LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

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\82X060722W.M
Title : SW846 8260

Signal : TIC: VX029509.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	72	90	95	rBV	26003	62717	3.68%	0.473%
2	2.429	211	220	235	rVB5	6050	25980	1.52%	0.196%
3	2.733	262	270	275	rBV2	19546	51617	3.03%	0.389%
4	2.776	275	277	289	rVB5	9614	21660	1.27%	0.163%
5	2.953	297	306	316	rBV	10125	29257	1.71%	0.221%
6	3.075	318	326	335	rVB4	7861	18663	1.09%	0.141%
7	5.391	694	706	721	rBV	175775	547156	32.07%	4.127%
8	5.550	721	732	751	rVB	275292	809972	47.47%	6.110%
9	5.824	766	777	788	rBV6	9165	31001	1.82%	0.234%
10	5.958	788	799	814	rBV	199276	560975	32.88%	4.232%
11	6.349	855	863	877	rBV7	8312	28062	1.64%	0.212%
12	6.763	920	931	949	rBV	396794	970166	56.86%	7.318%
13	7.129	979	991	1002	rVB5	16174	45741	2.68%	0.345%
14	7.373	1022	1031	1041	rVB2	30365	76177	4.46%	0.575%
15	7.489	1041	1050	1056	rBV4	7700	18388	1.08%	0.139%
16	7.769	1090	1096	1103	rVB3	15984	32976	1.93%	0.249%
17	7.952	1119	1126	1141	rVB4	14375	33169	1.94%	0.250%
18	8.598	1225	1232	1235	rBV2	26401	50241	2.94%	0.379%
19	8.647	1235	1240	1248	rVV	1033268	1706127	100.00%	12.870%
20	8.720	1248	1252	1257	rVV	35909	62026	3.64%	0.468%
21	8.769	1257	1260	1265	rVB3	13629	22081	1.29%	0.167%
22	8.909	1279	1283	1288	rVB5	11226	18001	1.06%	0.136%
23	8.976	1288	1294	1301	rBV	35416	58761	3.44%	0.443%
24	9.104	1309	1315	1321	rVB3	14315	27578	1.62%	0.208%
25	9.385	1357	1361	1365	rBV3	13361	21055	1.23%	0.159%
26	9.507	1375	1381	1386	rBV6	19416	48139	2.82%	0.363%
27	9.561	1386	1390	1395	rVB3	24786	38338	2.25%	0.289%
28	9.616	1395	1399	1404	rBV	43054	67145	3.94%	0.506%
29	9.836	1428	1435	1439	rBV3	24756	52722	3.09%	0.398%
30	10.006	1457	1463	1466	rBV	15735	25128	1.47%	0.190%
31	10.055	1466	1471	1478	rVV	742512	1035092	60.67%	7.808%
32	10.189	1487	1493	1498	rBV4	14698	31175	1.83%	0.235%
33	10.305	1503	1512	1518	rVV4	45785	127409	7.47%	0.961%
34	10.360	1518	1521	1532	rVB3	31219	58723	3.44%	0.443%
35	10.458	1532	1537	1542	rBV2	20263	32949	1.93%	0.249%
36	10.586	1551	1558	1565	rBV4	37636	85218	4.99%	0.643%

LSC Area Percent Report

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Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
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Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

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
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Title : SW846 8260

37	10.647	1565	1568	1571	rBV2	16918	23047	1.35%	0.174%
38	10.781	1582	1590	1594	rBV2	58948	97897	5.74%	0.738%
39	10.860	1594	1603	1607	rBV4	57298	119228	6.99%	0.899%
40	10.897	1607	1609	1613	rVB2	39454	45194	2.65%	0.341%
41	10.957	1614	1619	1623	rBV4	13100	25783	1.51%	0.194%
42	11.006	1623	1627	1629	rBV3	16138	24341	1.43%	0.184%
43	11.086	1635	1640	1645	rBV	794489	1054131	61.79%	7.951%
44	11.195	1650	1658	1659	rBV5	25878	49487	2.90%	0.373%
45	11.220	1659	1662	1667	rVB2	50869	68223	4.00%	0.515%
46	11.311	1673	1677	1679	rBV2	22172	31314	1.84%	0.236%
47	11.384	1685	1689	1694	rBV3	43794	83573	4.90%	0.630%
48	11.433	1694	1697	1699	rVV	34773	50482	2.96%	0.381%
49	11.482	1702	1705	1709	rVB2	54961	71001	4.16%	0.536%
50	11.622	1722	1728	1735	rBV4	34000	87834	5.15%	0.663%
51	11.689	1735	1739	1741	rVV5	16789	24089	1.41%	0.182%
52	11.720	1741	1744	1746	rVV	38714	43990	2.58%	0.332%
53	11.756	1746	1750	1760	rVB	93396	177285	10.39%	1.337%
54	11.890	1761	1772	1776	rBV9	42421	115027	6.74%	0.868%
55	11.945	1776	1781	1783	rBV3	36804	54766	3.21%	0.413%
56	11.976	1783	1786	1789	rVB2	28833	32919	1.93%	0.248%
57	12.024	1789	1794	1800	rBV	766845	964925	56.56%	7.279%
58	12.091	1801	1805	1810	rVB	38293	59737	3.50%	0.451%
59	12.158	1813	1816	1827	rVB9	30459	77472	4.54%	0.584%
60	12.268	1827	1834	1838	rBV4	37194	103591	6.07%	0.781%
61	12.317	1838	1842	1848	rBV3	70407	145825	8.55%	1.100%
62	12.427	1856	1860	1863	rBV3	46417	61293	3.59%	0.462%
63	12.469	1864	1867	1872	rVB4	57695	96956	5.68%	0.731%
64	12.561	1875	1882	1885	rBV6	44120	104021	6.10%	0.785%
65	12.683	1900	1902	1906	rBV5	20826	21787	1.28%	0.164%
66	12.817	1920	1924	1929	rBV3	69496	101485	5.95%	0.766%
67	12.890	1933	1936	1938	rBV	28186	34878	2.04%	0.263%
68	12.988	1949	1952	1955	rVB2	69280	78602	4.61%	0.593%
69	13.292	1999	2002	2007	rVB2	107210	155502	9.11%	1.173%
70	13.414	2020	2022	2025	rBV3	39298	50735	2.97%	0.383%
71	13.805	2083	2086	2089	rVB3	85322	105712	6.20%	0.797%
72	14.213	2151	2153	2158	rVB5	79184	102464	6.01%	0.773%
73	14.548	2206	2208	2210	rBV2	33889	40233	2.36%	0.303%
74	14.640	2217	2223	2226	rBV2	124832	206572	12.11%	1.558%
75	14.756	2239	2242	2244	rBV3	53707	61055	3.58%	0.461%
76	14.786	2244	2247	2254	rVB4	86764	134726	7.90%	1.016%

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Integrator: RTE
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Title : SW846 8260

77	14.847	2254	2257	2261	rBV3	56035	73958	4.33%	0.558%
78	15.182	2308	2312	2320	rVB8	49378	99057	5.81%	0.747%
79	15.377	2341	2344	2347	rBV4	58113	80495	4.72%	0.607%
80	15.420	2347	2351	2355	rVB2	110903	159760	9.36%	1.205%
81	15.481	2357	2361	2369	rVB2	96611	166446	9.76%	1.256%
82	15.615	2379	2383	2386	rBV	85521	142822	8.37%	1.077%
83	15.652	2386	2389	2398	rVV8	102560	227617	13.34%	1.717%
84	15.743	2401	2404	2409	rVB3	95747	145335	8.52%	1.096%
85	16.091	2457	2461	2466	rBV4	66589	118359	6.94%	0.893%
86	16.280	2487	2492	2501	rVB5	44644	124442	7.29%	0.939%

Sum of corrected areas: 13257058

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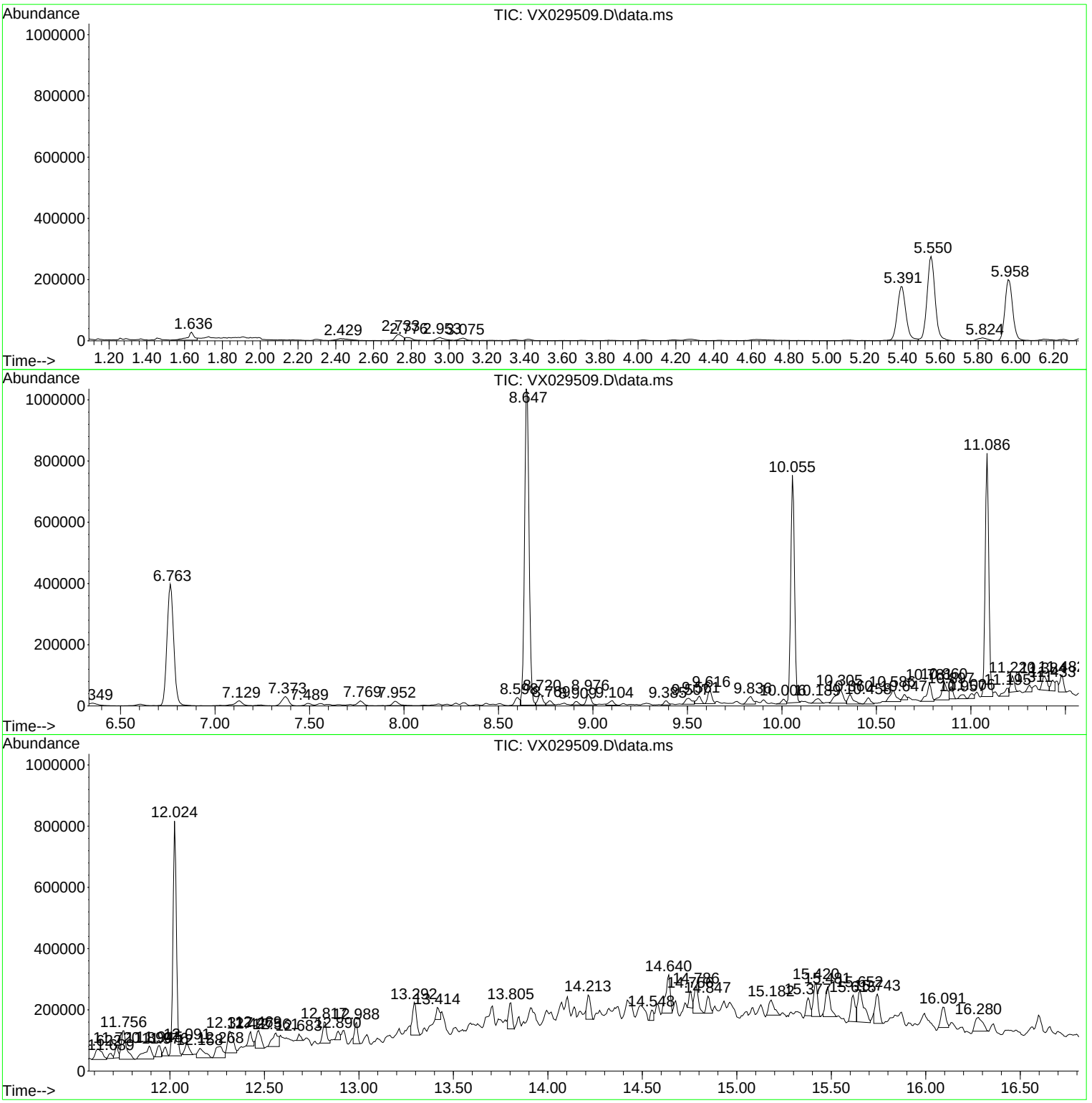
ClientSampleId :
WC-14A-1A-10-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
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WC-14A-1A-10-G

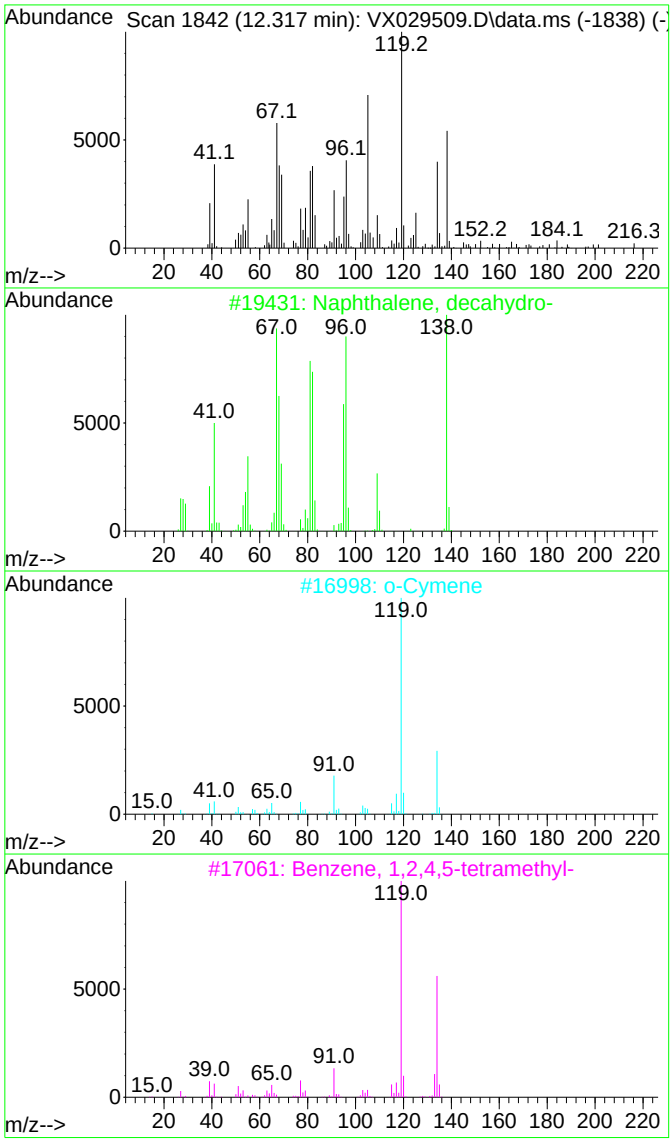
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

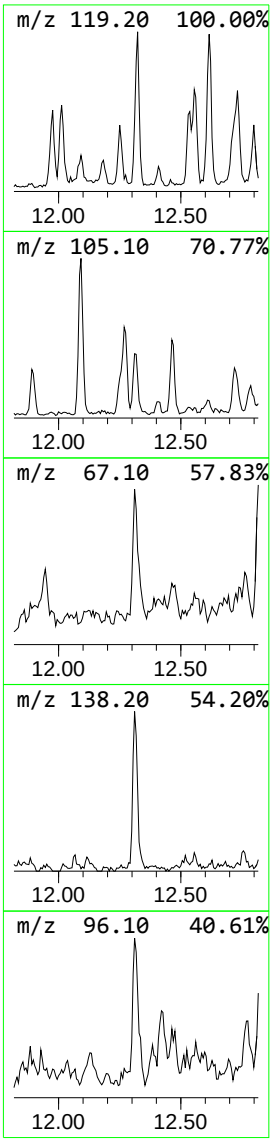
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, decahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	7.56 ug/l	145825	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	70
2	o-Cymene	134	C10H14	000527-84-4	49
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	42
4	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	42
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	42





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Operator : JC/MD
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Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

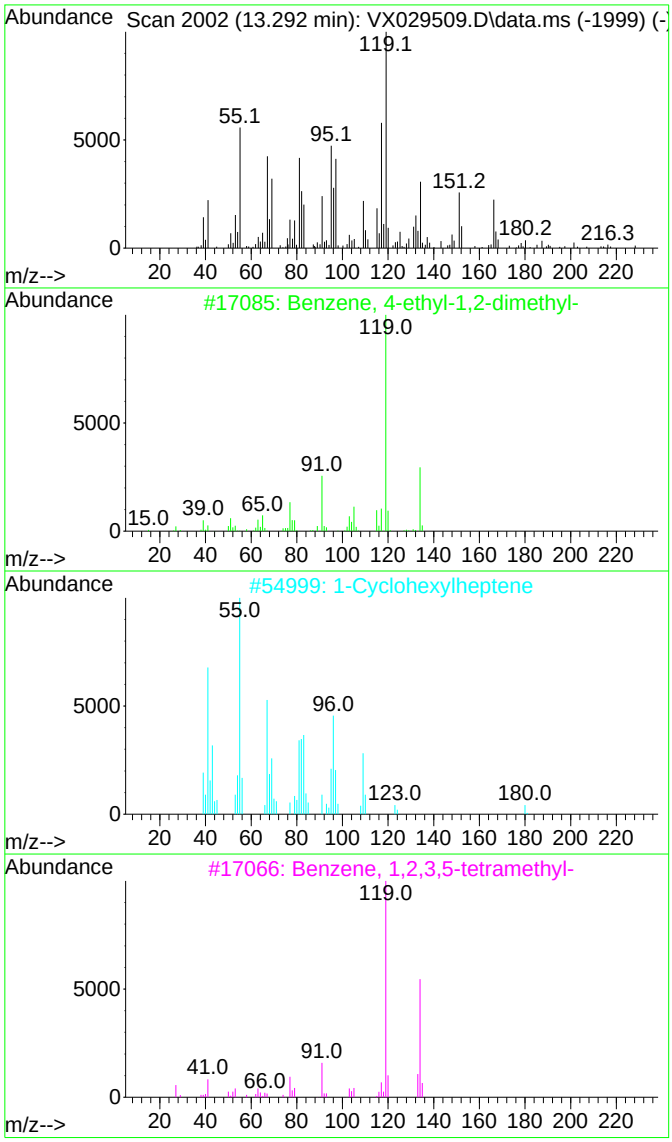
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

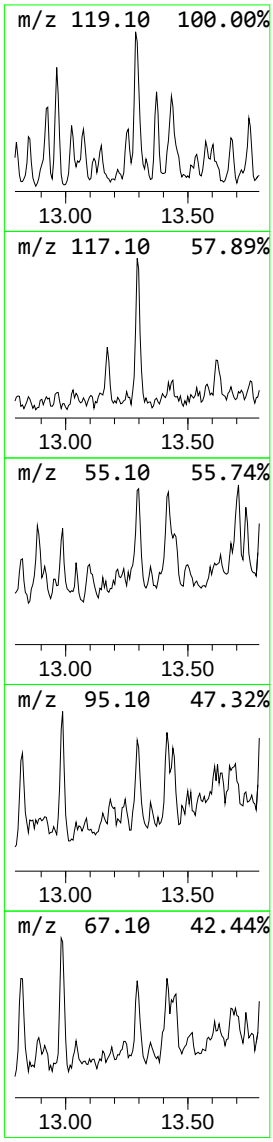
****

Peak Number 2 unknown13.292 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.06 ug/l	155502	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	35
2	1-Cyclohexylheptene	180	C13H24	114614-83-4	35
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	35
4	p-Cymene	134	C10H14	000099-87-6	35
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	35





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

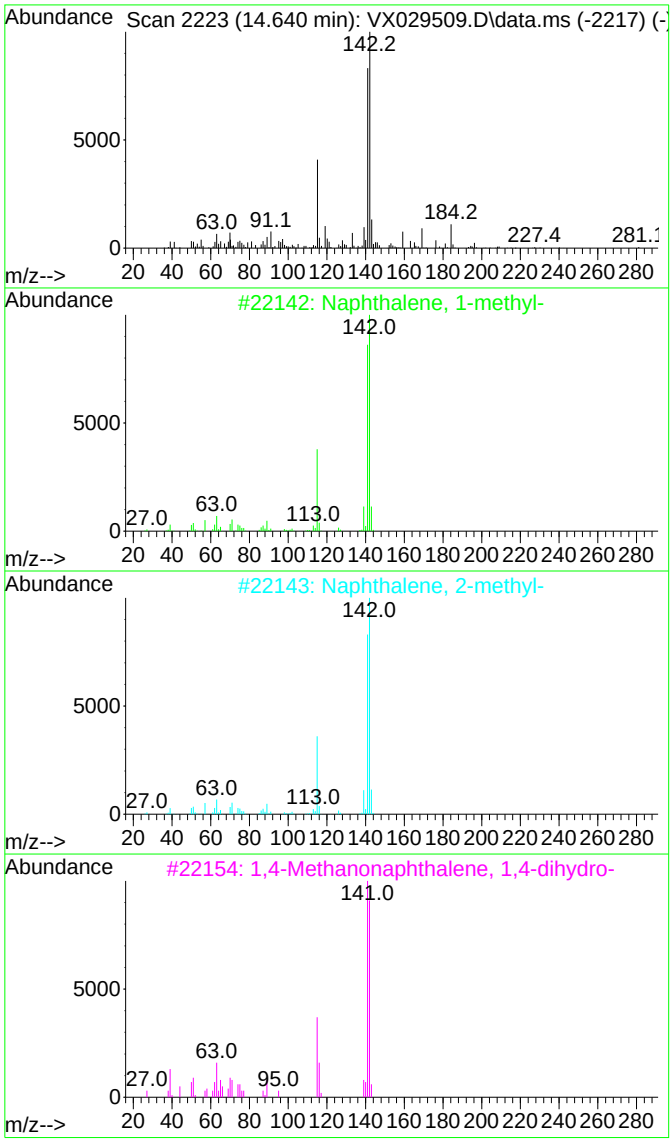
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

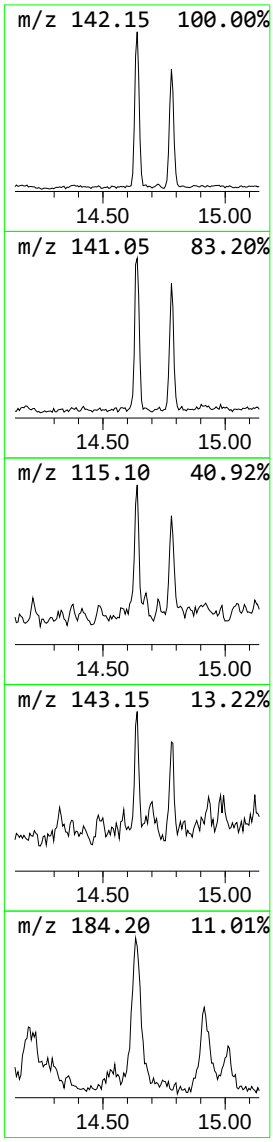
****

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	10.70 ug/l	206572	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	83
4	Benzocycloheptatriene	142	C11H10	000264-09-5	83
5	1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	47





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Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

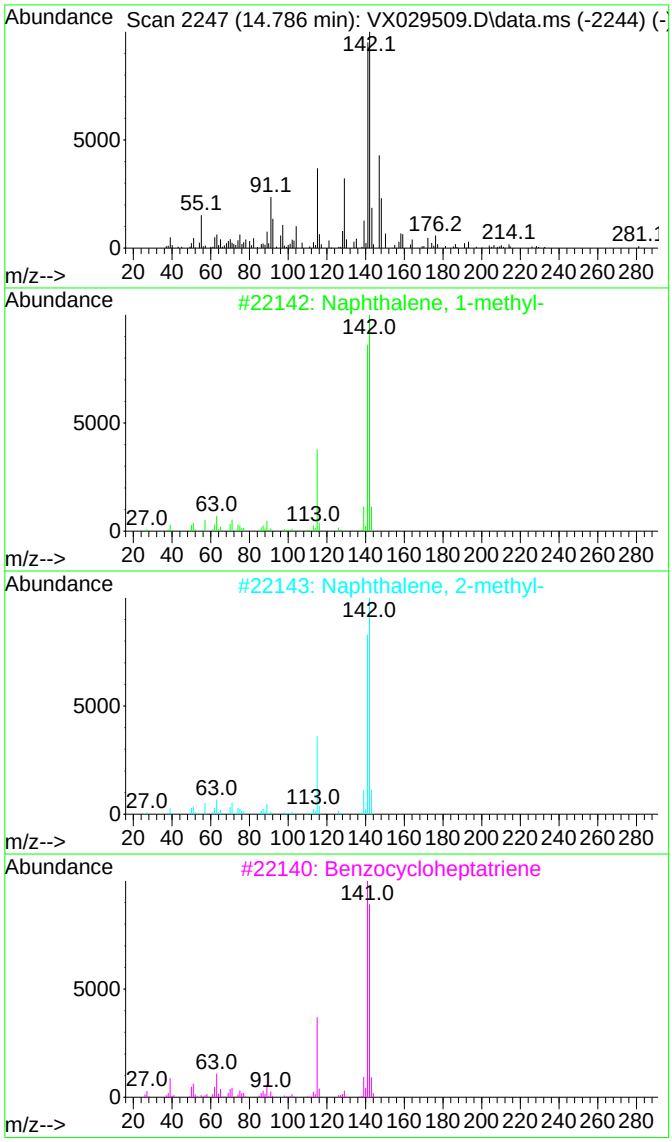
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

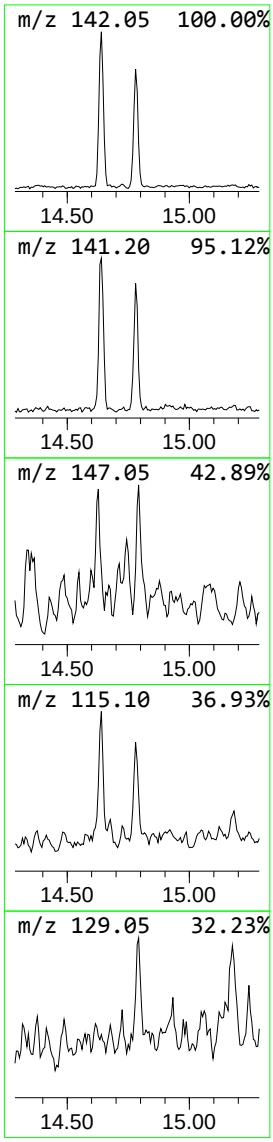
****

Peak Number 4 Benzocycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	6.98 ug/l	134726	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3	Benzocycloheptatriene	142	C11H10	000264-09-5	64
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	58
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	52





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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

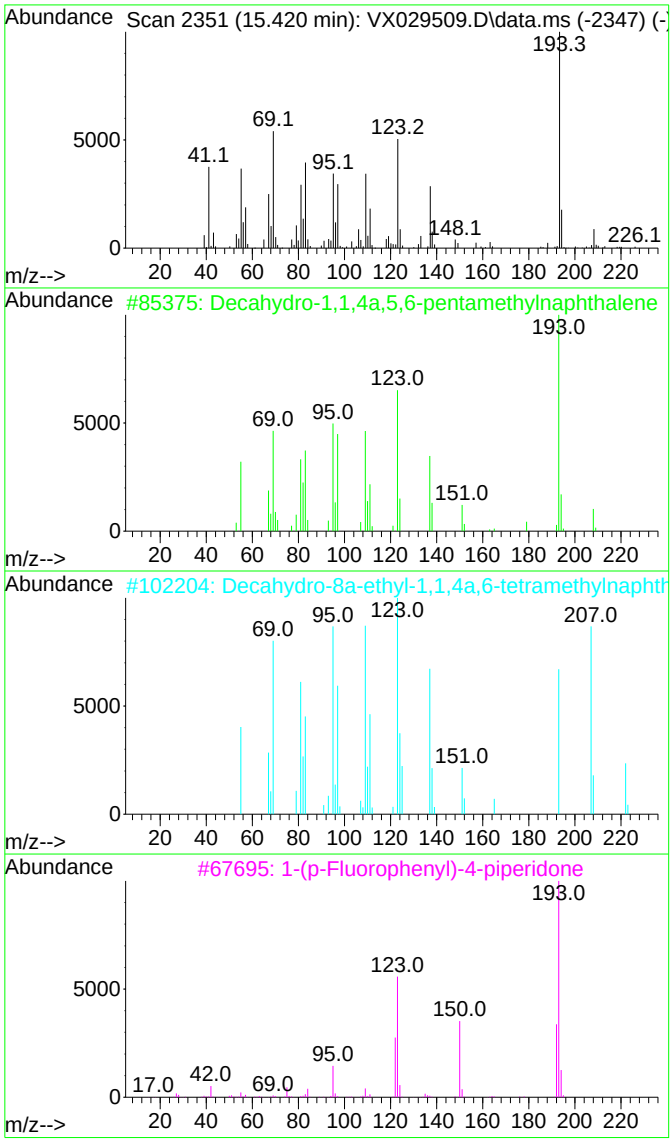
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

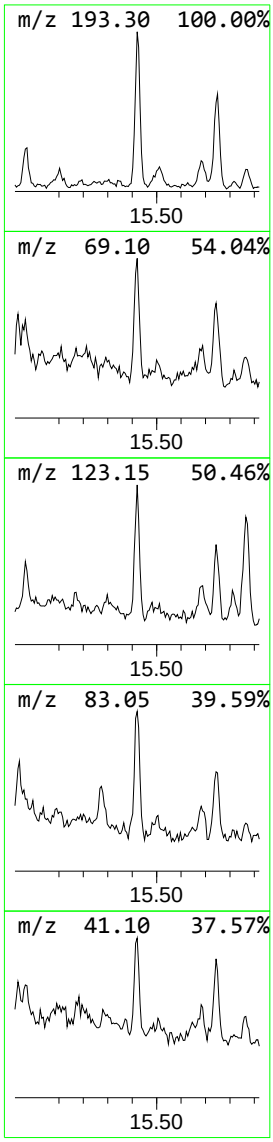
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	8.28 ug/l	159760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	89
2	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	38
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	35
5	n-Nonenylsuccinic anhydride	224	C13H20O3	028928-97-4	27





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ClientSampleId :
WC-14A-1A-10-G

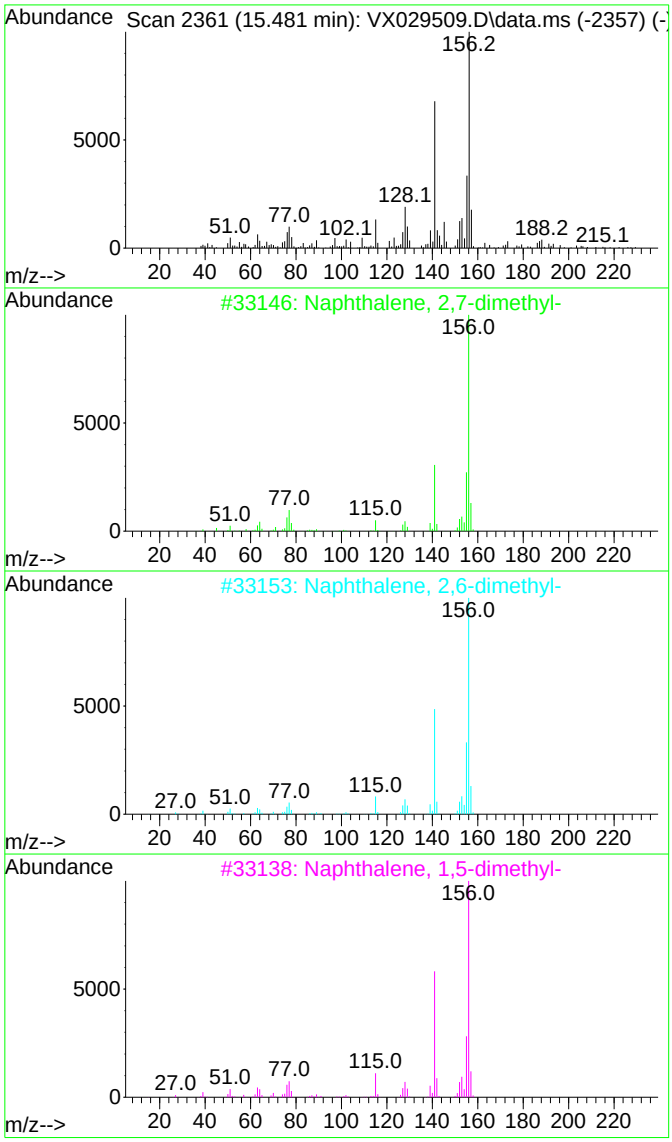
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

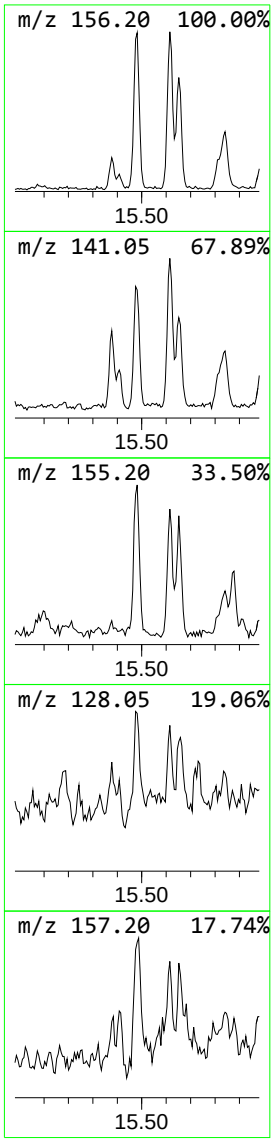
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	8.62 ug/l	166446	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	95
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	92
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

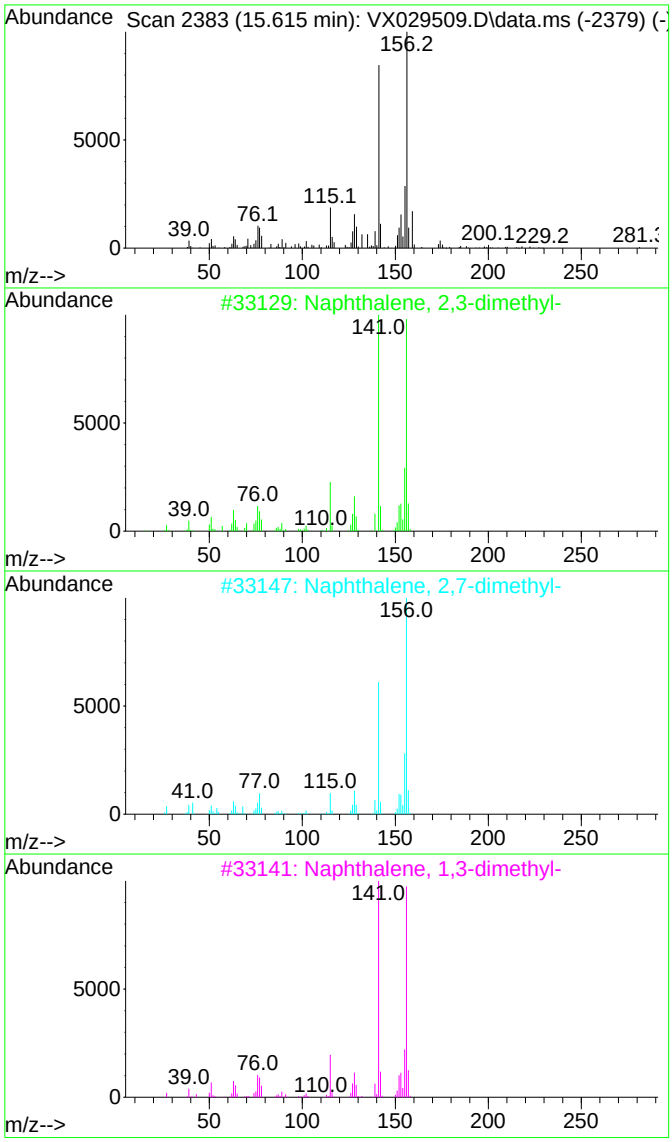
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

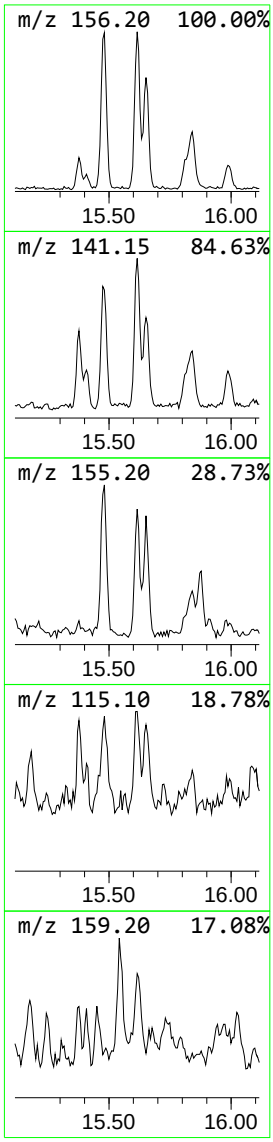
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	7.40 ug/l	142822	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	97
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

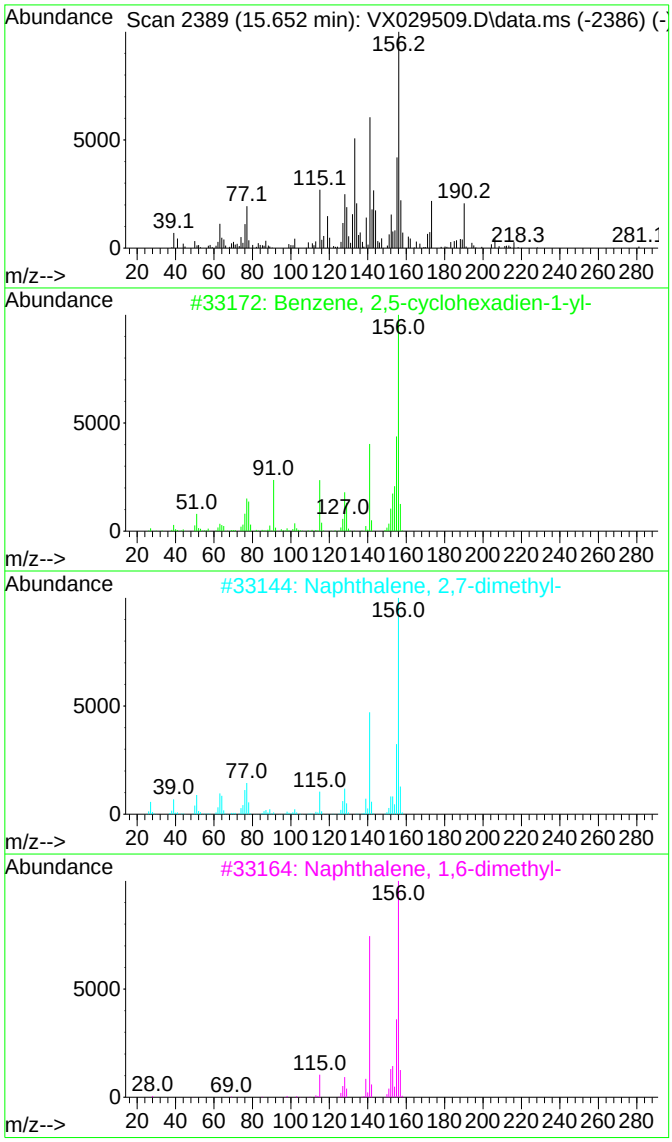
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

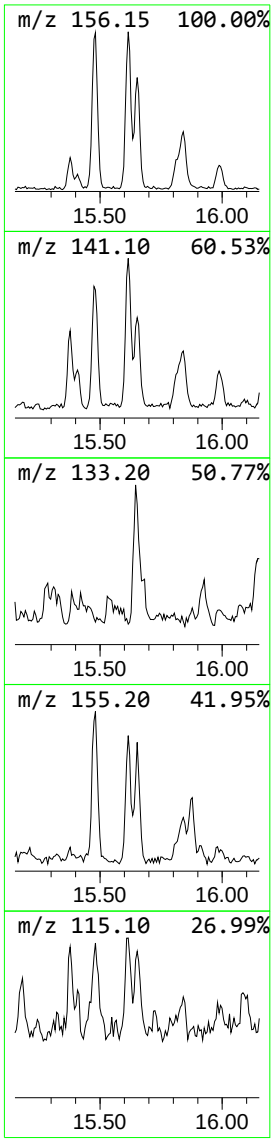
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2,5-cyclohexadien-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	11.79 ug/l	227617	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,5-cyclohexadien-1-yl-	156	C12H12	004794-05-2	60
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	55
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	55
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	46
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

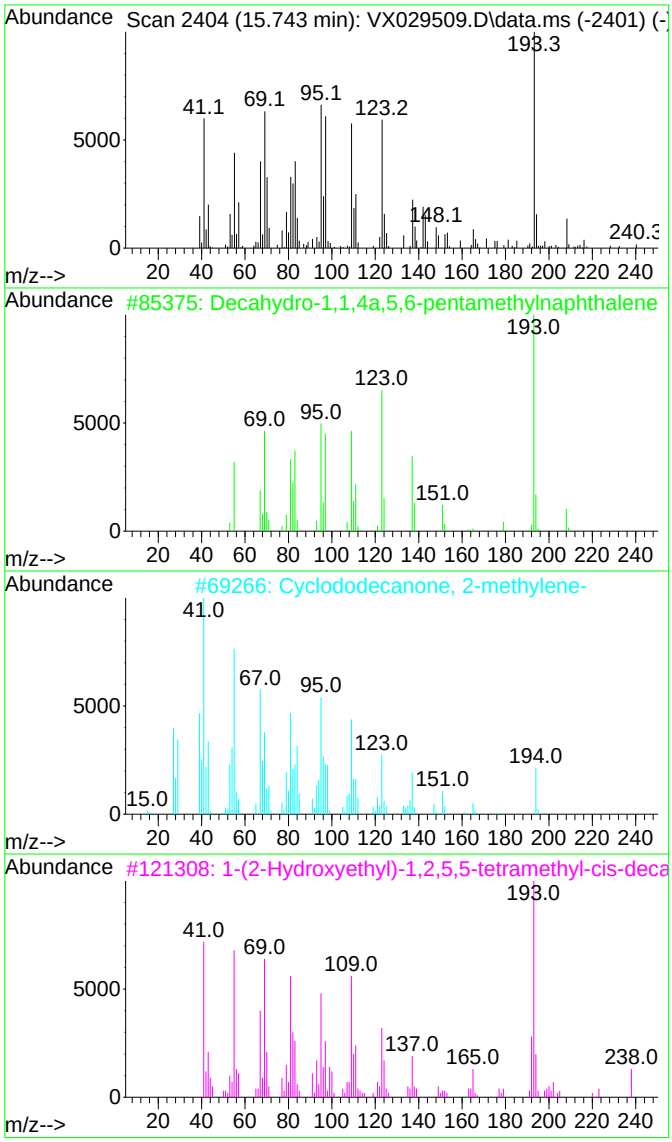
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

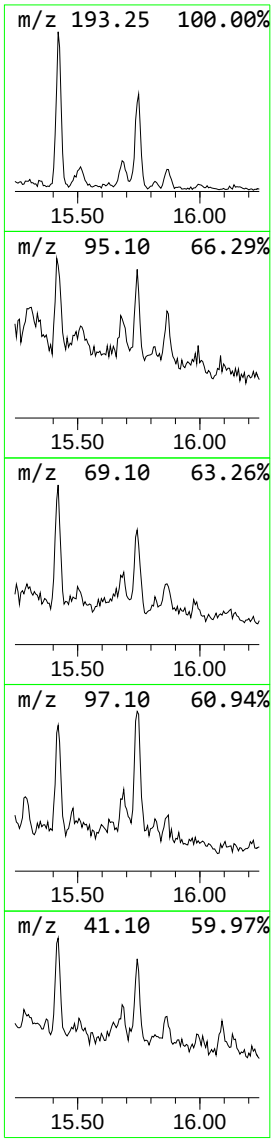
****

Peak Number 9 unknown15.743 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	7.53 ug/l	145335	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	91
2	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
3	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1010298-97-4	43
4	2-Anthracenamine	193	C14H11N	000613-13-8	38
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

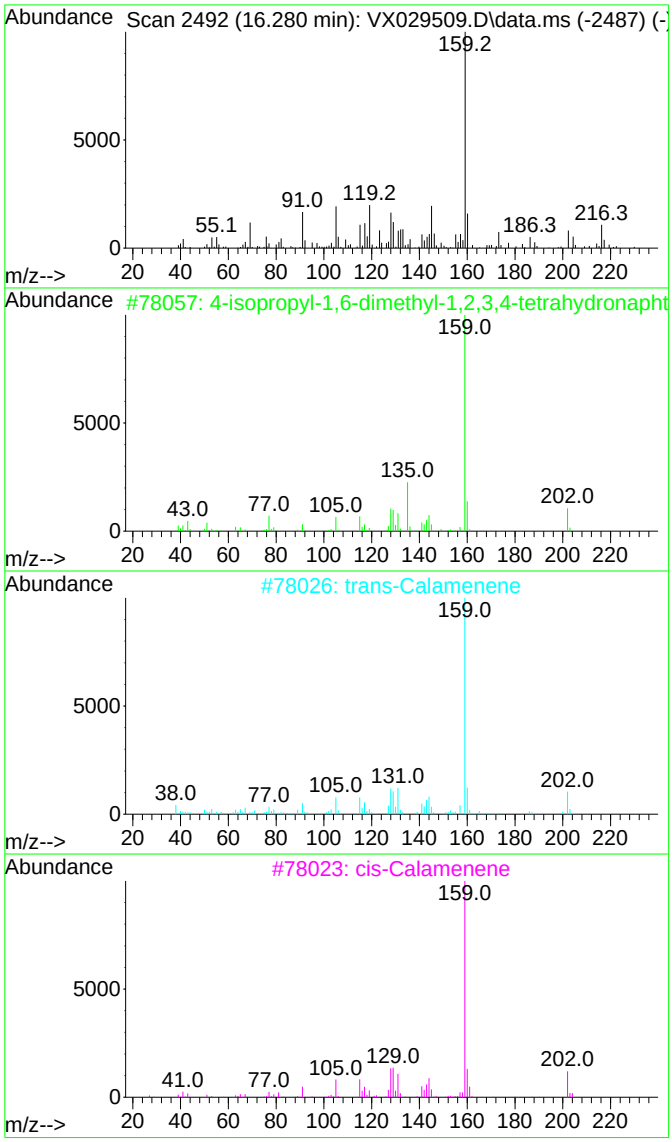
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

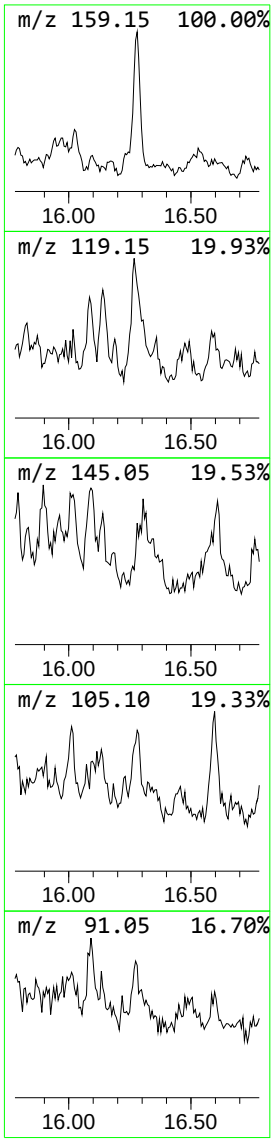
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 4-isopropyl-1,6-dimethyl-1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	6.45 ug/l	124442	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-isopropyl-1,6-dimethyl-1,2,3,4...	202	C15H22	1000378-99-6	55
2	trans-Calamenene	202	C15H22	073209-42-4	55
3	cis-Calamenene	202	C15H22	072937-55-4	49
4	Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	46
5	Cyclopropane, [(phenyl)(trimethy...	202	C13H18Si	1010154-11-9	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061522\
Data File : VX029509.D
Acq On : 15 Jun 2022 16:44
Operator : JC/MD
Sample : N3304-02
Misc : 4.71g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14A-1A-10-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.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
Naphthalene, de...	12.317	7.6	ug/l	145825	4	12.024	964925	50.0
unknown13.292	13.292	8.1	ug/l	155502	4	12.024	964925	50.0
Naphthalene, 1-...	14.640	10.7	ug/l	206572	4	12.024	964925	50.0
Benzocyclohepta...	14.786	7.0	ug/l	134726	4	12.024	964925	50.0
Decahydro-1,1,4...	15.420	8.3	ug/l	159760	4	12.024	964925	50.0
Naphthalene, 2,...	15.481	8.6	ug/l	166446	4	12.024	964925	50.0
Naphthalene, 2,...	15.615	7.4	ug/l	142822	4	12.024	964925	50.0
Benzene, 2,5-cy...	15.652	11.8	ug/l	227617	4	12.024	964925	50.0
unknown15.743	15.743	7.5	ug/l	145335	4	12.024	964925	50.0
4-isopropyl-1,6...	16.280	6.5	ug/l	124442	4	12.024	964925	50.0