LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080223\
Data File : VX036777.D
Acq On : 02 Aug 2023 17:53
Operator : JC/MD
Sample : 03815-01 10X
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUILDING-A-1-(0-5)

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\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036777.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.788	272	279	285	rBV2	3584	7398	1.02%	0.144%
2	2.946	296	305	315	rVB	11741	26918	3.71%	0.525%
3	4.580	561	573	586	rBV	12303	41204	5.67%	0.803%
4	5.385	695	705	721	rBV2	81311	241341	33.23%	4.706%
5	5.550	721	732	751	rVB	134107	381317	52.50%	7.435%
6	5.958	788	799	807	rBV	88425	235269	32.39%	4.588%
7	6.037	807	812	826	rVB2	14514	38746	5.33%	0.756%
8	6.763	921	931	943	rBV	217234	527069	72.57%	10.277%
9	8.647	1233	1240	1248	rBV	458316	726307	100.00%	14.162%
10	8.720	1248	1252	1262	rVB	11912	19845	2.73%	0.387%
11	10.055	1465	1471	1481	rBV	472529	645306	88.85%	12.583%
12	10.195	1490	1494	1499	rBV	14526	18953	2.61%	0.370%
13	10.305	1507	1512	1521	rBV	9524	14162	1.95%	0.276%
14	10.646	1562	1568	1576	rBV3	6572	12396	1.71%	0.242%
15	11.079	1634	1639	1653	rBV	389891	493293	67.92%	9.619%
16	11.756	1745	1750	1755	rBV	6749	8763	1.21%	0.171%
17	12.024	1788	1794	1801	rBV	486377	621503	85.57%	12.119%
18	12.085	1801	1804	1809	rVB	5900	7400	1.02%	0.144%
19	12.244	1823	1830	1838	rBV	41860	53878	7.42%	1.051%
20	12.414	1853	1858	1864	rBV	12870	16329	2.25%	0.318%
21	13.292	1992	2002	2006	rBV2	12595	18782	2.59%	0.366%
22	13.341	2006	2010	2014	rVV	9104	11463	1.58%	0.224%
23	13.426	2018	2024	2033	rVB	10468	15114	2.08%	0.295%
24	13.774	2073	2081	2090	rBV	164971	208468	28.70%	4.065%
25	13.865	2090	2096	2102	rVB	8613	12321	1.70%	0.240%
26	14.316	2164	2170	2176	rBV	5712	9938	1.37%	0.194%
27	14.597	2211	2216	2219	rBV	9059	12395	1.71%	0.242%
28	14.633	2219	2222	2231	rVB	48877	65306	8.99%	1.273%
29	14.780	2240	2246	2255	rVB	185346	243054	33.46%	4.739%
30	15.206	2306	2316	2321	rBV	15178	21503	2.96%	0.419%
31	15.347	2334	2339	2341	rBV2	6299	9349	1.29%	0.182%
32	15.371	2341	2343	2346	rVV	8833	11446	1.58%	0.223%
33	15.408	2346	2349	2354	rVV4	6872	10466	1.44%	0.204%
34	15.475	2354	2360	2364	rVV	35714	59581	8.20%	1.162%
35	15.511	2364	2366	2372	rVV2	12047	16196	2.23%	0.316%
36	15.615	2377	2383	2386	rVV	59589	97227	13.39%	1.896%

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Integrator: RTE
Smoothing : ON Filtering: 5
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Peak separation: 5

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Title : SW846 8260

37	15.652	2386	2389	2395	rVV	30716	45692	6.29%	0.891%
38	15.737	2399	2403	2409	rVV6	4926	9351	1.29%	0.182%
39	15.810	2409	2415	2417	rVV3	13809	22702	3.13%	0.443%
40	15.834	2417	2419	2430	rVB3	15171	25832	3.56%	0.504%
41	15.987	2438	2444	2454	rBV3	8550	15543	2.14%	0.303%
42	16.090	2456	2461	2467	rVB2	10275	17053	2.35%	0.333%
43	16.328	2488	2500	2506	rBV	15432	32272	4.44%	0.629%

Sum of corrected areas: 5128451

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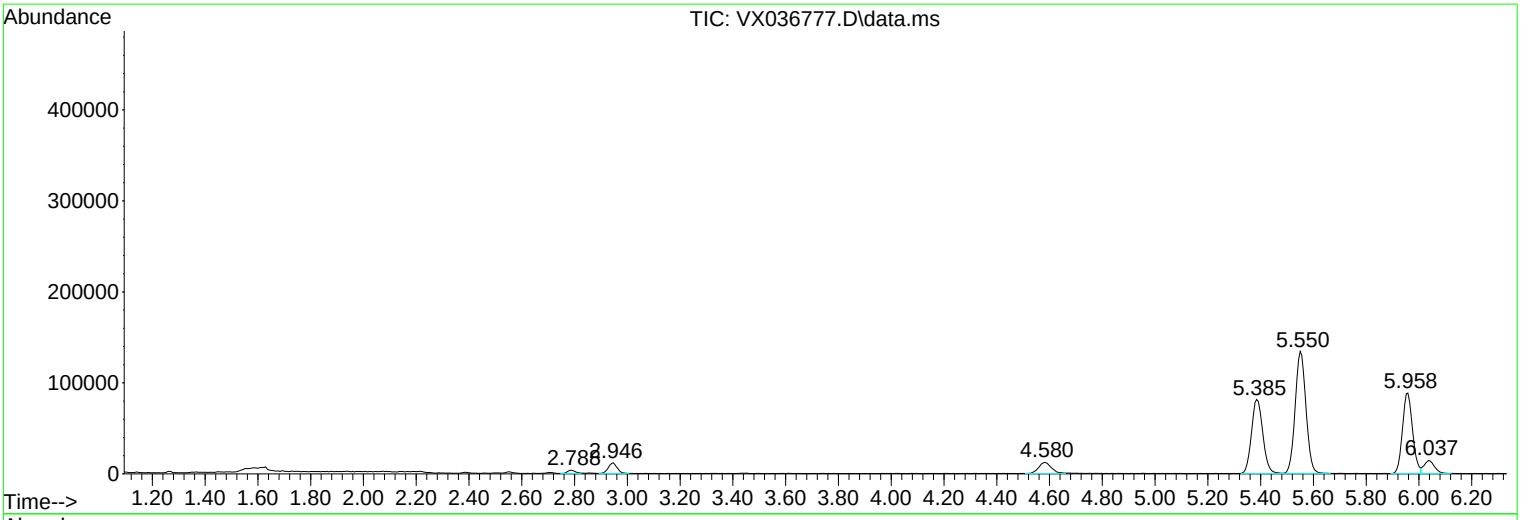
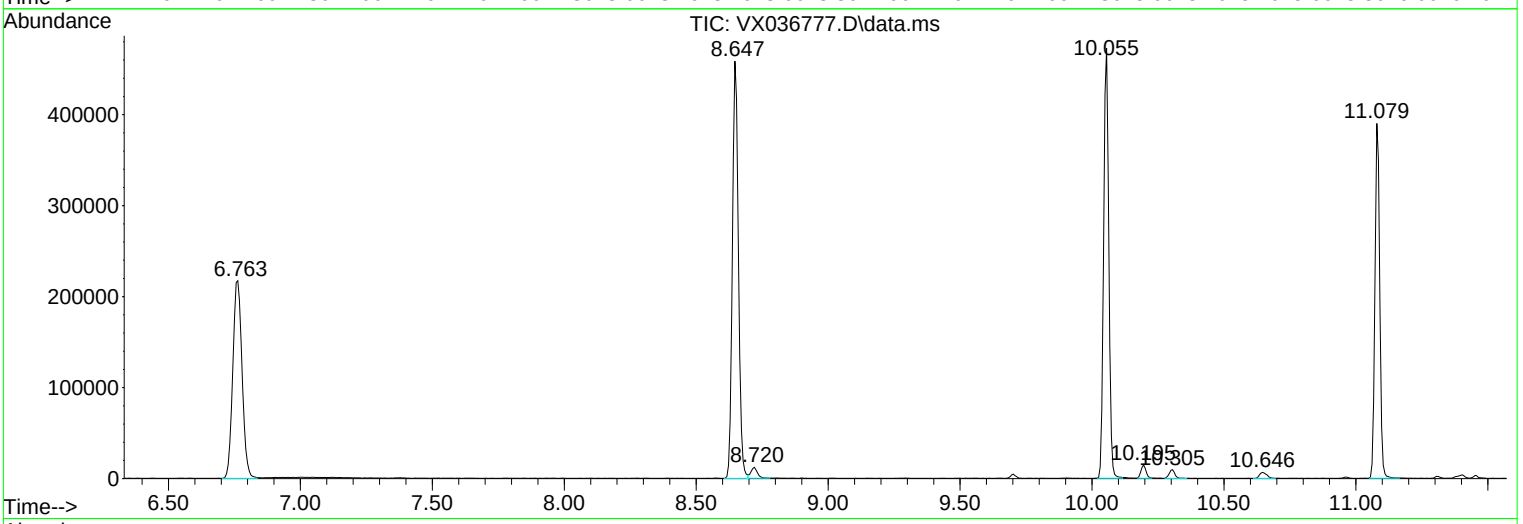
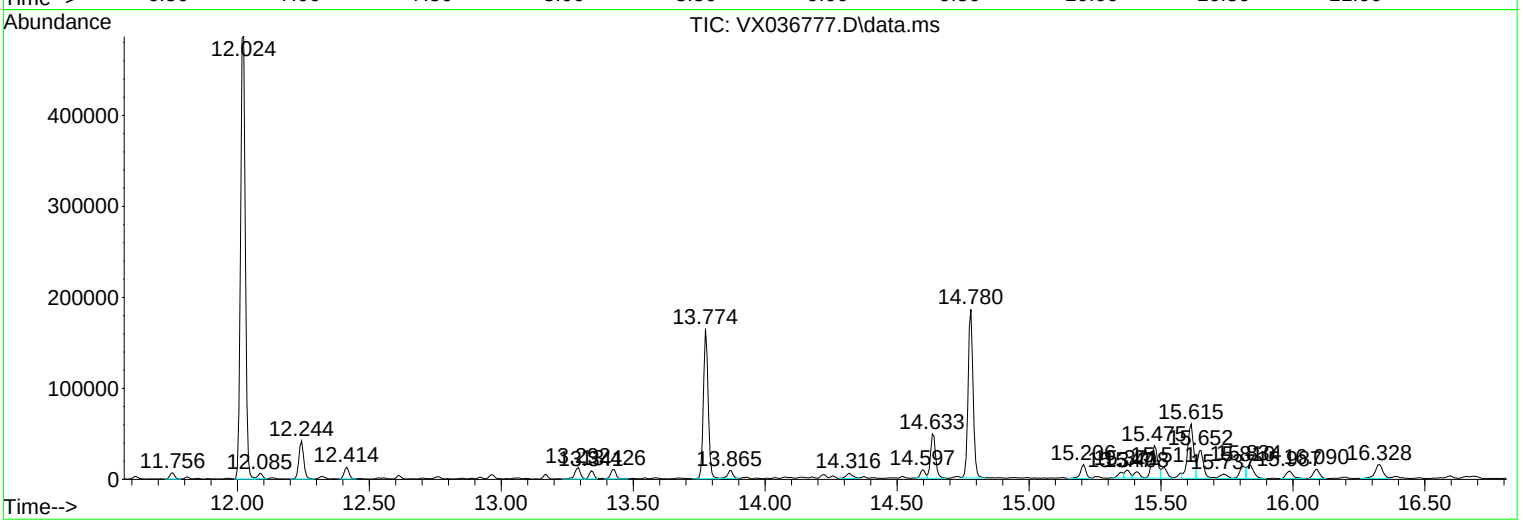
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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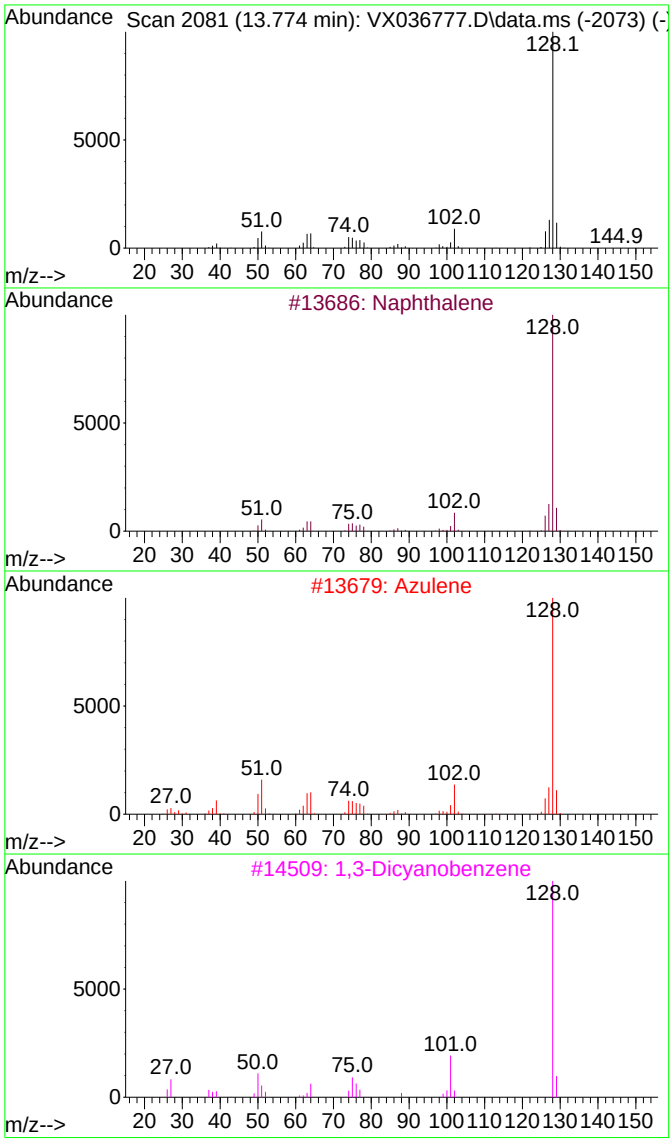
TIC Integration Parameters: LSCINT.P

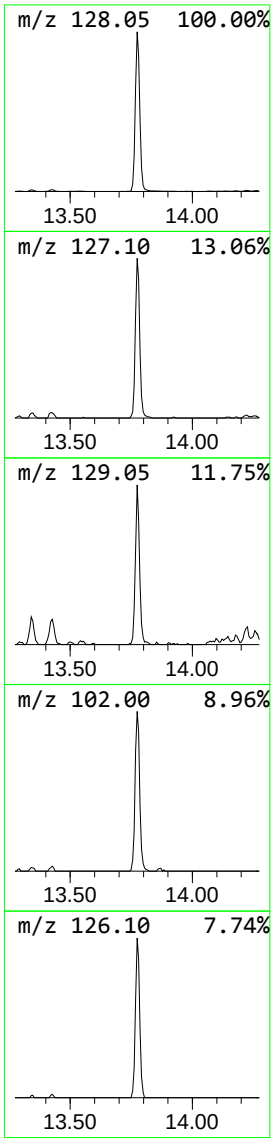
****

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	16.77 ug/l	208468	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	91
3	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50





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MSVOA_X
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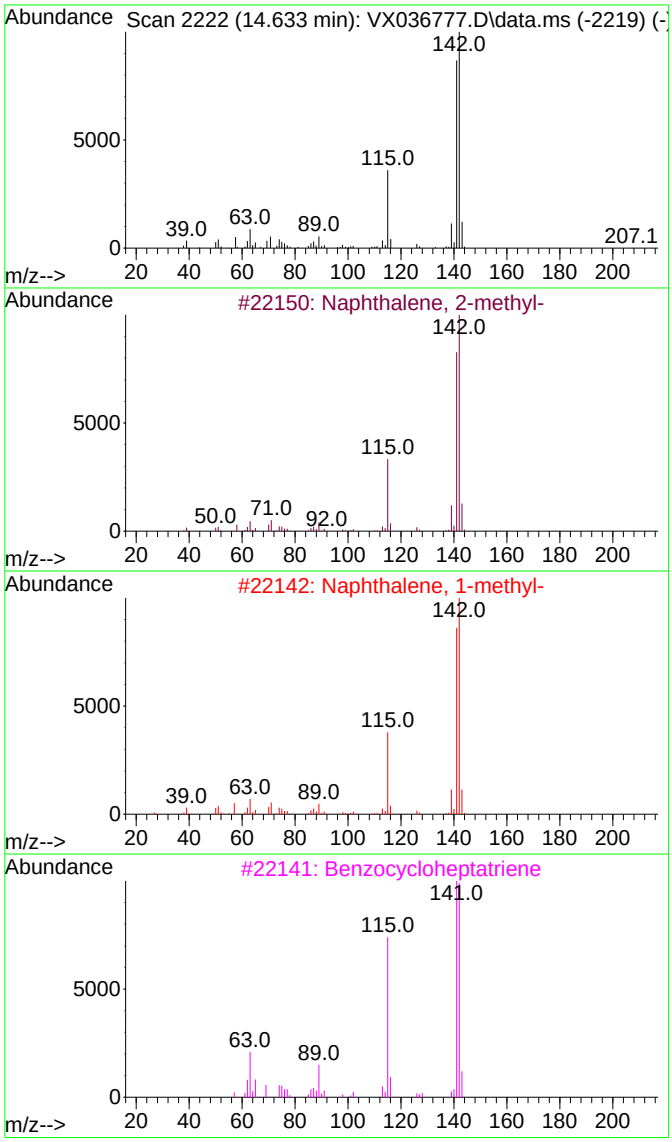
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

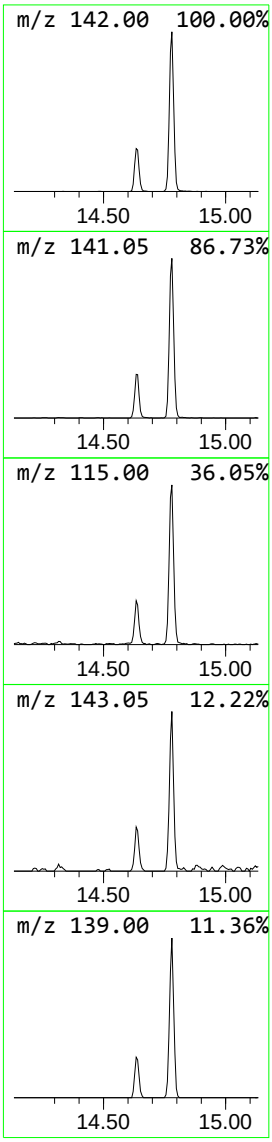
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	5.25 ug/l	65306	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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64





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ClientSampleId :
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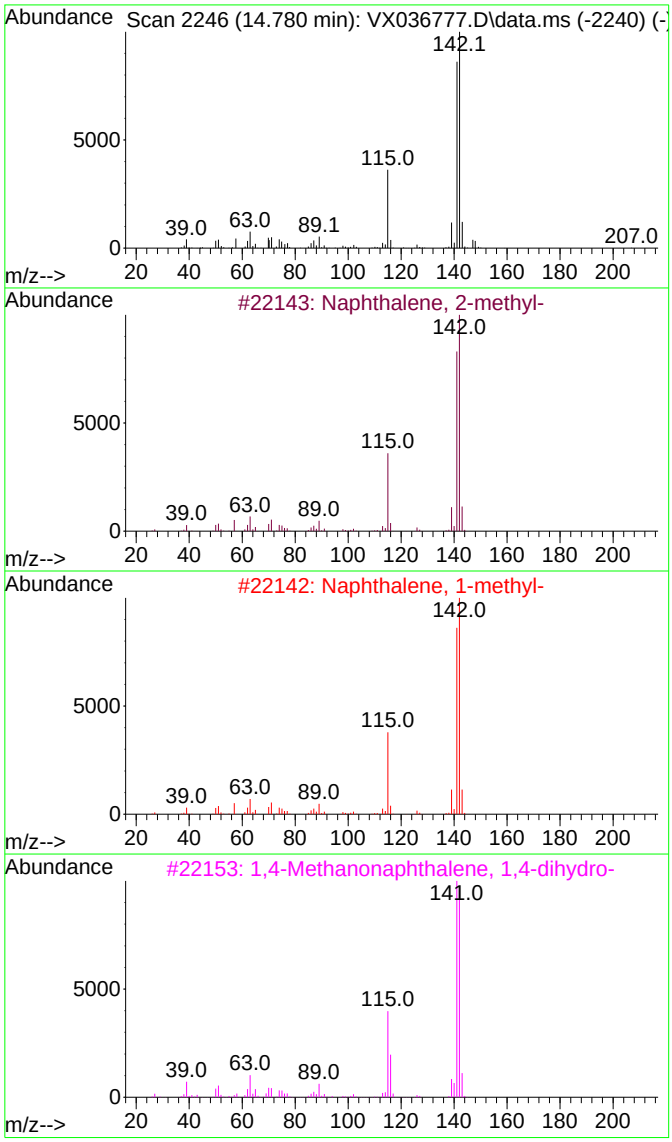
Quant Title : SW846 8260

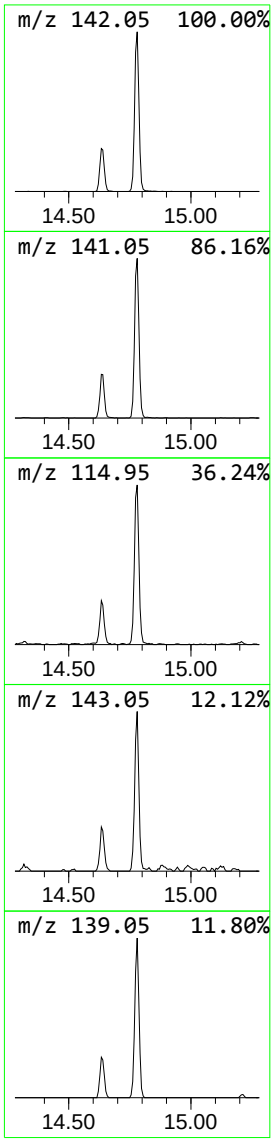
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	19.55 ug/l	243054	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	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





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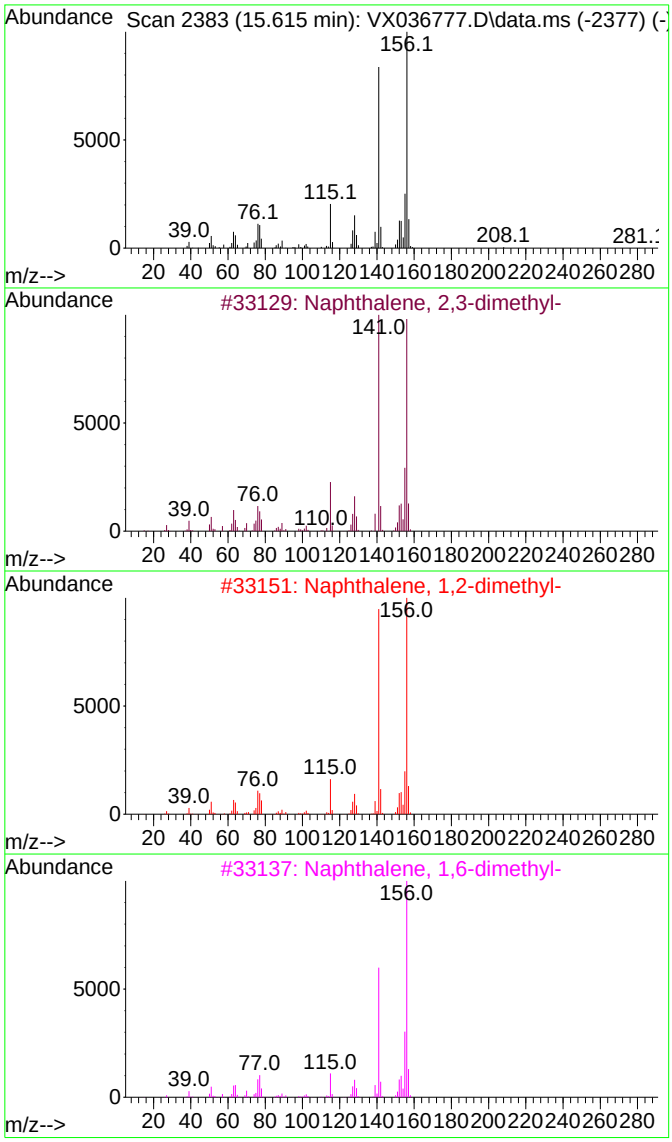
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

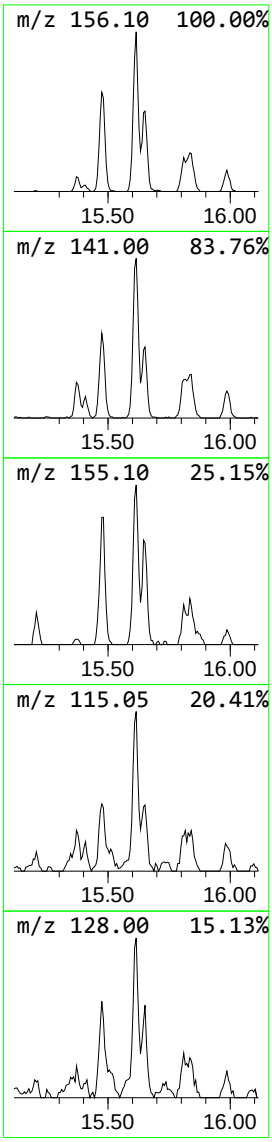
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	7.82 ug/l	97227	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, 1,2-dimethyl-	156	C12H12	000573-98-8	98
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Azulene	13.774	16.8	ug/l	208468	4	12.024	621503	50.0
Benzocycloheptа...	14.633	5.3	ug/l	65306	4	12.024	621503	50.0
1,4-Methanonaph...	14.780	19.6	ug/l	243054	4	12.024	621503	50.0
Naphthalene, 2,...	15.615	7.8	ug/l	97227	4	12.024	621503	50.0