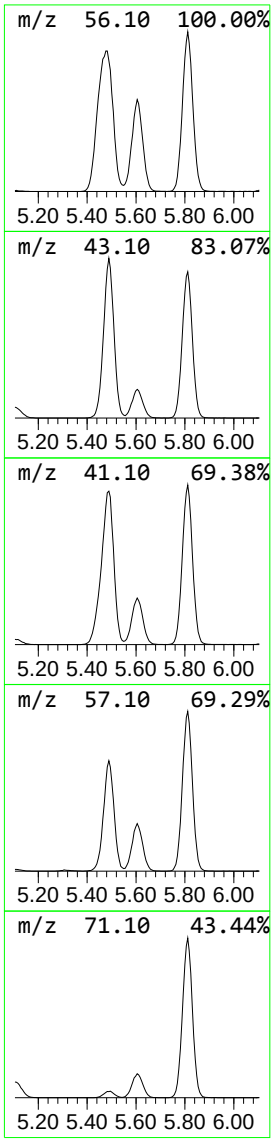
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.604	50.00 ug/l	1070800	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	50
3	Ethane, isocyanato-	71	C3H5NO	000109-90-0	42
4	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

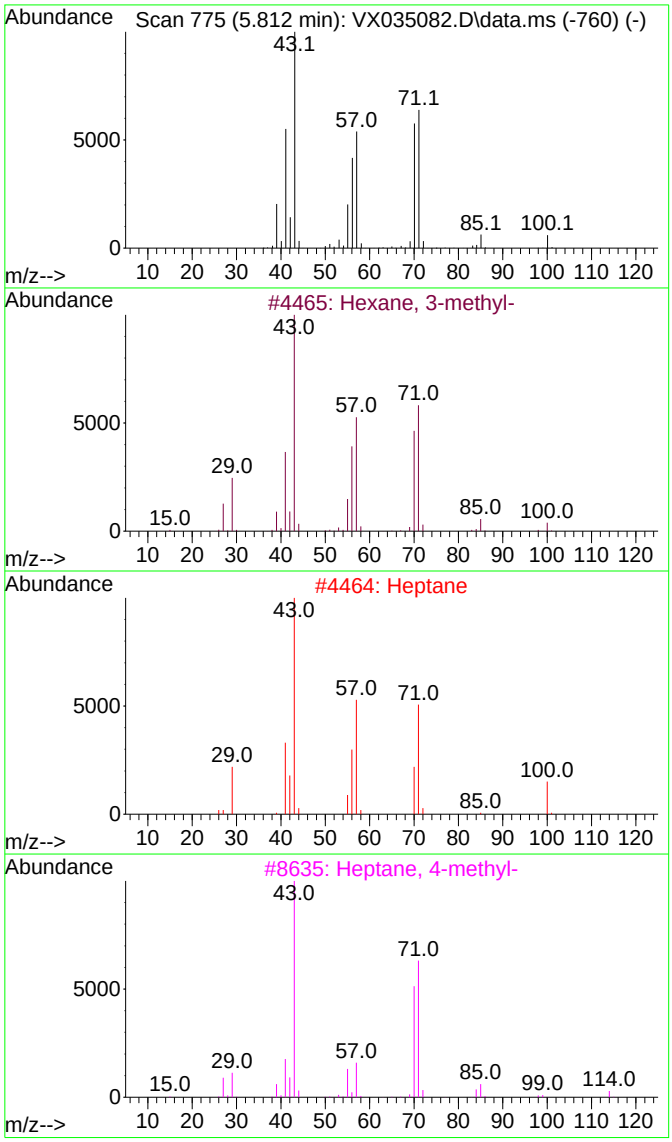
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

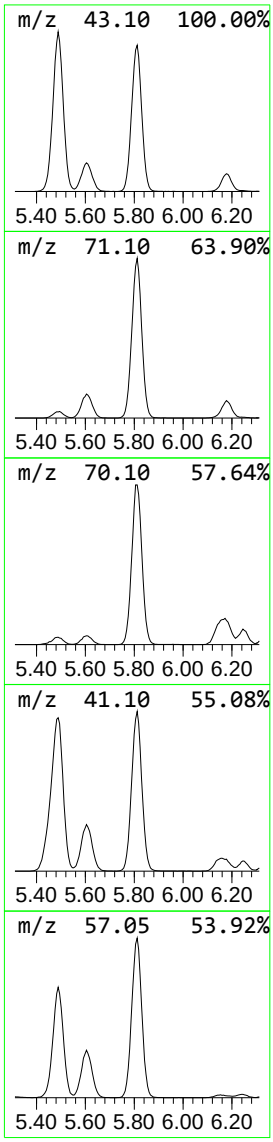
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	201.44 ug/l	4314080	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

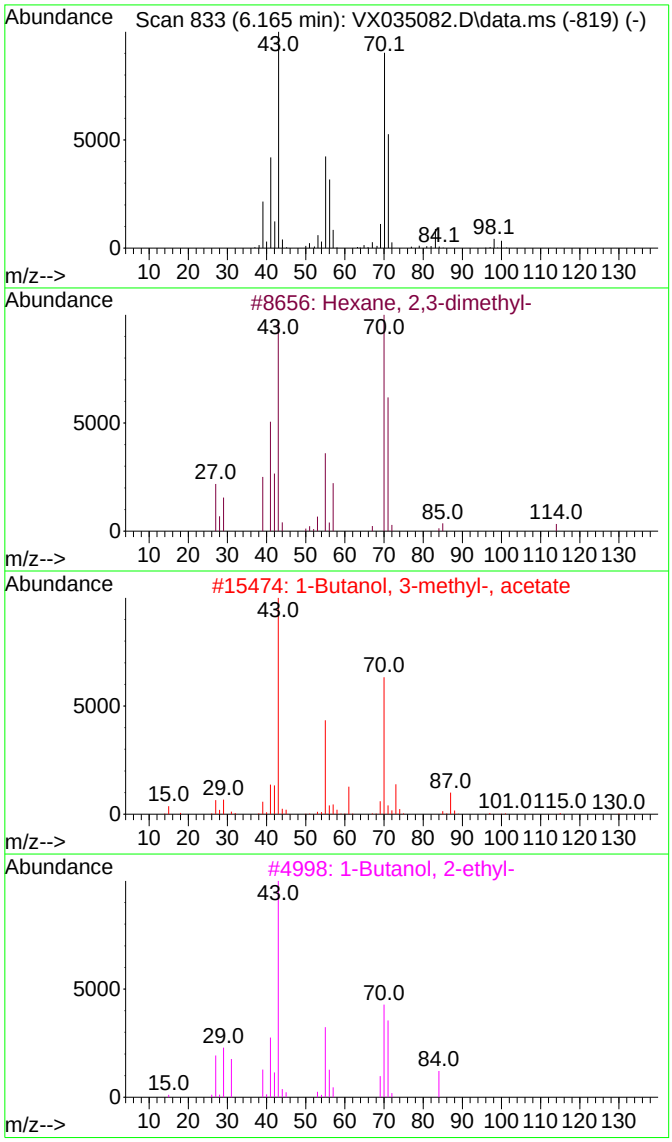
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

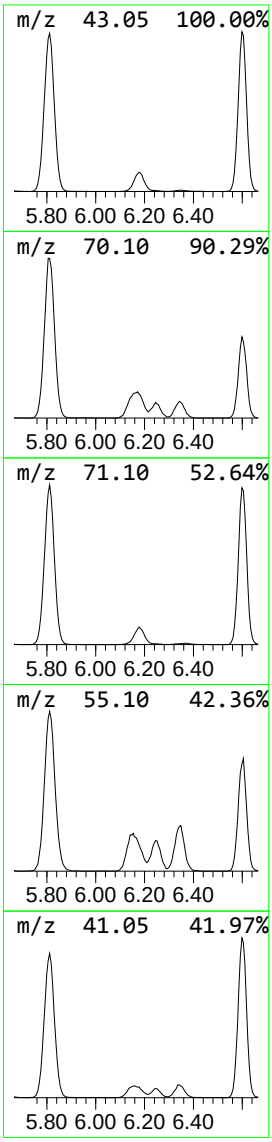
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.165	27.07 ug/l	617386	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	59
2	1-Butanol, 3-methyl-, acetate	130	C7H14O2	000123-92-2	53
3	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53
4	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

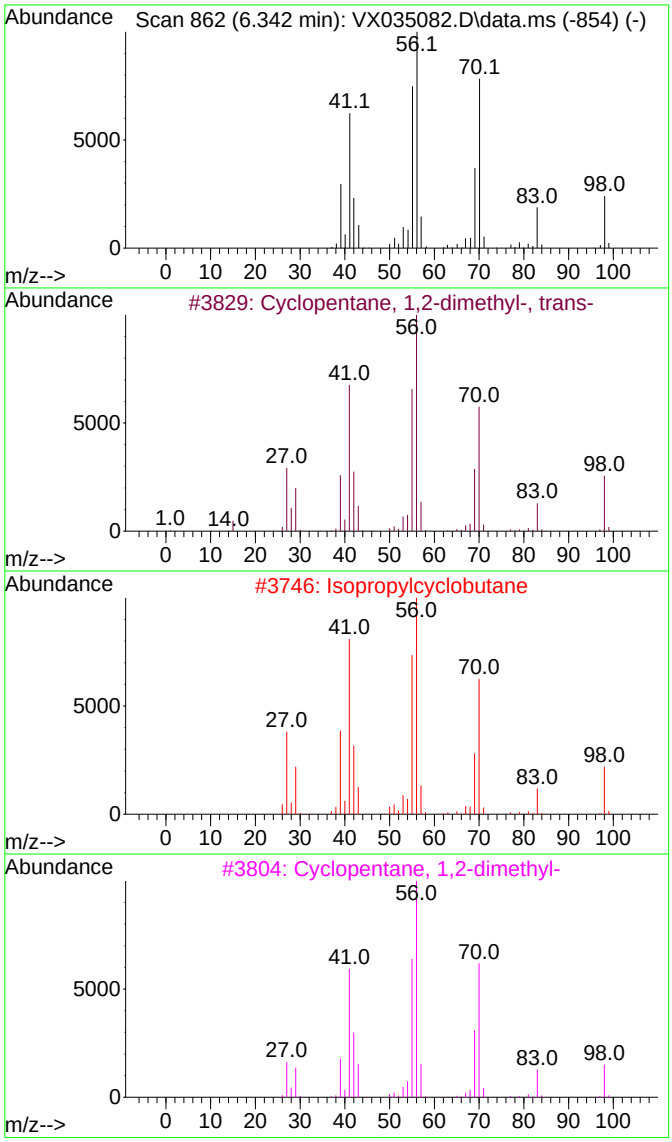
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

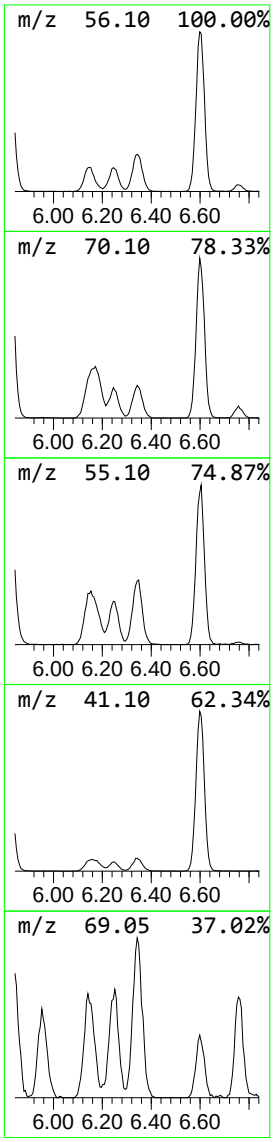
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.342	16.62 ug/l	378946	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	94
2	Isopropylcyclobutane	98	C7H14	000872-56-0	94
3	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	87
5	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

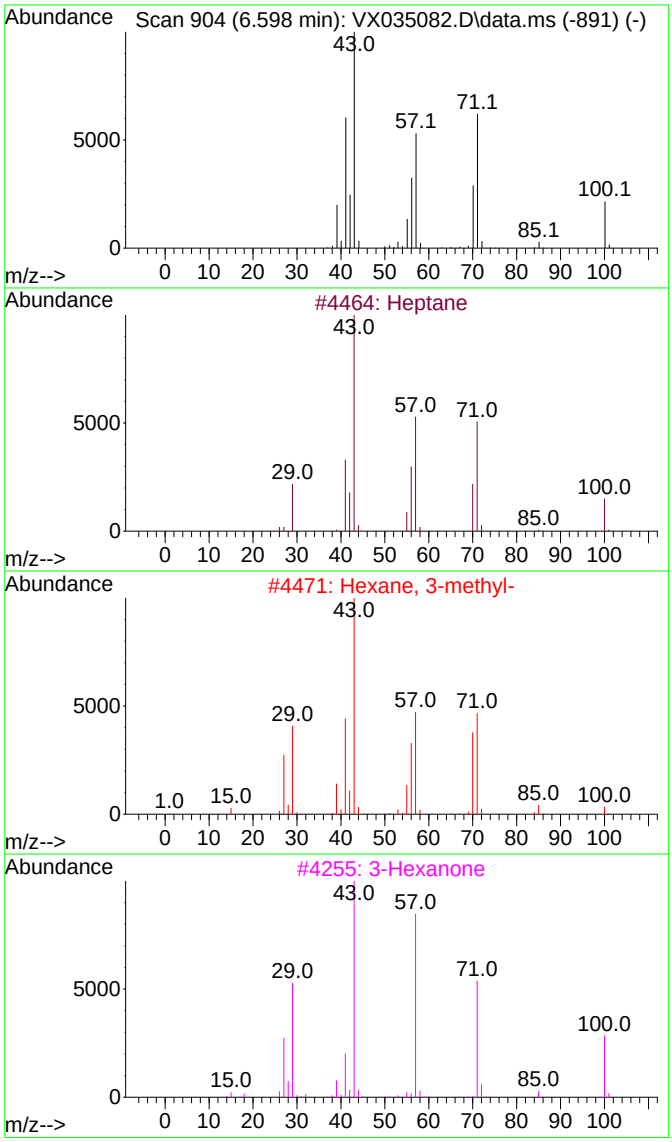
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

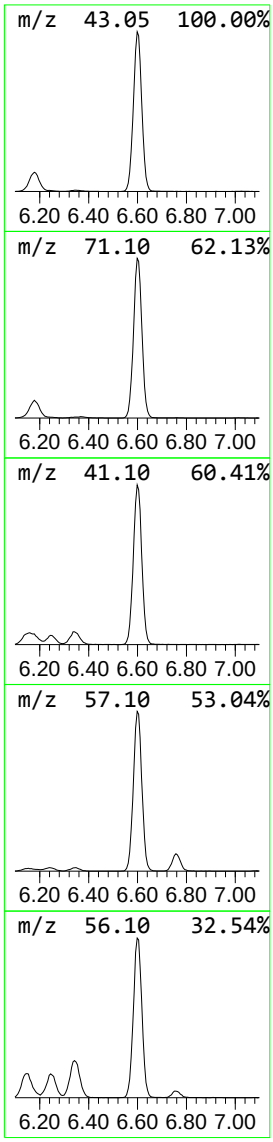
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	149.54 ug/l	3410290	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
3	3-Hexanone	100	C6H12O	000589-38-8	46
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	43
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

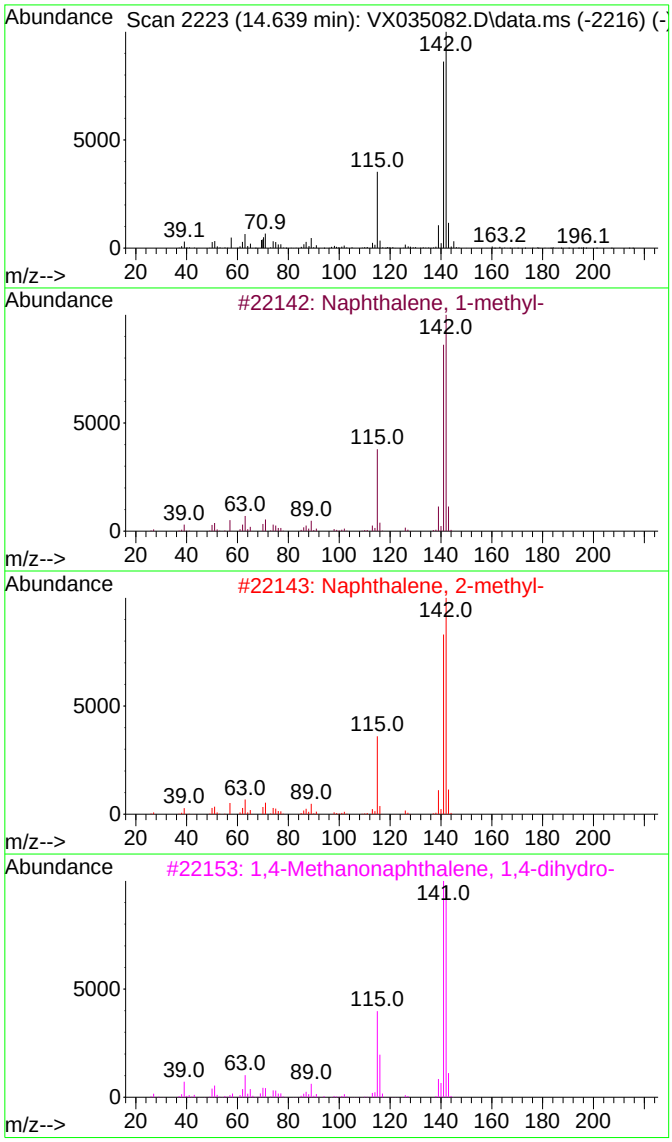
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

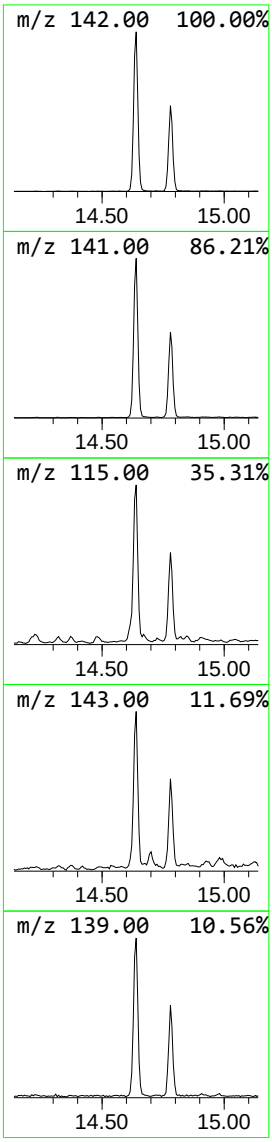
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	43.44 ug/l	1072030	1,4-Dichlorobenzene-d4	12.024

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

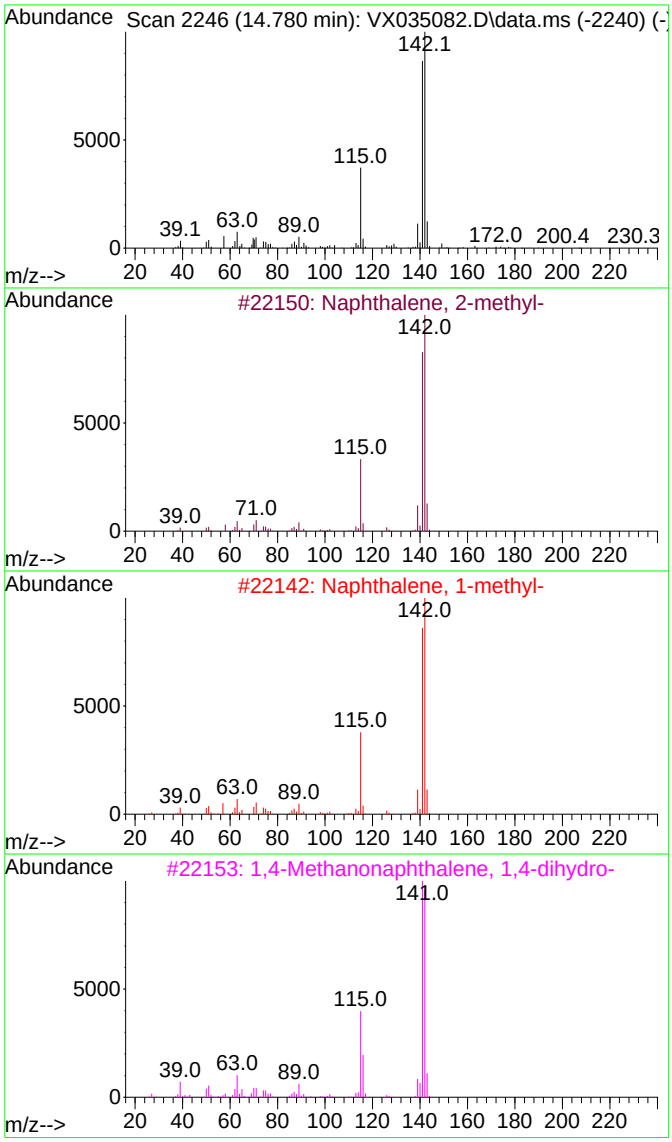
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

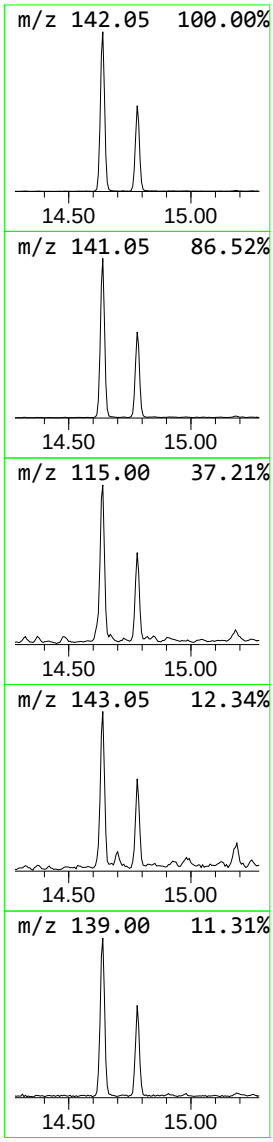
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	19.86 ug/l	490207	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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

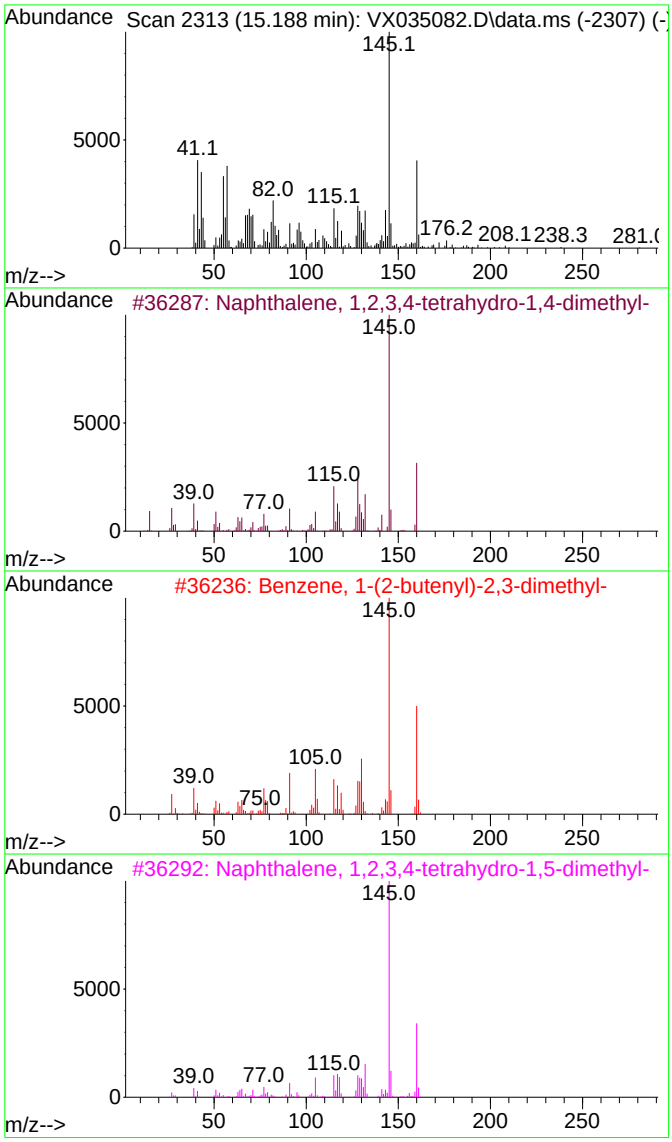
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

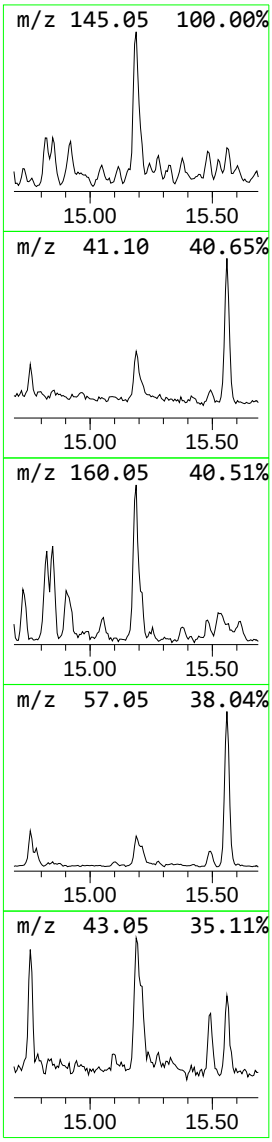
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.188	16.15 ug/l	398649	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	87
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	81
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

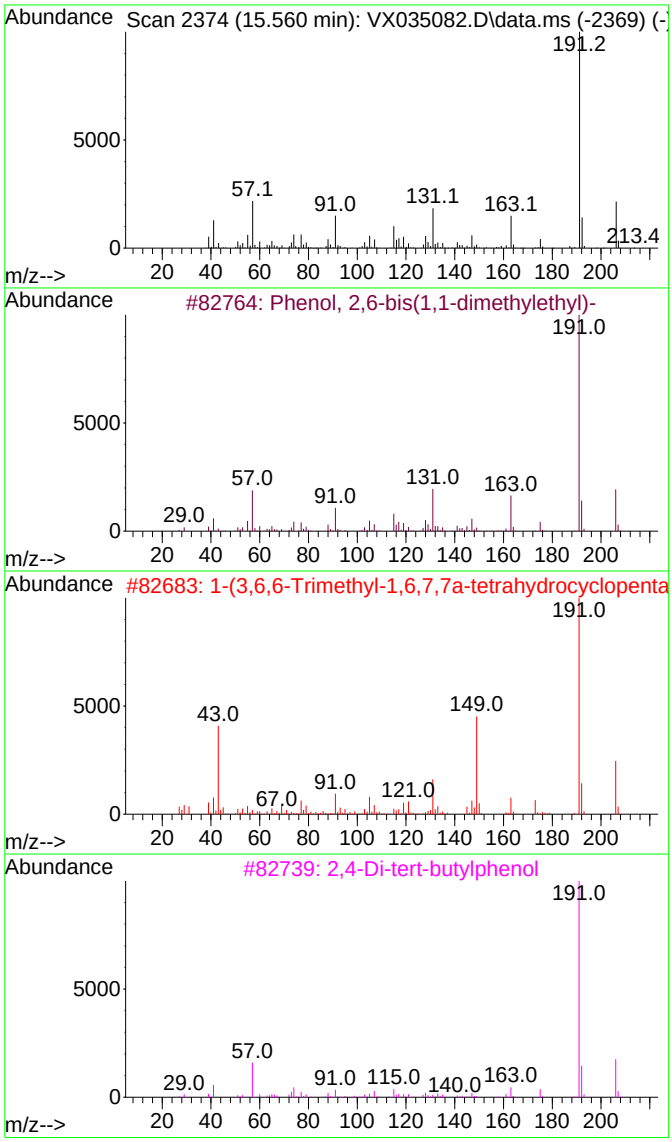
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

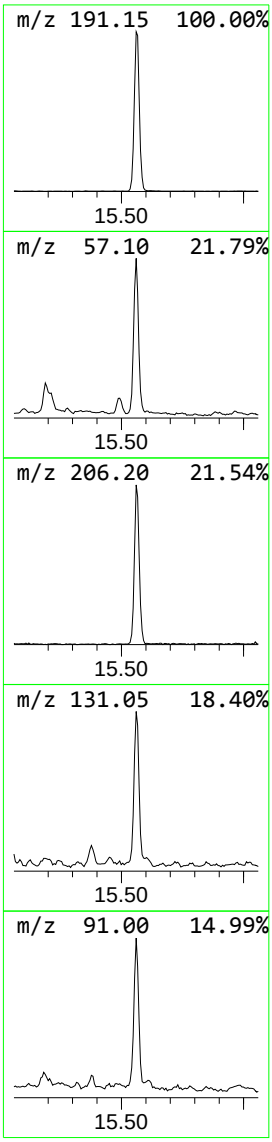
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	43.14 ug/l	1064690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
2	1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	90
3	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	86
5	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035082.D
Acq On : 14 Apr 2023 14:46
Operator : JC/MD
Sample : 02345-02
Misc : 1.62g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1611

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 2-methyl-	5.489	258.5	ug/l	5536190	1	5.550	1070800	50.0
Pentane, 2,3-di...	5.604	50.0	ug/l	1070800	1	5.550	1070800	50.0
Hexane, 3-methyl-	5.812	201.4	ug/l	4314080	1	5.550	1070800	50.0
Hexane, 2,3-dim...	6.165	27.1	ug/l	617386	2	6.757	1140220	50.0
Cyclopentane, 1...	6.342	16.6	ug/l	378946	2	6.757	1140220	50.0
Heptane	6.598	149.5	ug/l	3410290	2	6.757	1140220	50.0
Naphthalene, 1-...	14.640	43.4	ug/l	1072030	4	12.024	1234060	50.0
Naphthalene, 2-...	14.780	19.9	ug/l	490207	4	12.024	1234060	50.0
Naphthalene, 1,...	15.188	16.1	ug/l	398649	4	12.024	1234060	50.0
Phenol, 2,6-bis...	15.560	43.1	ug/l	1064690	4	12.024	1234060	50.0