LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

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\82X021723W.M
Title : SW846 8260

Signal : TIC: VX034252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV3	12984	26593	1.87%	0.257%
2	1.581	72	81	82	rBV7	10112	24455	1.72%	0.237%
3	2.941	295	304	313	rBV	7611	18138	1.27%	0.175%
4	5.385	694	705	721	rBV	158104	461465	32.41%	4.463%
5	5.550	721	732	747	rVB	274101	771636	54.20%	7.463%
6	5.952	787	798	812	rBV	178027	475378	33.39%	4.598%
7	6.763	920	931	945	rBV	425426	1021093	71.72%	9.876%
8	8.647	1232	1240	1259	rBV	894961	1423633	100.00%	13.769%
9	10.055	1465	1471	1483	rBV	844162	1170813	82.24%	11.324%
10	11.079	1634	1639	1652	rBV	697903	887689	62.35%	8.585%
11	11.750	1745	1749	1755	rVB	14952	20947	1.47%	0.203%
12	12.018	1788	1793	1802	rBV	803923	1048598	73.66%	10.142%
13	12.244	1825	1830	1837	rBV2	46034	62234	4.37%	0.602%
14	12.317	1837	1842	1848	rBV2	16474	25453	1.79%	0.246%
15	12.616	1886	1891	1895	rBV	17853	22451	1.58%	0.217%
16	12.701	1899	1905	1911	rBV2	18588	33916	2.38%	0.328%
17	12.963	1945	1948	1955	rVB2	10681	15837	1.11%	0.153%
18	13.049	1955	1962	1964	rBV2	10724	16174	1.14%	0.156%
19	13.170	1977	1982	1986	rBV	28858	39189	2.75%	0.379%
20	13.292	1993	2002	2007	rBV2	34260	57403	4.03%	0.555%
21	13.341	2007	2010	2013	rVB2	14228	16220	1.14%	0.157%
22	13.426	2019	2024	2028	rVB	37401	52571	3.69%	0.508%
23	13.542	2039	2043	2047	rBV	21241	28876	2.03%	0.279%
24	13.774	2077	2081	2089	rBV	257171	334574	23.50%	3.236%
25	13.847	2089	2093	2100	rVV9	8374	16535	1.16%	0.160%
26	13.926	2100	2106	2110	rVB5	14253	23703	1.66%	0.229%
27	14.067	2126	2129	2132	rBV4	11254	16681	1.17%	0.161%
28	14.219	2150	2154	2157	rBV3	30794	45071	3.17%	0.436%
29	14.256	2158	2160	2165	rVV4	15965	19708	1.38%	0.191%
30	14.317	2165	2170	2176	rVV	30736	60009	4.22%	0.580%
31	14.524	2200	2204	2210	rVB3	14933	25026	1.76%	0.242%
32	14.634	2216	2222	2227	rBV	202036	264031	18.55%	2.554%
33	14.780	2239	2246	2253	rBV	303105	388942	27.32%	3.762%
34	14.957	2273	2275	2283	rVB5	17328	27877	1.96%	0.270%
35	15.207	2313	2316	2321	rVB	18573	24903	1.75%	0.241%
36	15.377	2339	2344	2347	rBV	57102	82452	5.79%	0.797%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

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\82X021723W.M
Title : SW846 8260

37	15.414	2347	2350	2355	rVB2	37454	56367	3.96%	0.545%
38	15.475	2355	2360	2373	rVB	100206	181397	12.74%	1.754%
39	15.615	2377	2383	2386	rVV	150453	222027	15.60%	2.147%
40	15.652	2386	2389	2396	rVV	46763	83176	5.84%	0.804%
41	15.743	2400	2404	2409	rVB4	27327	46294	3.25%	0.448%
42	15.816	2410	2416	2417	rBV2	37563	59163	4.16%	0.572%
43	15.835	2417	2419	2430	rVB4	49255	114265	8.03%	1.105%
44	15.987	2438	2444	2454	rVB	54505	96012	6.74%	0.929%
45	16.091	2456	2461	2467	rBV3	17926	32185	2.26%	0.311%
46	16.194	2476	2478	2484	rVB6	10289	15076	1.06%	0.146%
47	16.328	2494	2500	2510	rVB3	127473	264230	18.56%	2.556%
48	16.475	2520	2524	2529	rVB2	9783	18146	1.27%	0.176%
49	16.560	2531	2538	2541	rVV7	13260	31480	2.21%	0.304%
50	16.597	2541	2544	2549	rVB2	21887	35536	2.50%	0.344%
51	16.658	2549	2554	2559	rBV2	17781	33935	2.38%	0.328%

Sum of corrected areas: 10339563

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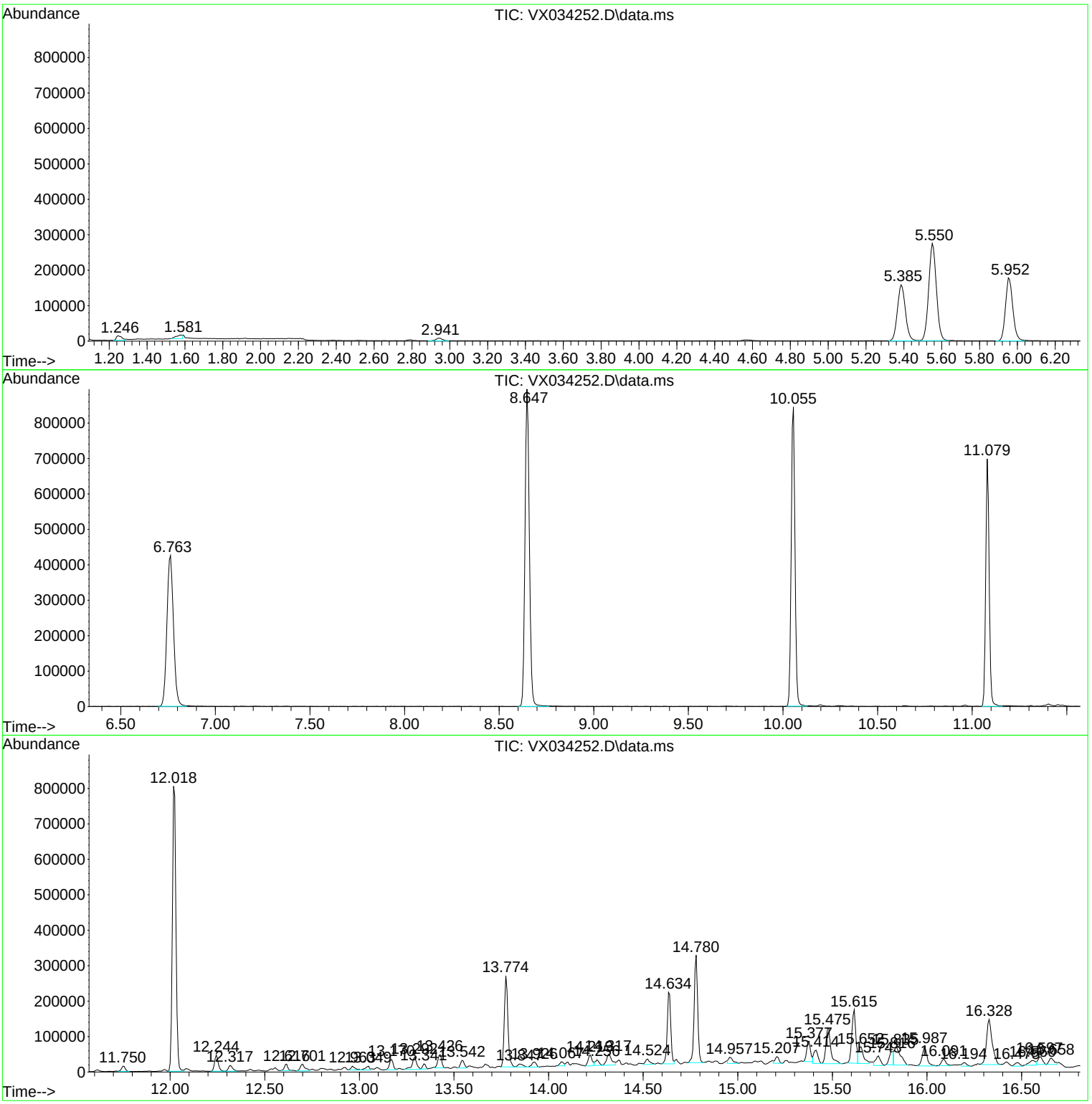
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

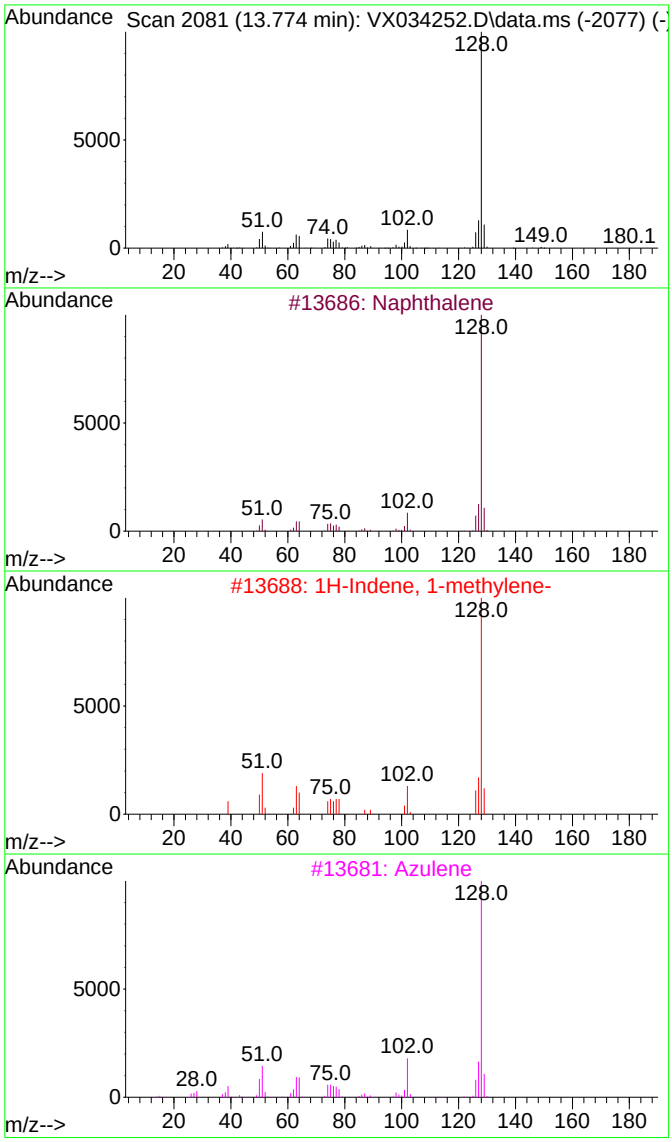
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

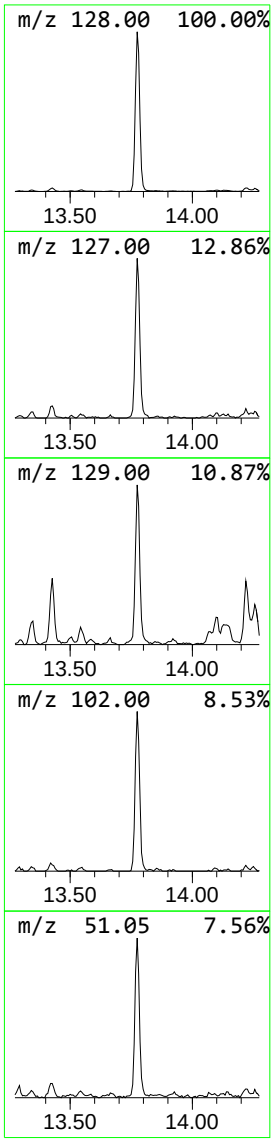
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1H-Indene, 1-methylene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	15.95 ug/l	334574	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	94
3	Azulene	128	C10H8	000275-51-4	91
4	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

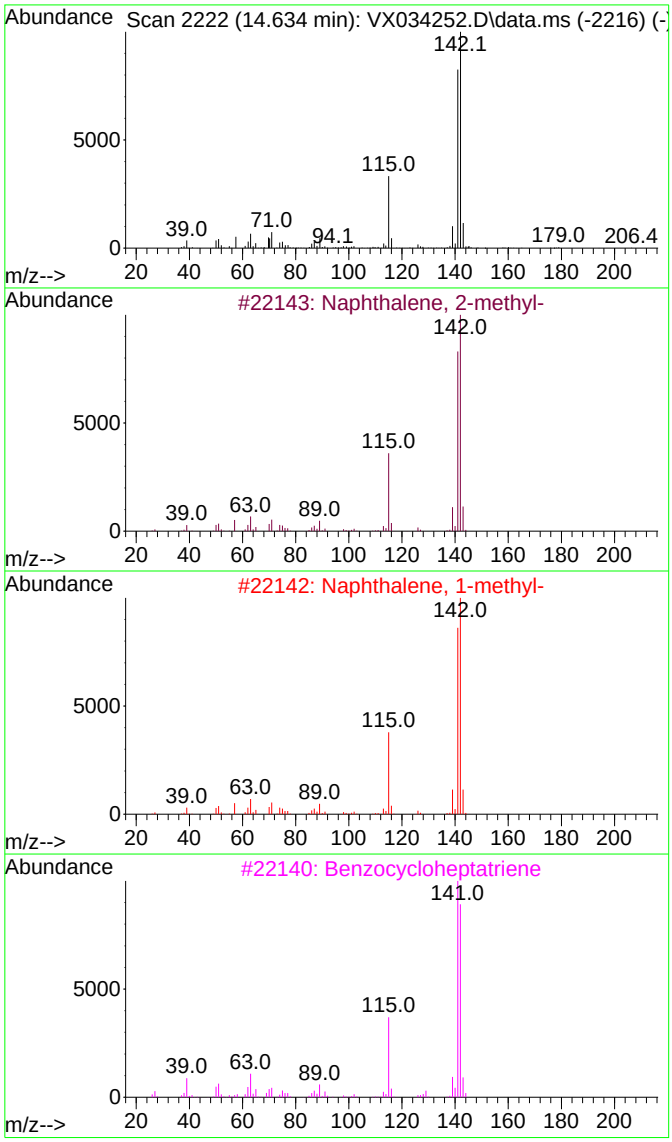
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

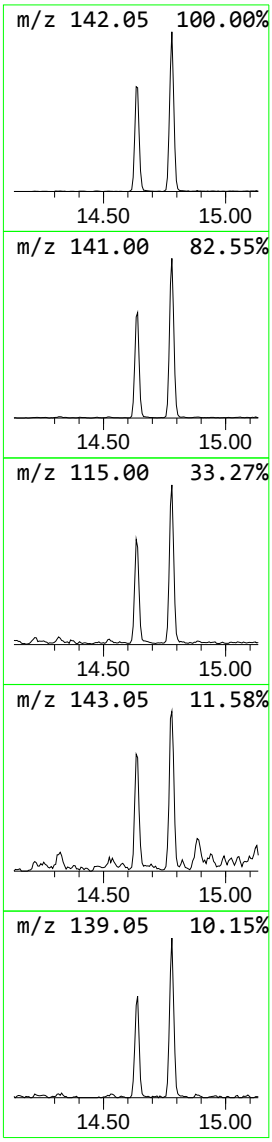
****

Peak Number 2 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	12.59 ug/l	264031	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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	86
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

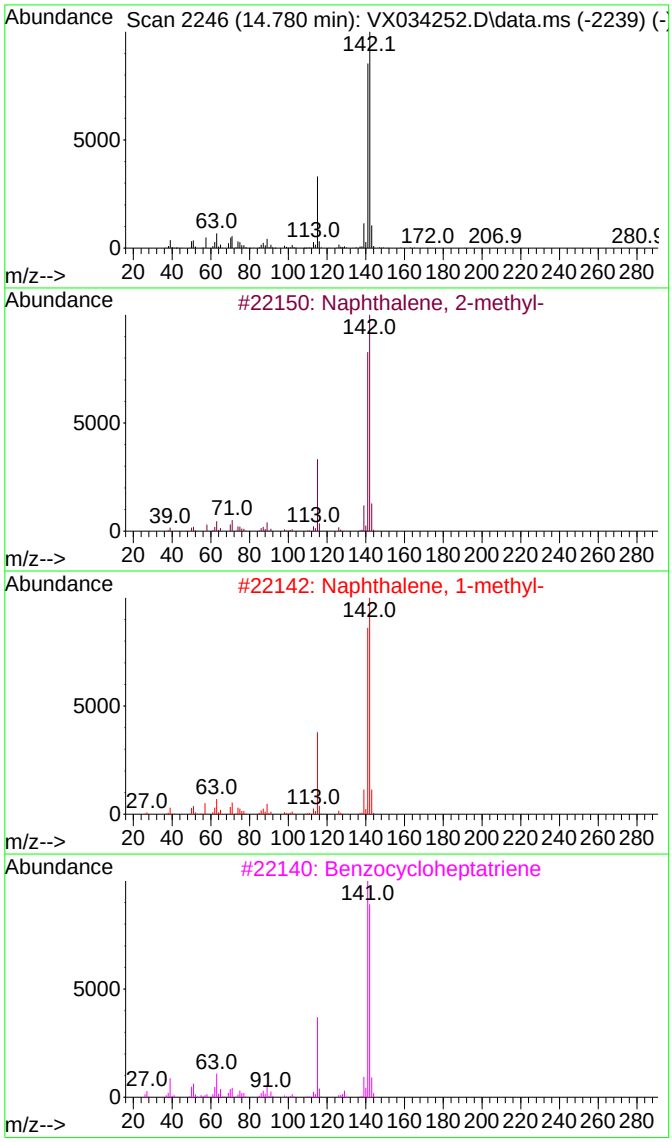
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

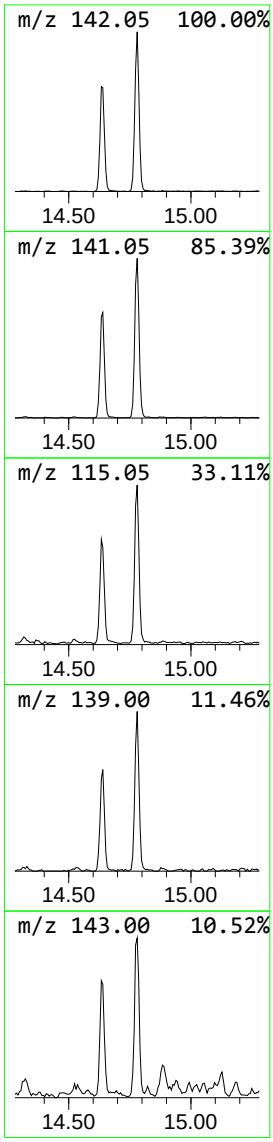
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	18.55 ug/l	388942	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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

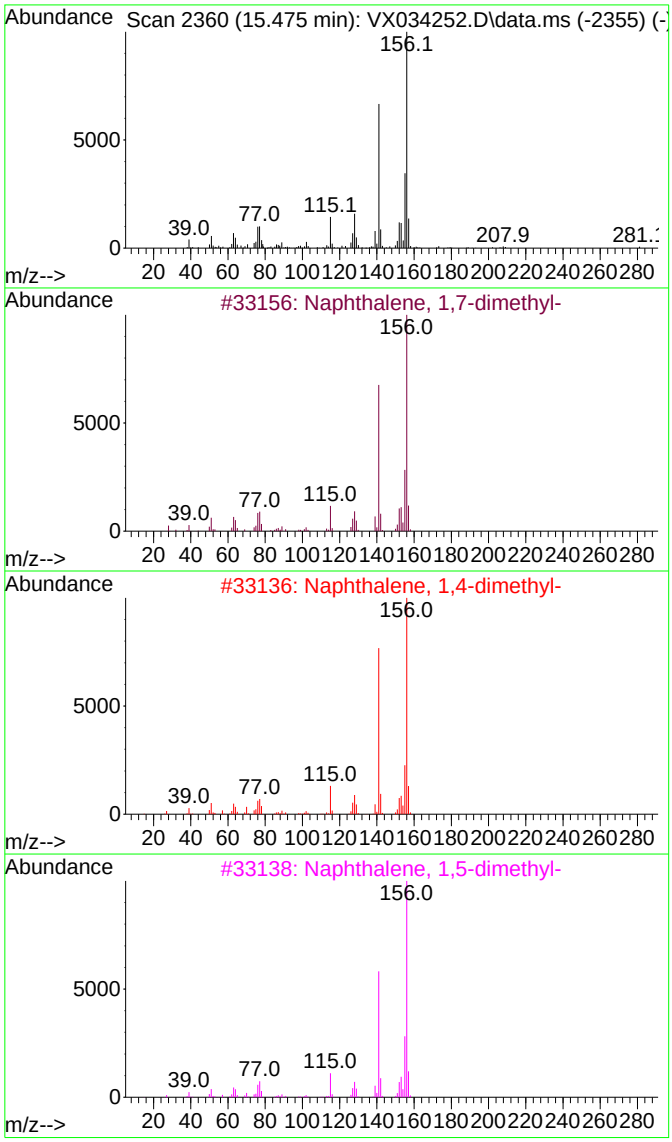
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

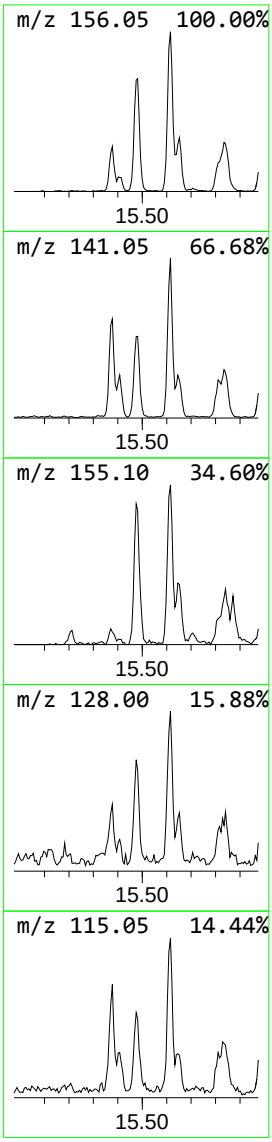
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	8.65 ug/l	181397	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
Acq On : 23 Feb 2023 16:38
Operator : JC/MD
Sample : 01638-01 20X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

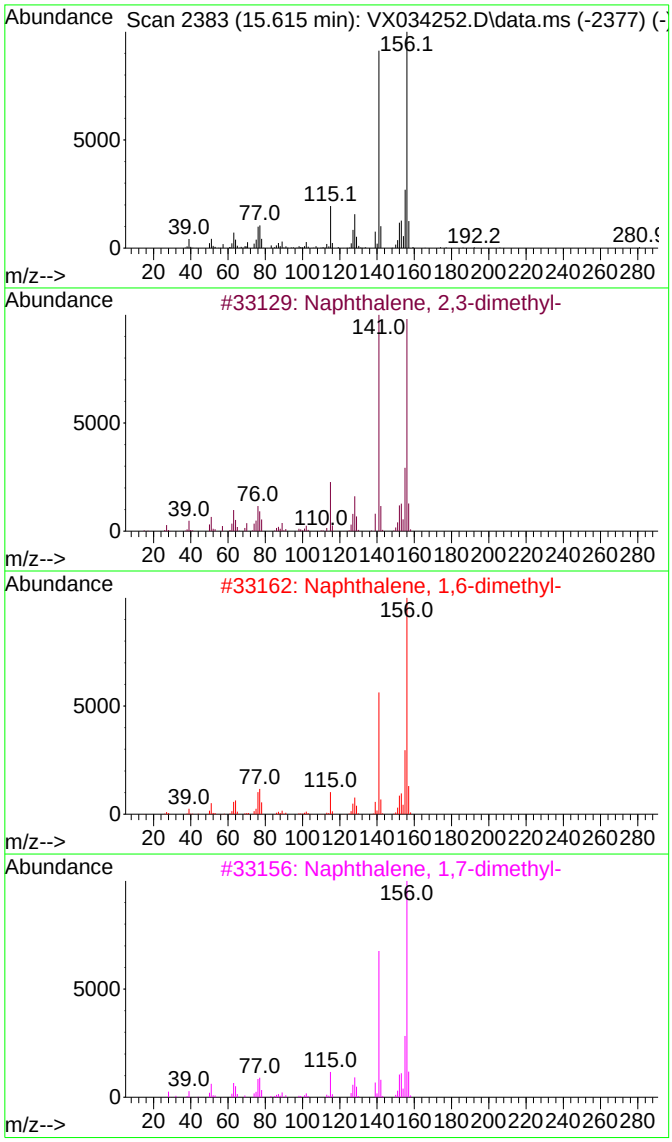
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

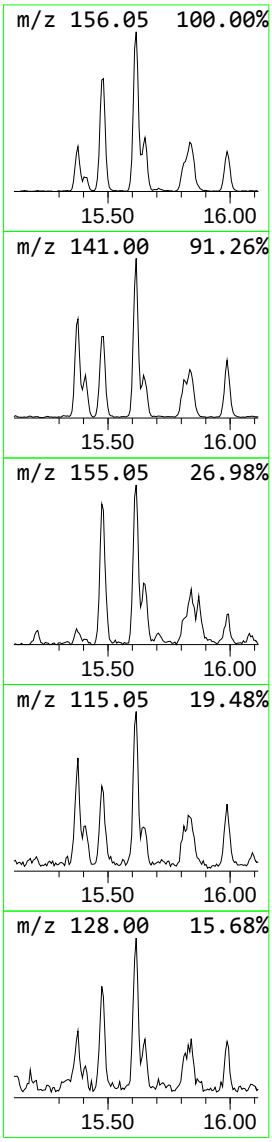
****

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	10.59 ug/l	222027	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

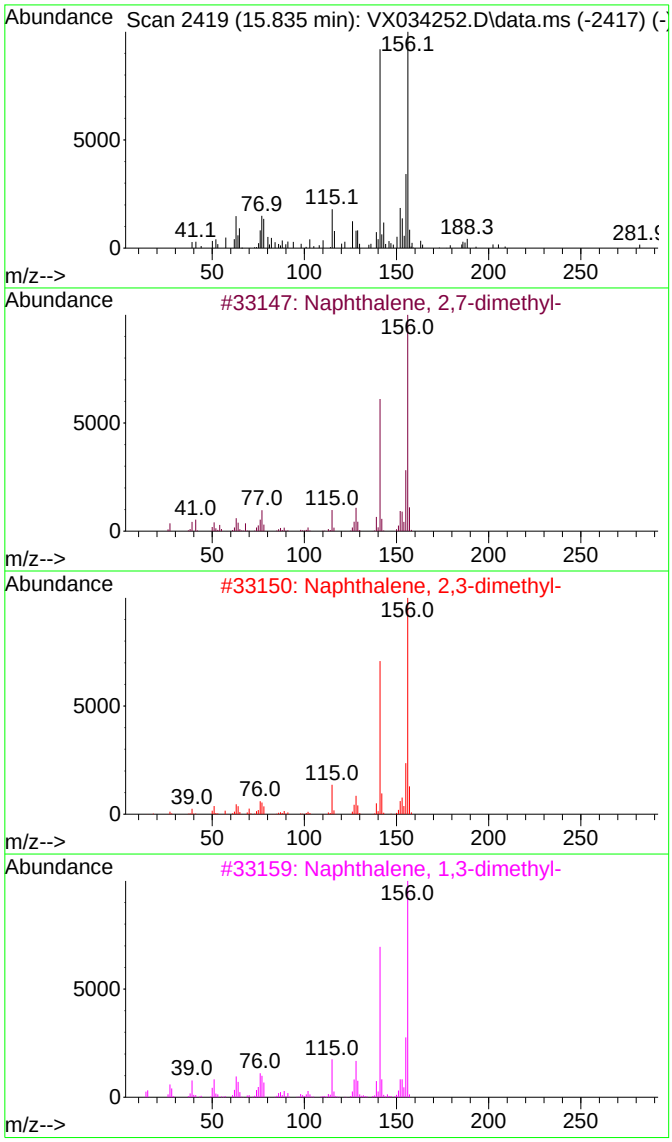
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

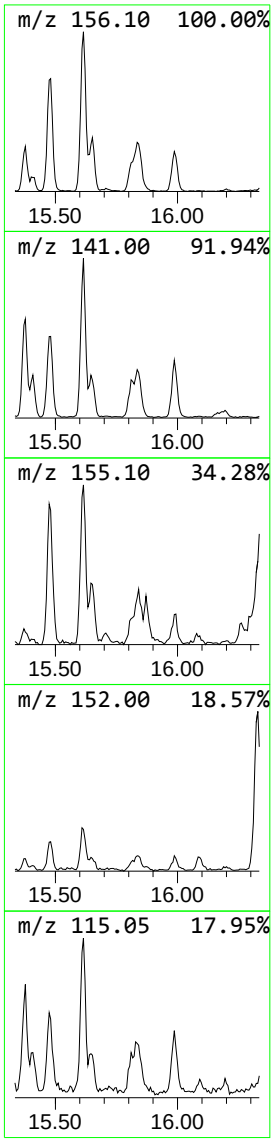
****

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	5.45 ug/l	114265	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	90
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	87
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	81
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	81
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	76





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

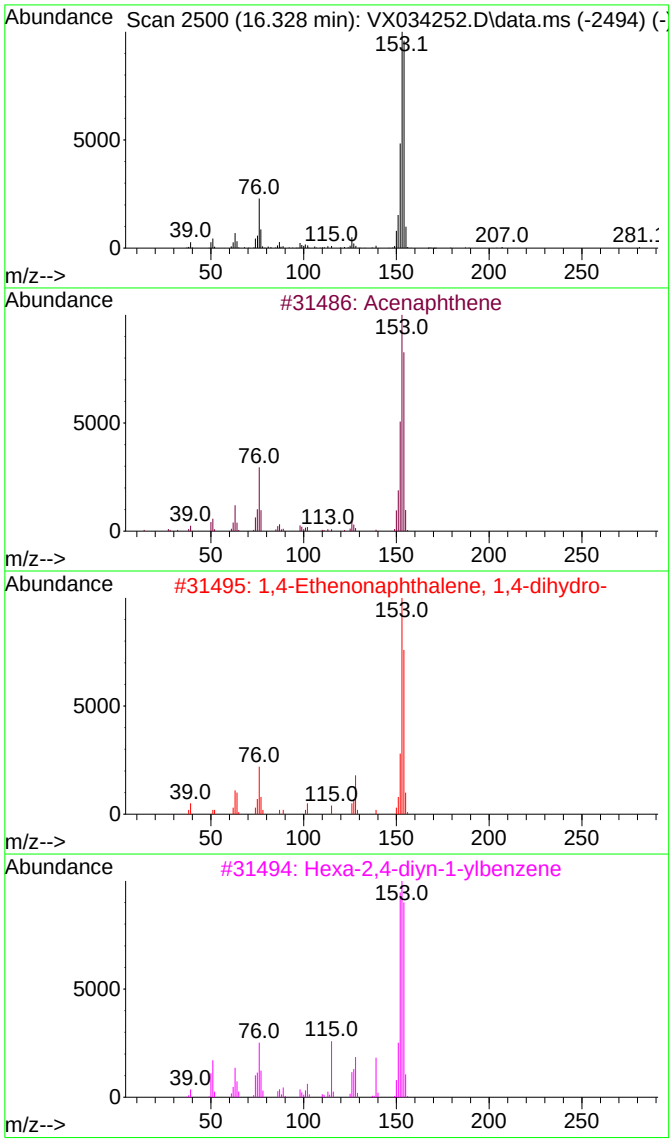
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

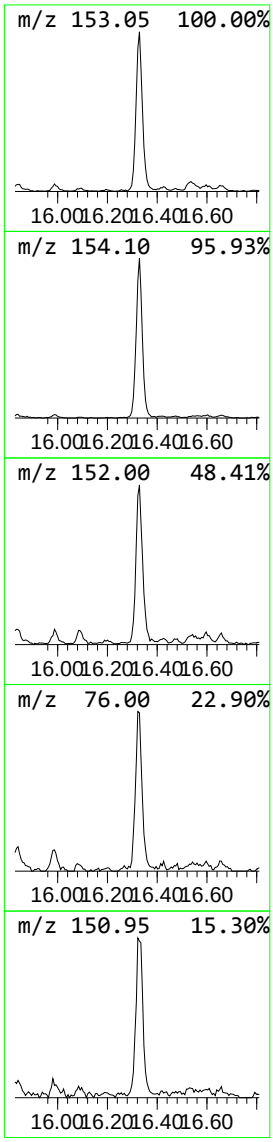
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	12.60 ug/l	264230	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	89
2	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
5	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034252.D
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VB-15-241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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
1H-Indene, 1-me...	13.774	15.9	ug/l	334574	4	12.024	1048600	50.0
Benzocyclohepta...	14.634	12.6	ug/l	264031	4	12.024	1048600	50.0
1,4-Methanonaph...	14.780	18.6	ug/l	388942	4	12.024	1048600	50.0
Naphthalene, 1,...	15.475	8.7	ug/l	181397	4	12.024	1048600	50.0
Naphthalene, 2,...	15.615	10.6	ug/l	222027	4	12.024	1048600	50.0
Naphthalene, 2,...	15.835	5.5	ug/l	114265	4	12.024	1048600	50.0
1,4-Ethenonapht...	16.328	12.6	ug/l	264230	4	12.024	1048600	50.0