LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

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_N\methods\82N030524W.M
Title : SW846 8260

Signal : TIC: VN081359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.836	135	150	151	rBV7	49494	144302	3.17%	0.610%
2	2.895	151	160	162	rVV10	26445	75254	1.66%	0.318%
3	8.165	1044	1056	1060	rBV	247595	593694	13.06%	2.511%
4	8.218	1060	1065	1076	rVB	483264	1052288	23.15%	4.450%
5	8.577	1115	1126	1137	rBV	291831	652607	14.35%	2.760%
6	9.100	1206	1215	1231	rBV	664445	1377387	30.30%	5.825%
7	10.565	1456	1464	1472	rBV	998037	1840126	40.47%	7.783%
8	11.865	1677	1685	1696	rBV	839164	1531409	33.68%	6.477%
9	11.965	1696	1702	1708	rBV	188581	326814	7.19%	1.382%
10	12.076	1713	1721	1729	rVB2	53712	104381	2.30%	0.441%
11	12.400	1765	1776	1782	rBV	128973	230428	5.07%	0.975%
12	12.694	1821	1826	1833	rBV2	70950	118618	2.61%	0.502%
13	12.853	1846	1853	1861	rVB	669889	1140181	25.08%	4.822%
14	13.035	1877	1884	1889	rBV2	50518	89573	1.97%	0.379%
15	13.100	1889	1895	1897	rVV	100116	163453	3.60%	0.691%
16	13.129	1897	1900	1904	rVV	218743	383240	8.43%	1.621%
17	13.176	1904	1908	1915	rVB	251831	408097	8.98%	1.726%
18	13.335	1928	1935	1943	rBV	110302	202589	4.46%	0.857%
19	13.482	1951	1960	1965	rBV	641985	1076884	23.69%	4.555%
20	13.535	1965	1969	1974	rVV	146026	240195	5.28%	1.016%
21	13.676	1988	1993	1998	rBV3	26169	49014	1.08%	0.207%
22	13.794	2006	2013	2031	rVB2	914154	2067668	45.48%	8.745%
23	13.953	2033	2040	2043	rBV3	68011	126734	2.79%	0.536%
24	13.994	2043	2047	2058	rVB2	287449	559220	12.30%	2.365%
25	14.106	2062	2066	2071	rVB2	42994	62889	1.38%	0.266%
26	14.176	2072	2078	2085	rVB	219446	352835	7.76%	1.492%
27	14.253	2085	2091	2092	rBV2	32088	56803	1.25%	0.240%
28	14.329	2100	2104	2109	rVB	79784	112545	2.48%	0.476%
29	14.470	2120	2128	2133	rBV2	134943	247077	5.43%	1.045%
30	14.523	2133	2137	2141	rVB6	31267	50349	1.11%	0.213%
31	14.658	2157	2160	2163	rVV2	55898	81353	1.79%	0.344%
32	14.694	2163	2166	2171	rVV2	99593	151038	3.32%	0.639%
33	14.794	2178	2183	2188	rBV4	74547	126026	2.77%	0.533%
34	14.929	2201	2206	2209	rBV2	96750	171106	3.76%	0.724%
35	14.958	2209	2211	2218	rVB2	92062	133652	2.94%	0.565%
36	15.041	2218	2225	2232	rBV3	126919	339897	7.48%	1.438%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

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_N\methods\82N030524W.M
Title : SW846 8260

37	15.117	2233	2238	2246	rVB	266295	485346	10.68%	2.053%
38	15.206	2246	2253	2261	rBV2	317842	622563	13.69%	2.633%
39	15.311	2266	2271	2280	rBV5	66240	141371	3.11%	0.598%
40	15.435	2288	2292	2301	rVB5	25607	58766	1.29%	0.249%
41	15.641	2320	2327	2338	rVB	2300528	4546368	100.00%	19.228%
42	15.835	2355	2360	2369	rVB2	108414	215997	4.75%	0.914%
43	16.547	2478	2481	2484	rVB5	36395	49446	1.09%	0.209%
44	16.782	2513	2521	2522	rBV	760722	1084695	23.86%	4.588%

Sum of corrected areas: 23644278

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
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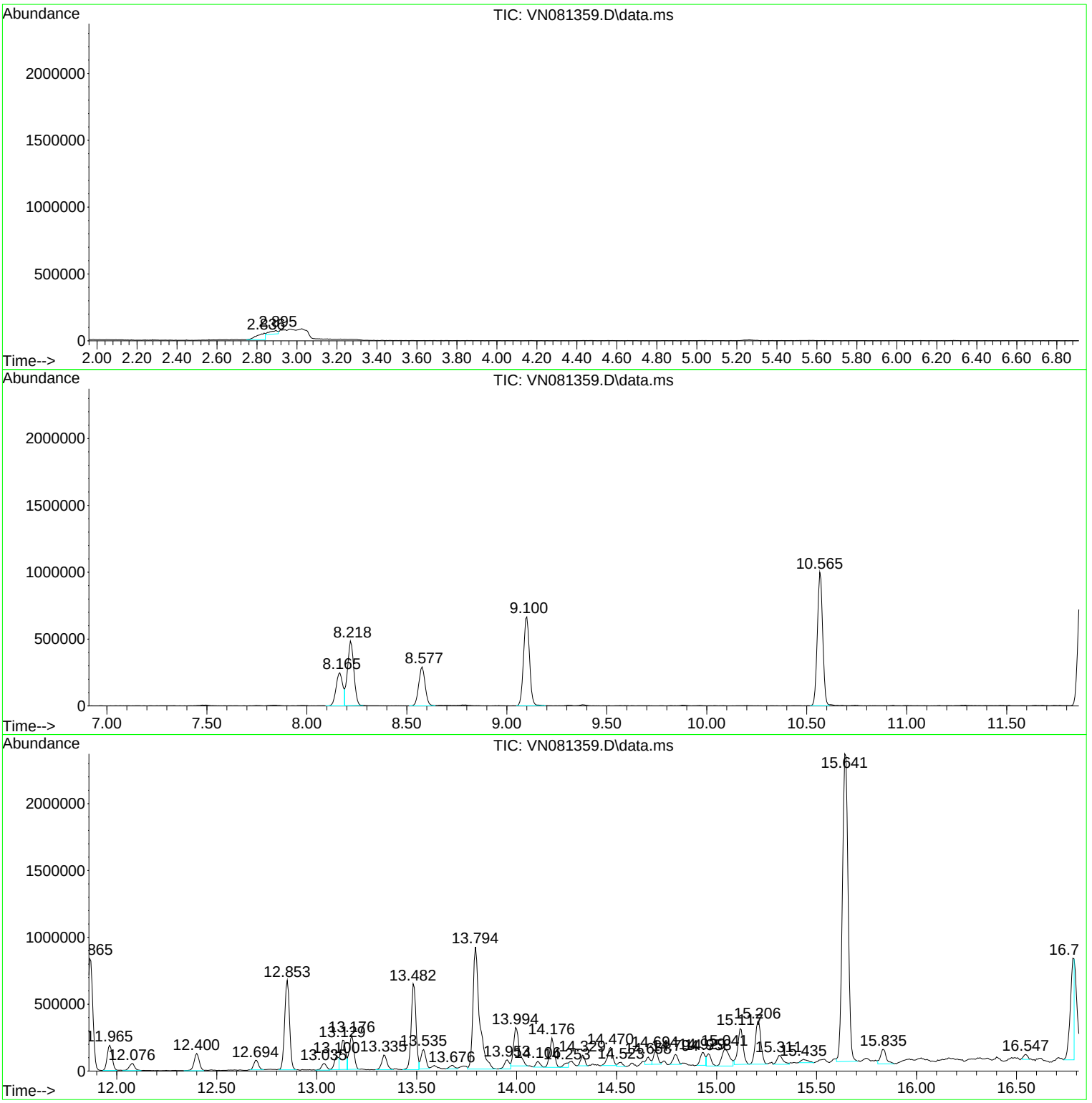
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

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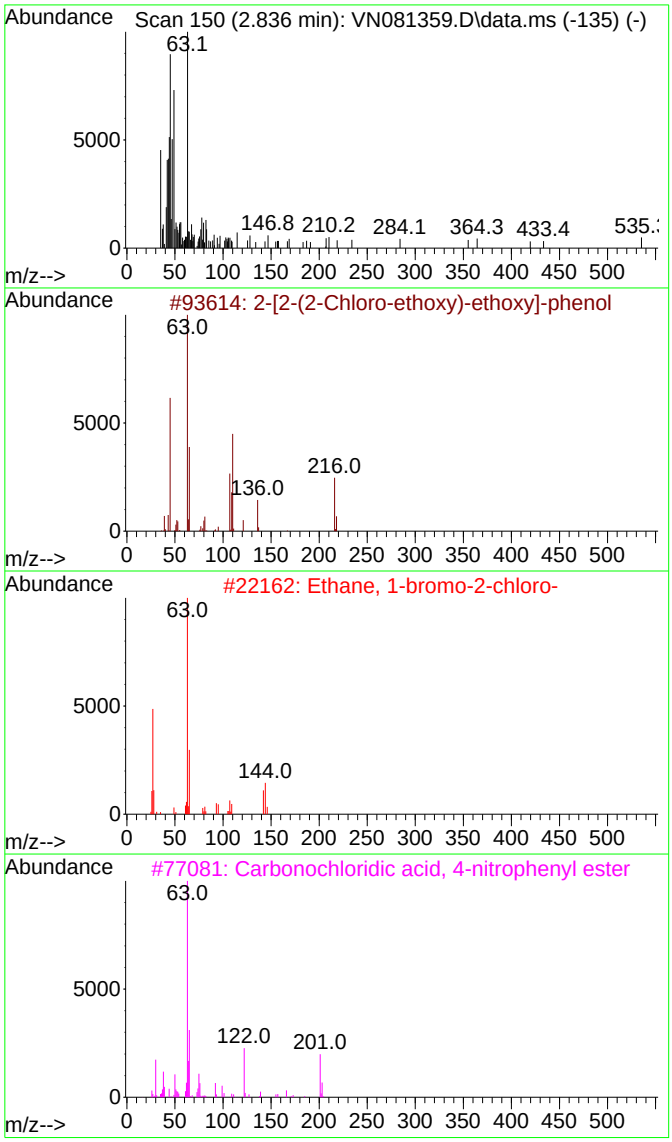
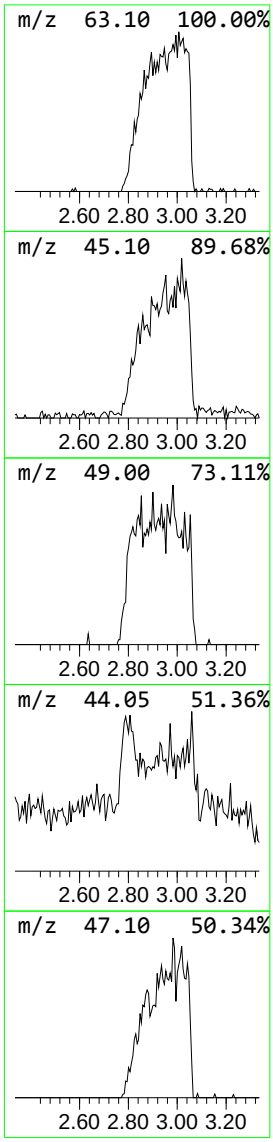
Peak Number 1 unknown2.836 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	6.86 ug/l	144302	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	25
2	Ethane, 1-bromo-2-chloro-	142	C2H4BrCl	000107-04-0	10
3	Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	10
4	Benzaldehyde, 5-bromo-2-hydroxy-...	359	C13H9BrF3N3O	1000276-33-1	10
5	2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

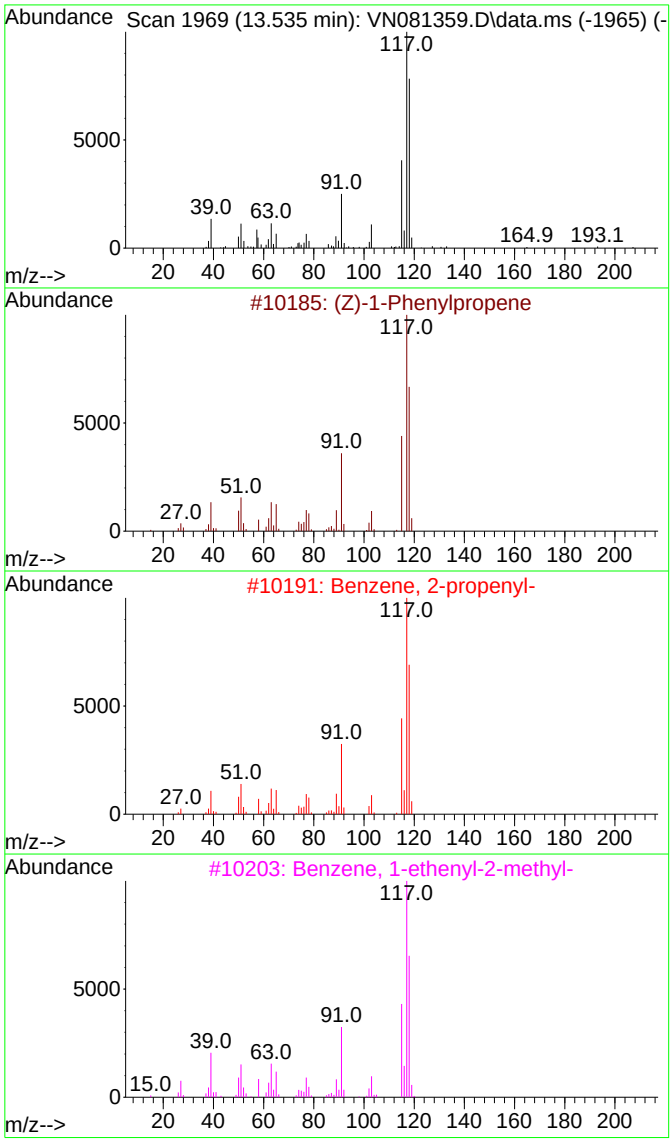
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

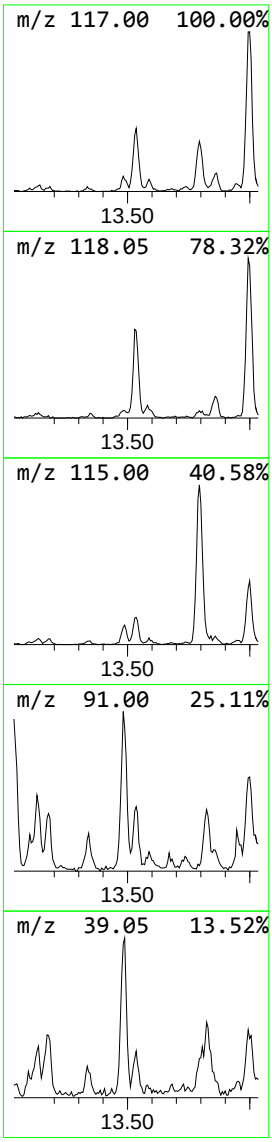
****

Peak Number 2 (Z)-1-Phenylpropene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.535	5.81 ug/l	240195	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	90
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
4	Indane	118	C9H10	000496-11-7	81
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

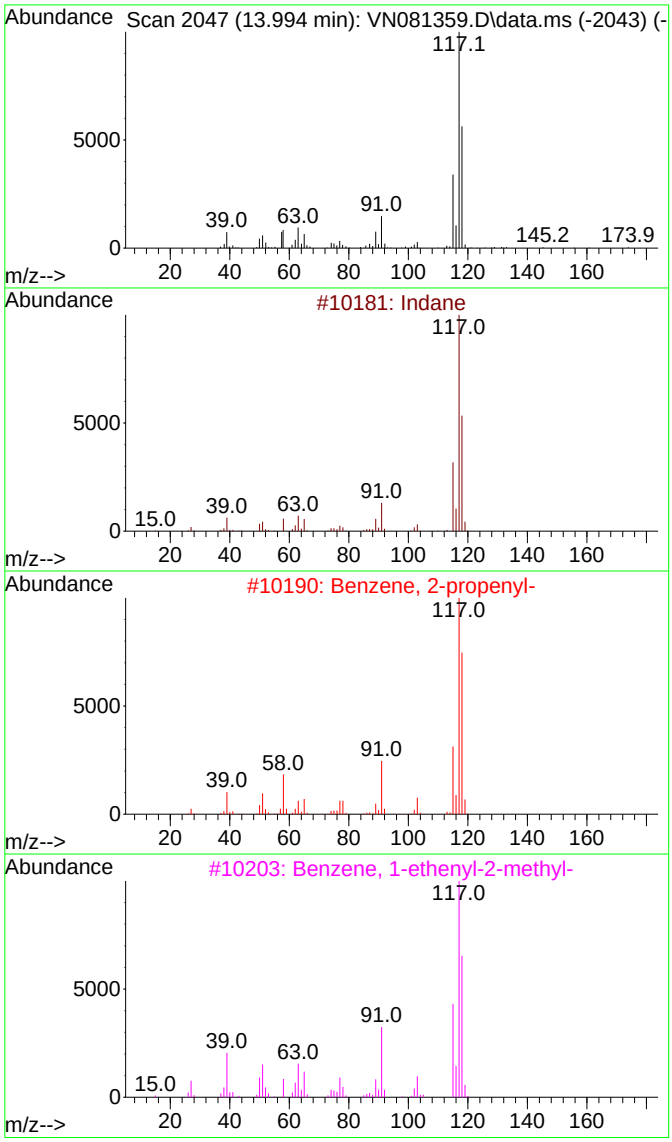
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

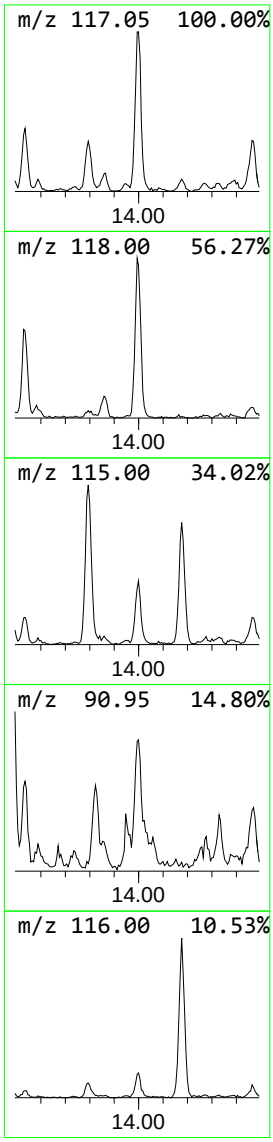
****

Peak Number 3 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	13.52 ug/l	559220	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

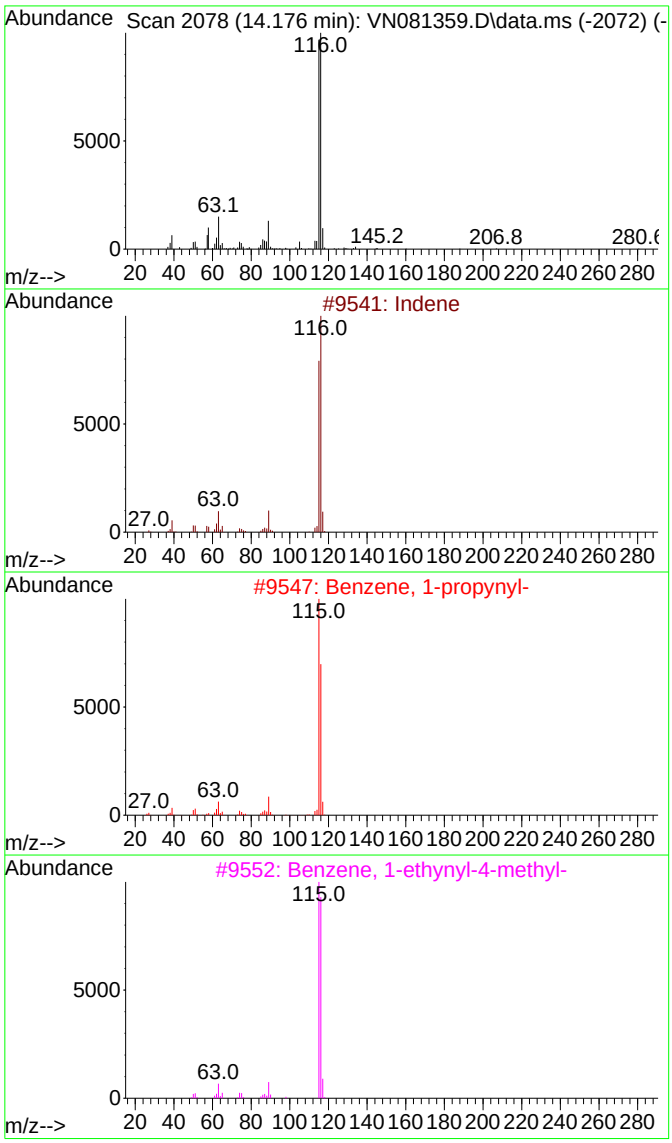
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

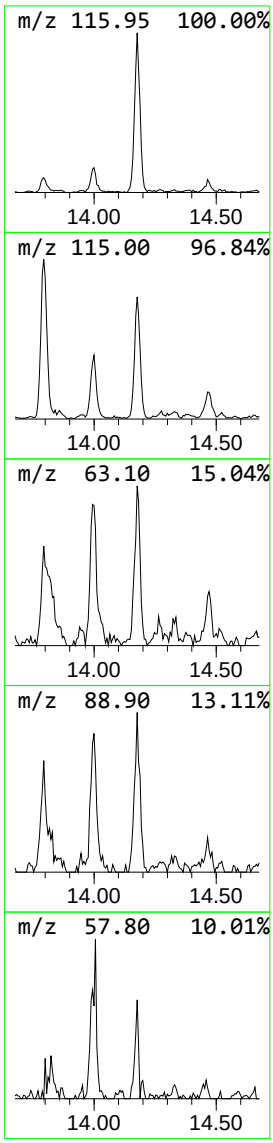
****

Peak Number 4 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	8.53 ug/l	352835	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	94
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	86
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	83
5	6-Phenyl-5-hexyn-3-ol	174	C12H14O	135663-98-8	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

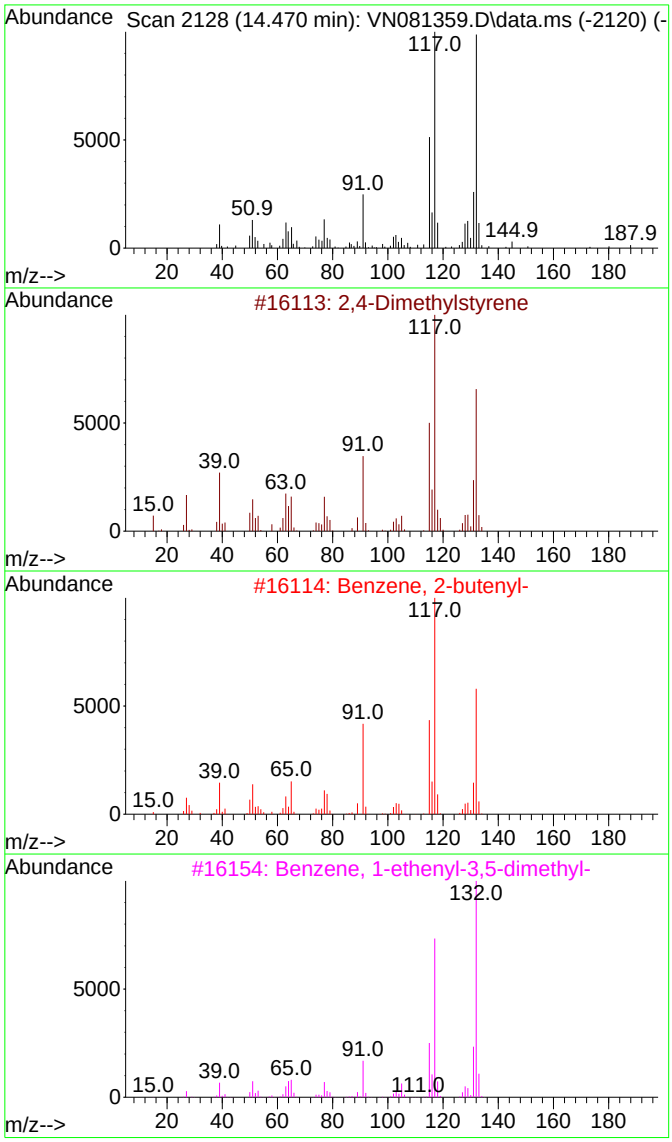
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

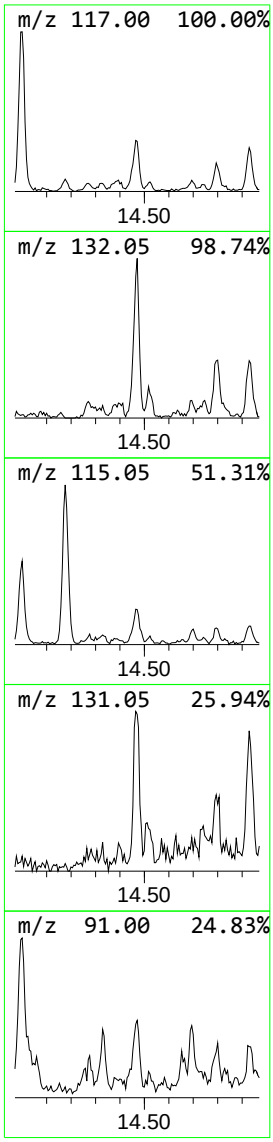
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4-Dimethylstyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.470	5.97 ug/l	247077	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	95
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	94
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	94
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

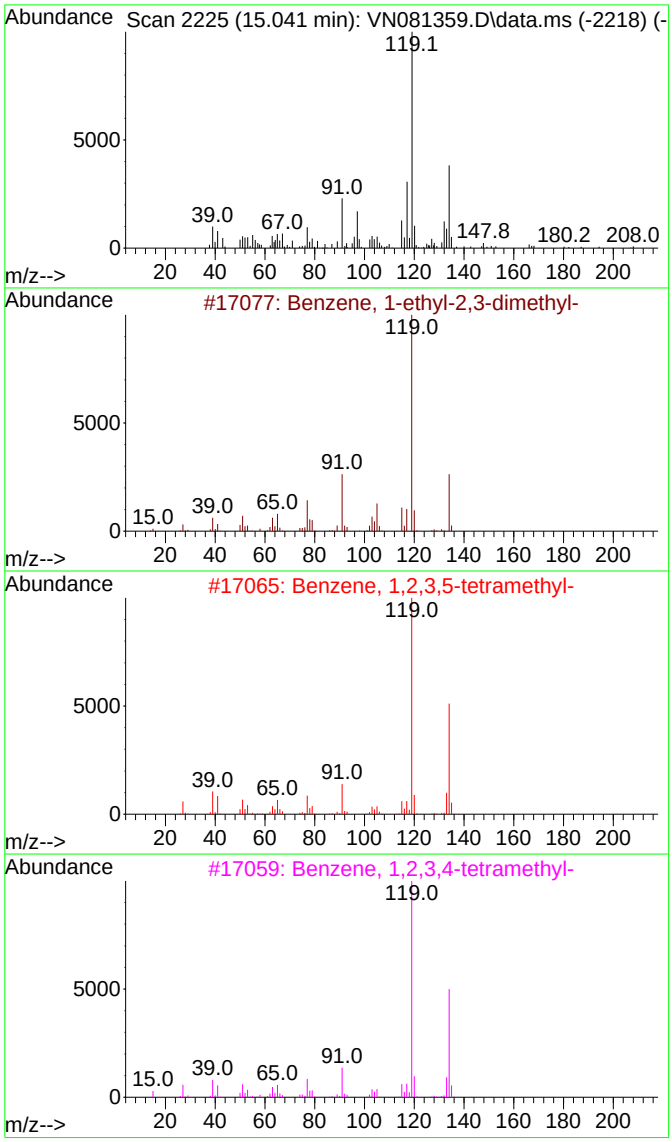
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

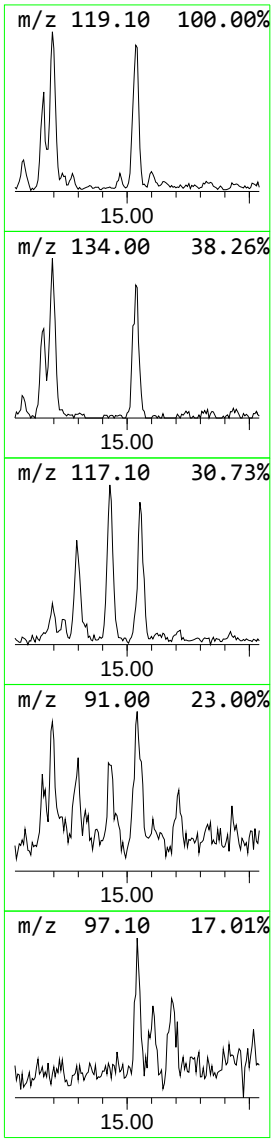
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	8.22 ug/l	339897	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	76
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	76
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76
4	o-Cymene	134	C10H14	000527-84-4	76
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

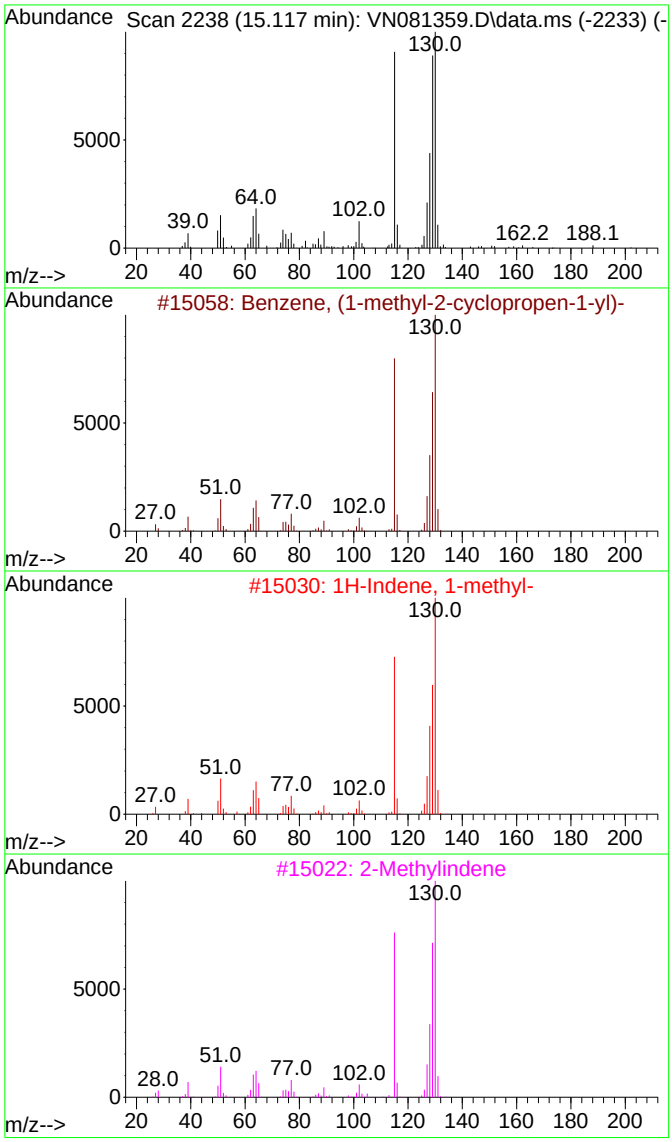
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

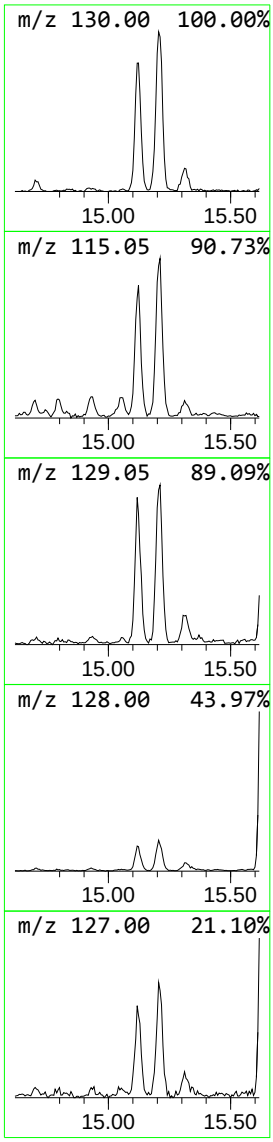
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (1-methyl-2-cyclop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.117	11.74 ug/l	485346	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	97
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	2-Methylindene	130	C10H10	002177-47-1	95
4	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	94
5	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	92





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

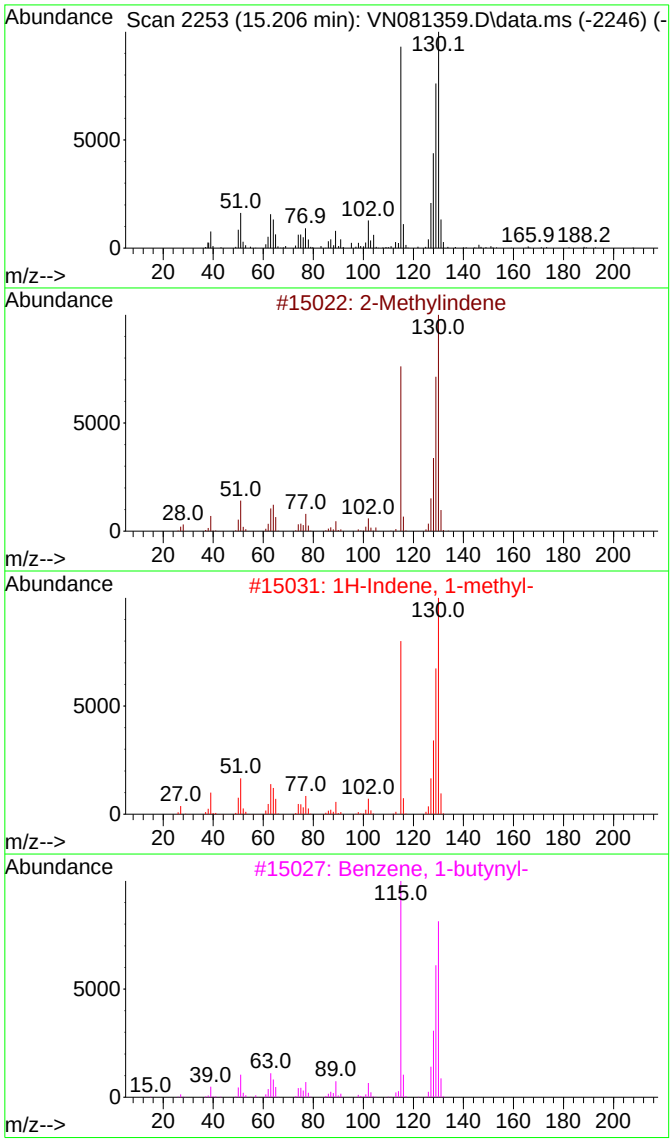
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

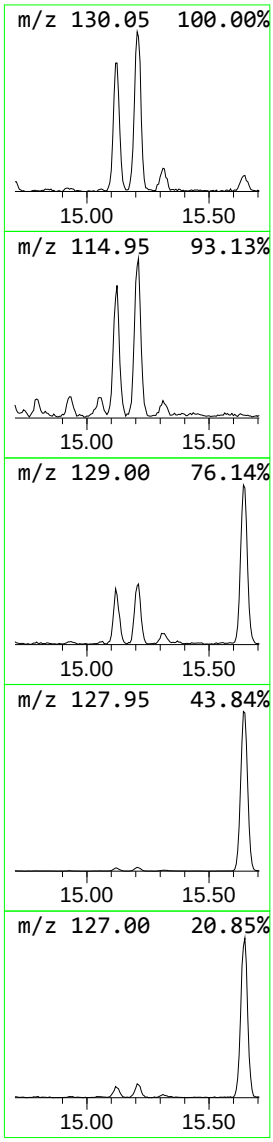
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Methylindene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	15.05 ug/l	622563	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	96
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

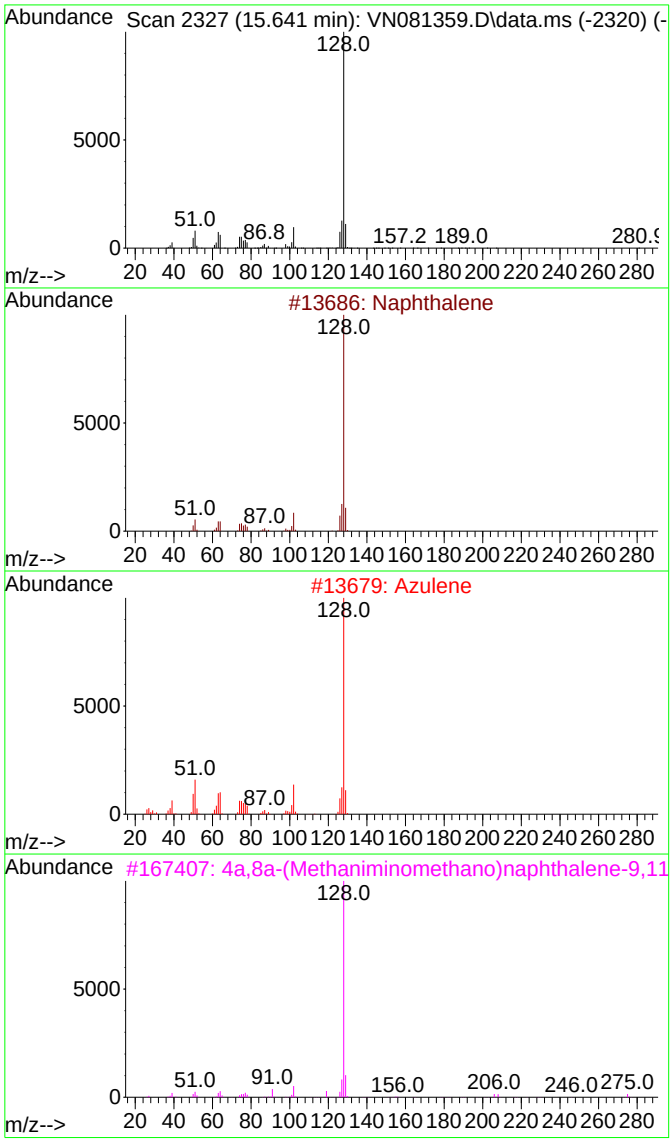
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

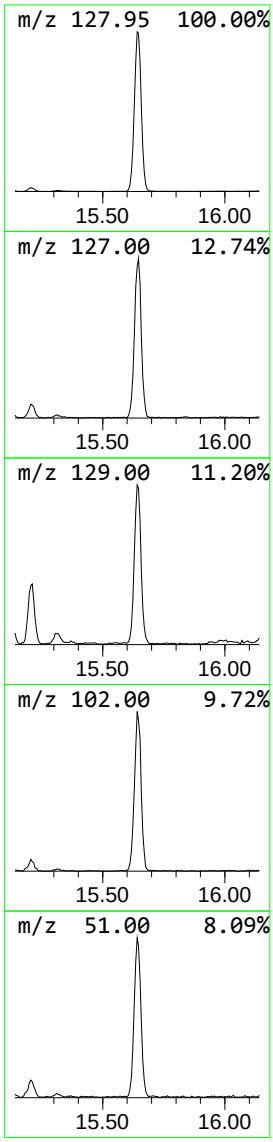
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	109.94 ug/l	4546370	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

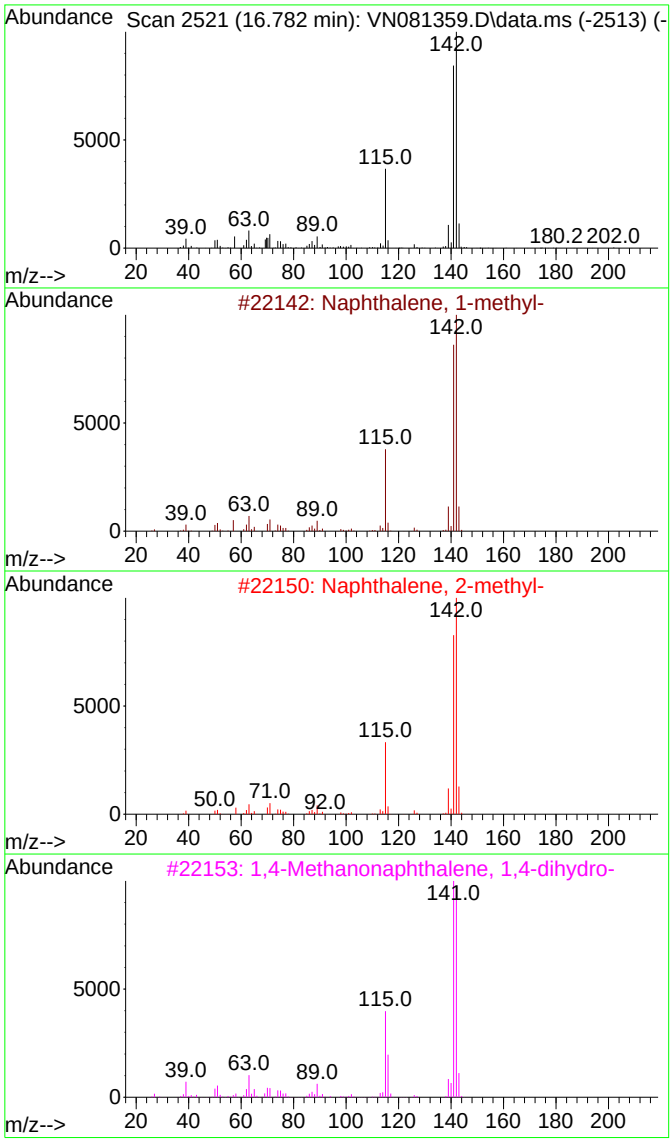
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

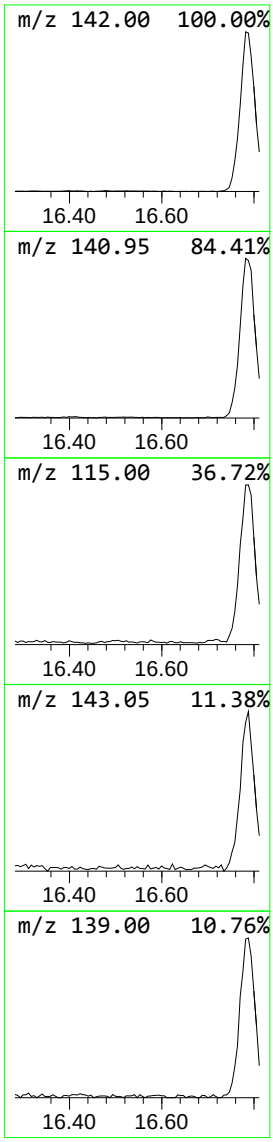
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	26.23 ug/l	1084700	1,4-Dichlorobenzene-d4	13.794

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	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031124\
Data File : VN081359.D
Acq On : 11 Mar 2024 13:28
Operator : JC\MD
Sample : P1705-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-2B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.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
unknown2.836	2.836	6.9	ug/l	144302	1	8.218	1052290	50.0
(Z)-1-Phenylpro...	13.535	5.8	ug/l	240195	4	13.794	2067670	50.0
Indane	13.994	13.5	ug/l	559220	4	13.794	2067670	50.0
Indene	14.176	8.5	ug/l	352835	4	13.794	2067670	50.0
2,4-Dimethylsty...	14.470	6.0	ug/l	247077	4	13.794	2067670	50.0
Benzene, 1-ethy...	15.041	8.2	ug/l	339897	4	13.794	2067670	50.0
Benzene, (1-met...	15.117	11.7	ug/l	485346	4	13.794	2067670	50.0
2-Methylindene	15.206	15.1	ug/l	622563	4	13.794	2067670	50.0
Azulene	15.641	109.9	ug/l	4546370	4	13.794	2067670	50.0
1,4-Methanonaph...	16.782	26.2	ug/l	1084700	4	13.794	2067670	50.0