LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052423\
Data File : VN077889.D
Acq On : 25 May 2023 08:11
Operator : JC\MD
Sample : 02888-01
Misc : 4.99g/10mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

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\82N051523W.M
Title : SW846 8260

Signal : TIC: VN077889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.306	727	740	755	rBV	679097	2048721	1.21%	0.204%
2	8.224	1060	1066	1078	rVB4	1349926	3601109	2.12%	0.359%
3	8.447	1095	1104	1111	rBV	973122	2238871	1.32%	0.223%
4	8.612	1121	1132	1144	rBV	15541500	35911567	21.19%	3.577%
5	8.859	1168	1174	1184	rVB	1354182	2828056	1.67%	0.282%
6	8.971	1184	1193	1207	rVB	3591837	7288083	4.30%	0.726%
7	9.106	1207	1216	1222	rBV2	1011510	2334724	1.38%	0.233%
8	9.606	1283	1301	1307	rBV	2759626	6946946	4.10%	0.692%
9	10.212	1398	1404	1419	rVB2	1675380	3978975	2.35%	0.396%
10	10.347	1419	1427	1437	rBV	1285964	2998200	1.77%	0.299%
11	10.459	1440	1446	1452	rBV	1077750	1890297	1.12%	0.188%
12	10.577	1457	1466	1469	rVV	2329478	4749849	2.80%	0.473%
13	10.641	1469	1477	1489	rVV2	67727089	143057502	84.41%	14.251%
14	10.753	1489	1496	1510	rVB	6099371	10841597	6.40%	1.080%
15	11.012	1531	1540	1549	rBV6	884180	2651935	1.56%	0.264%
16	11.647	1642	1648	1653	rBV2	1180443	2368571	1.40%	0.236%
17	11.753	1660	1666	1671	rBV	1140453	1735821	1.02%	0.173%
18	11.877	1680	1687	1692	rBV2	1448217	2733079	1.61%	0.272%
19	11.971	1696	1703	1709	rVV2	50379525	89107225	52.58%	8.876%
20	12.024	1709	1712	1715	rVV	4041732	6163874	3.64%	0.614%
21	12.077	1715	1721	1732	rVB3	89860532	169474911	100.00%	16.882%
22	12.406	1765	1777	1786	rBV	40360022	70385704	41.53%	7.011%
23	12.706	1819	1828	1834	rBV3	3918140	8128090	4.80%	0.810%
24	12.859	1848	1854	1858	rBV	1053166	1987832	1.17%	0.198%
25	12.977	1864	1874	1879	rBV	2332942	3965755	2.34%	0.395%
26	13.041	1879	1885	1890	rVV	6110185	10042556	5.93%	1.000%
27	13.106	1890	1896	1904	rVV	18224137	45245015	26.70%	4.507%
28	13.176	1904	1908	1915	rVB2	12001537	21861917	12.90%	2.178%
29	13.347	1929	1937	1944	rBV3	6611100	12753733	7.53%	1.270%
30	13.488	1951	1961	1967	rBV	28473349	46176346	27.25%	4.600%
31	13.535	1967	1969	1974	rVV	2500482	3516636	2.08%	0.350%
32	13.594	1974	1979	1988	rVV5	1032854	2662804	1.57%	0.265%
33	13.682	1989	1994	1999	rVV2	1446693	2990558	1.76%	0.298%
34	13.741	2001	2004	2009	rVV3	988161	1764555	1.04%	0.176%
35	13.824	2009	2018	2022	rVV2	6655198	13975949	8.25%	1.392%
36	13.865	2022	2025	2034	rVB	7921526	11866064	7.00%	1.182%

LSC Area Percent Report

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S-H4(BHF)

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Title : SW846 8260

37	13.959	2034	2041	2042	rBV3	1322362	2157754	1.27%	0.215%
38	14.000	2042	2048	2057	rVV3	8544846	21209856	12.52%	2.113%
39	14.071	2057	2060	2064	rVV2	1738321	2954419	1.74%	0.294%
40	14.112	2064	2067	2072	rVV	1405983	2172642	1.28%	0.216%
41	14.182	2072	2079	2086	rVV2	48358110	82492895	48.68%	8.217%
42	14.253	2086	2091	2093	rVV	1083689	1769214	1.04%	0.176%
43	14.282	2093	2096	2100	rVV	1419212	2374103	1.40%	0.236%
44	14.335	2100	2105	2110	rVV2	2220445	3694480	2.18%	0.368%
45	14.400	2110	2116	2120	rVV2	1150434	2496033	1.47%	0.249%
46	14.453	2120	2125	2134	rVB3	908103	2109310	1.24%	0.210%
47	14.659	2151	2160	2163	rBV	953544	1953864	1.15%	0.195%
48	14.700	2163	2167	2171	rVB	1895503	2726880	1.61%	0.272%
49	14.800	2177	2184	2189	rBV4	1007567	2206486	1.30%	0.220%
50	14.935	2202	2207	2218	rVB5	1287791	2864965	1.69%	0.285%
51	15.047	2218	2226	2232	rBV2	1445787	3976764	2.35%	0.396%
52	15.123	2232	2239	2247	rVB2	5833266	11084203	6.54%	1.104%
53	15.212	2247	2254	2262	rVB	4951663	9232143	5.45%	0.920%
54	15.318	2266	2272	2279	rVV2	955838	1802377	1.06%	0.180%
55	15.647	2317	2328	2340	rVB2	40509099	82317755	48.57%	8.200%

Sum of corrected areas: 1003869570

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Instrument :
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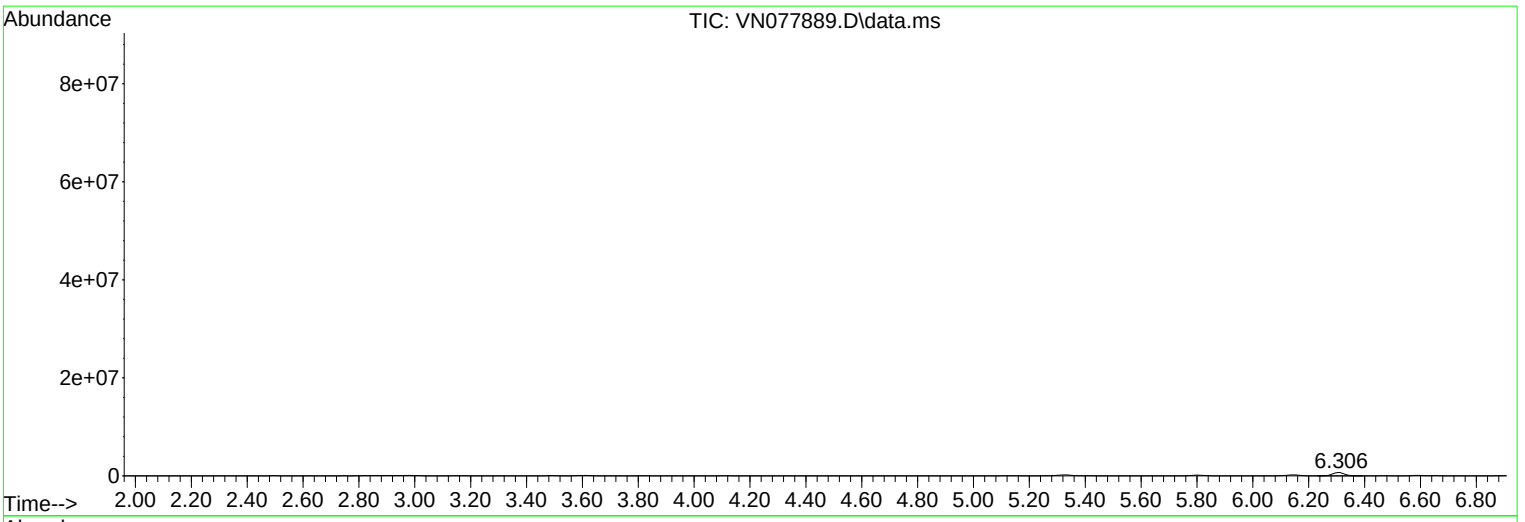
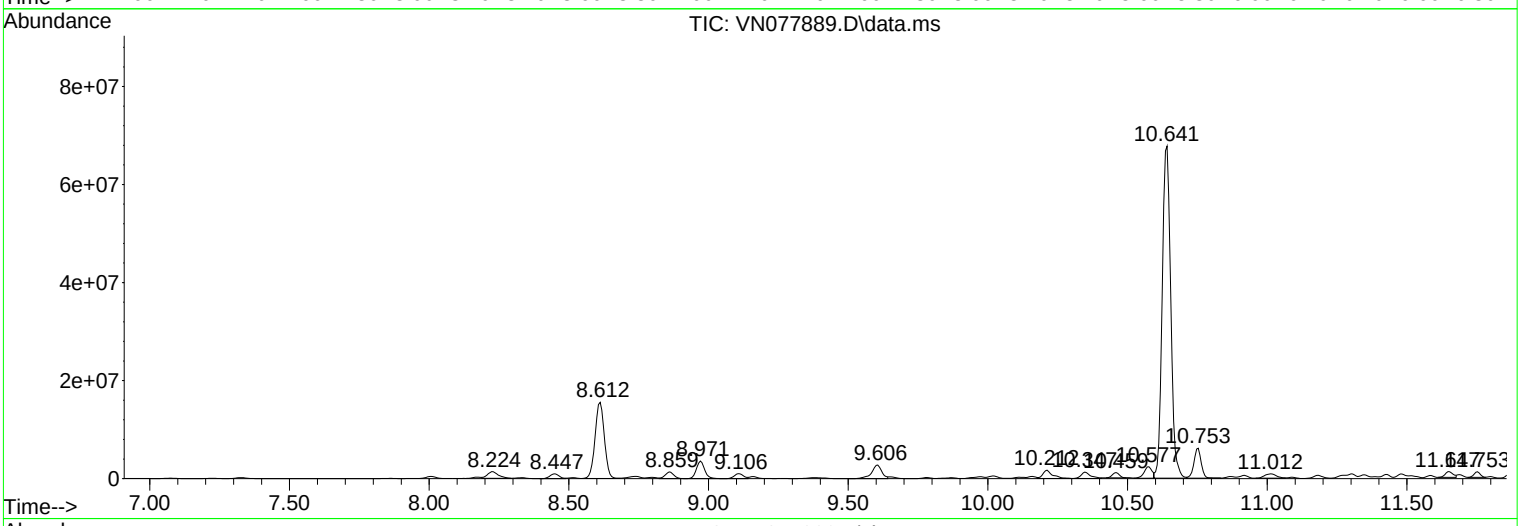
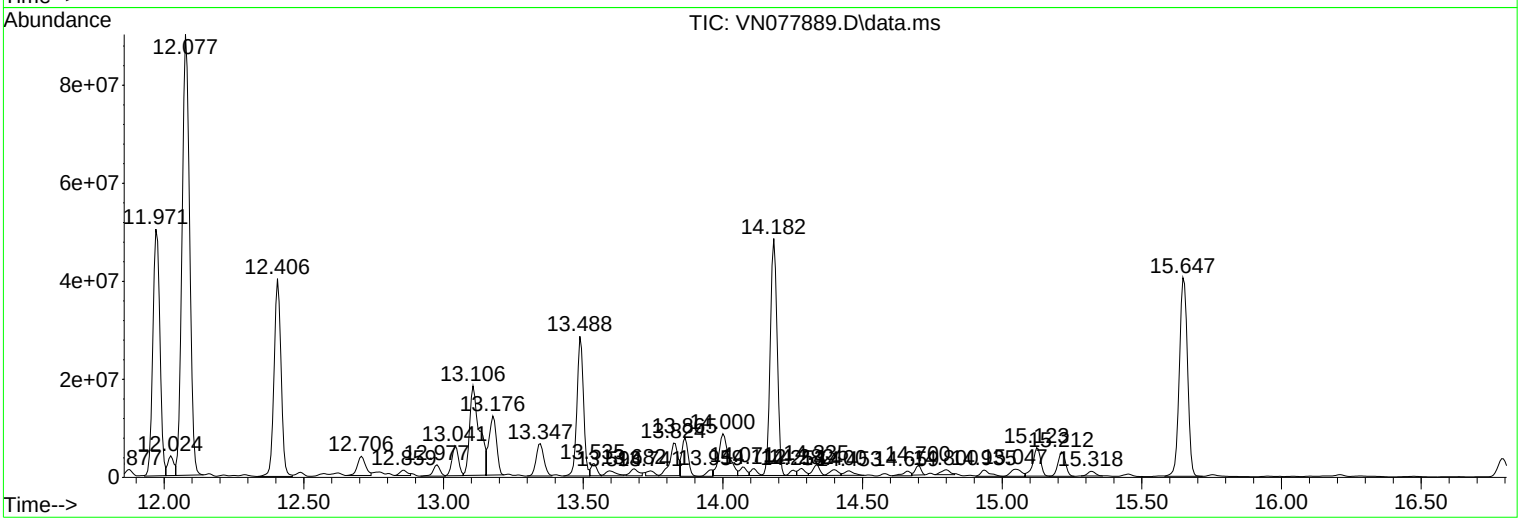
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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







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ClientSampleId :
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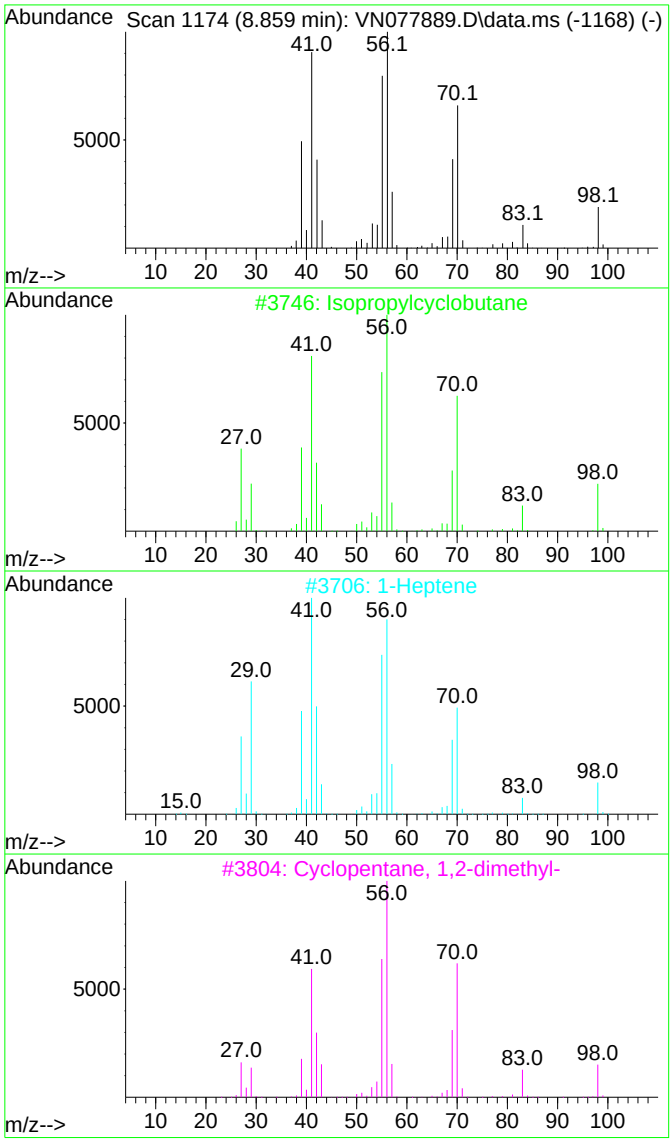
Quant Title : SW846 8260

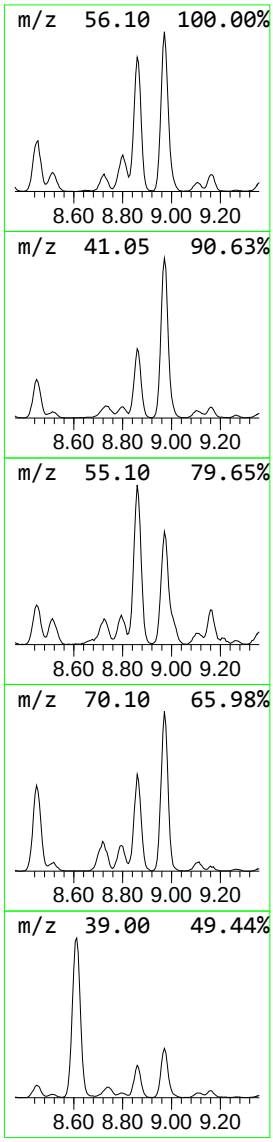
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isopropylcyclobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.859	60.57 ug/l	2828060	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	95
2	1-Heptene	98	C7H14	000592-76-7	95
3	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	72
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	68
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	58





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ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

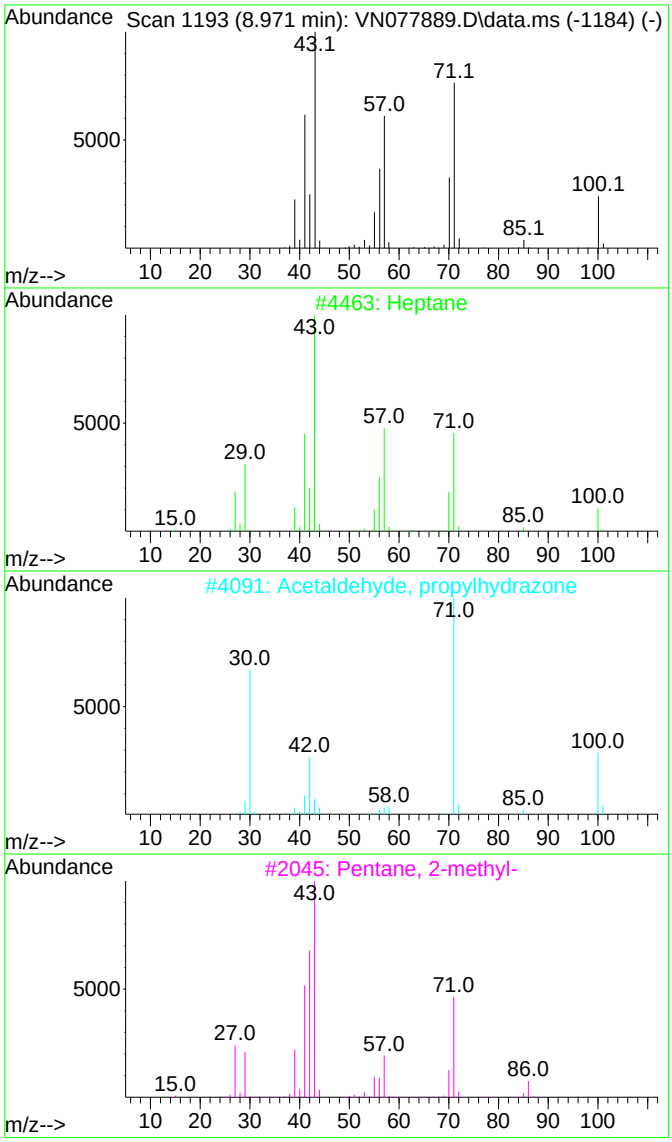
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

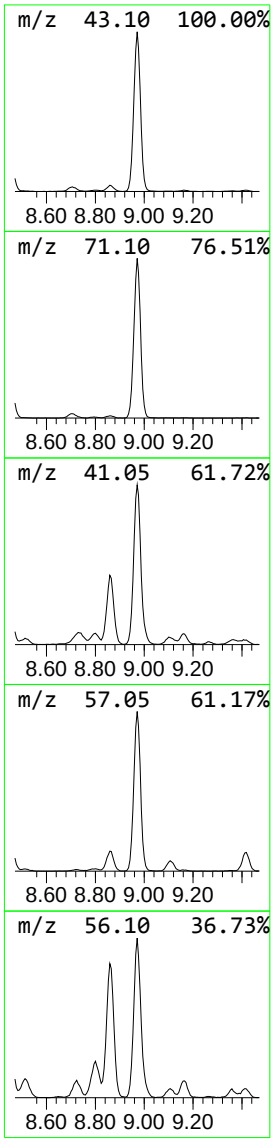
****

Peak Number 2 Heptane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	156.08 ug/l	7288080	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	53
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
4	3-Hexanone	100	C6H12O	000589-38-8	43
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	43





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Misc : 4.99g/10mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

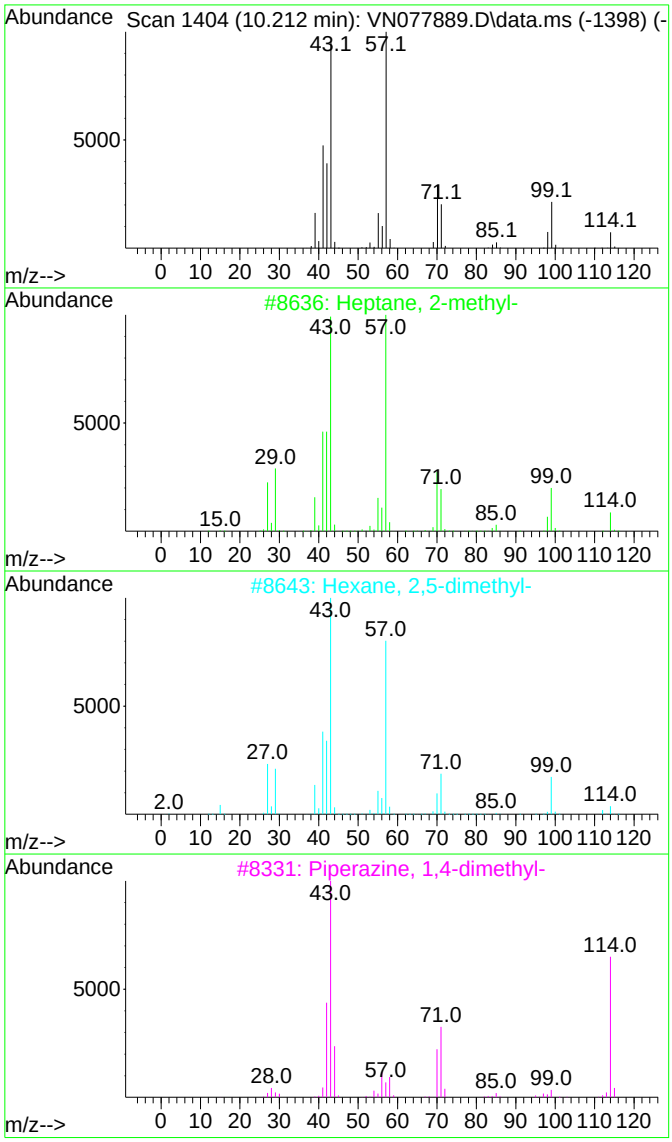
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

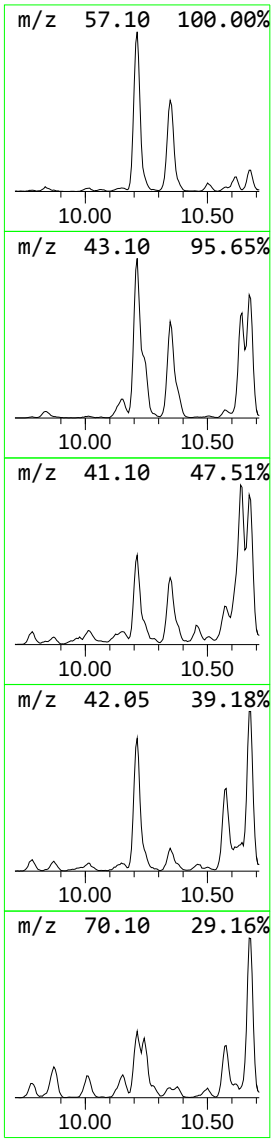
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.212	85.21 ug/l	3978980	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	97
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	90
3	Piperazine, 1,4-dimethyl-	114	C6H14N2	000106-58-1	50
4	Nonane, 4-methyl-	142	C10H22	017301-94-9	43
5	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	38





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ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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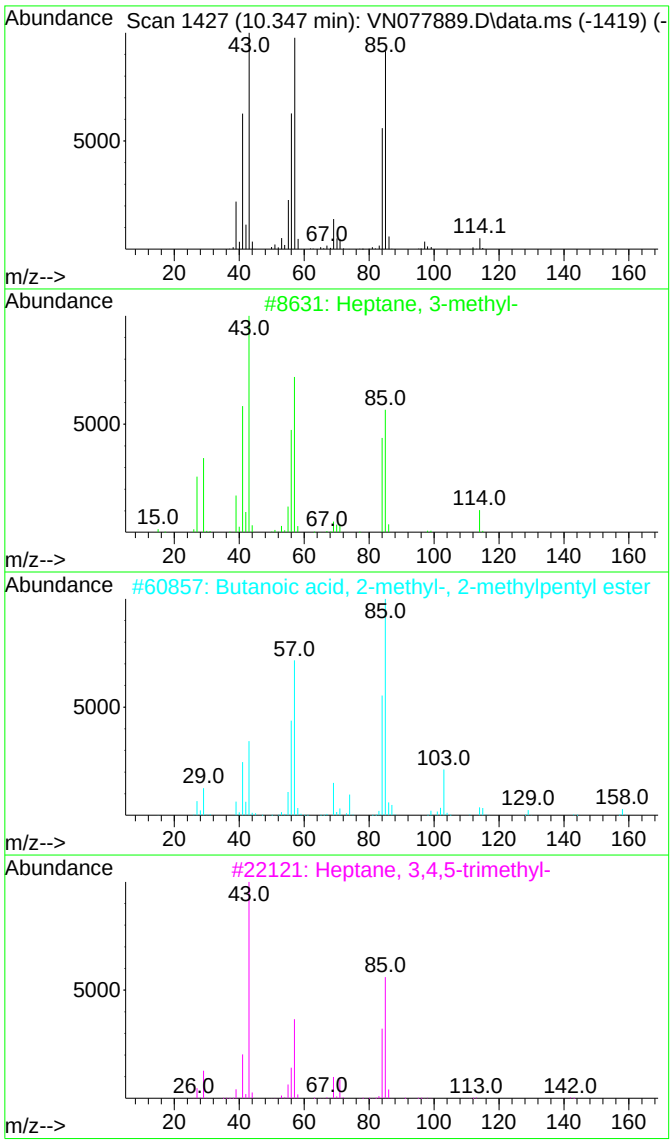
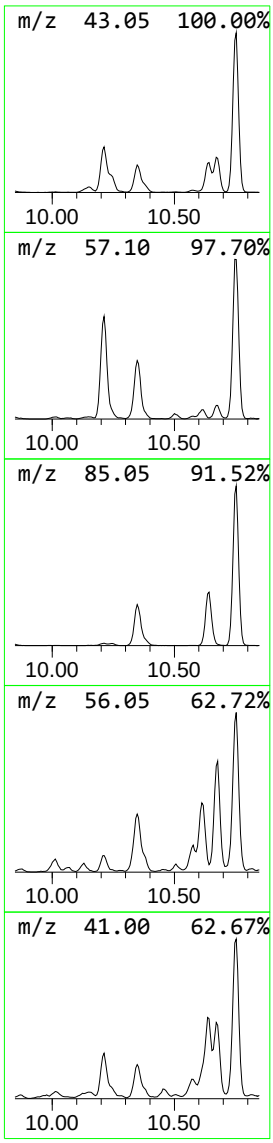
****
Peak Number 4 Heptane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.347	64.21 ug/l	2998200	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Butanoic acid, 2-methyl-, 2-meth...	186	C11H22O2	083783-88-4	64
3	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	64
4	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	64
5	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	64





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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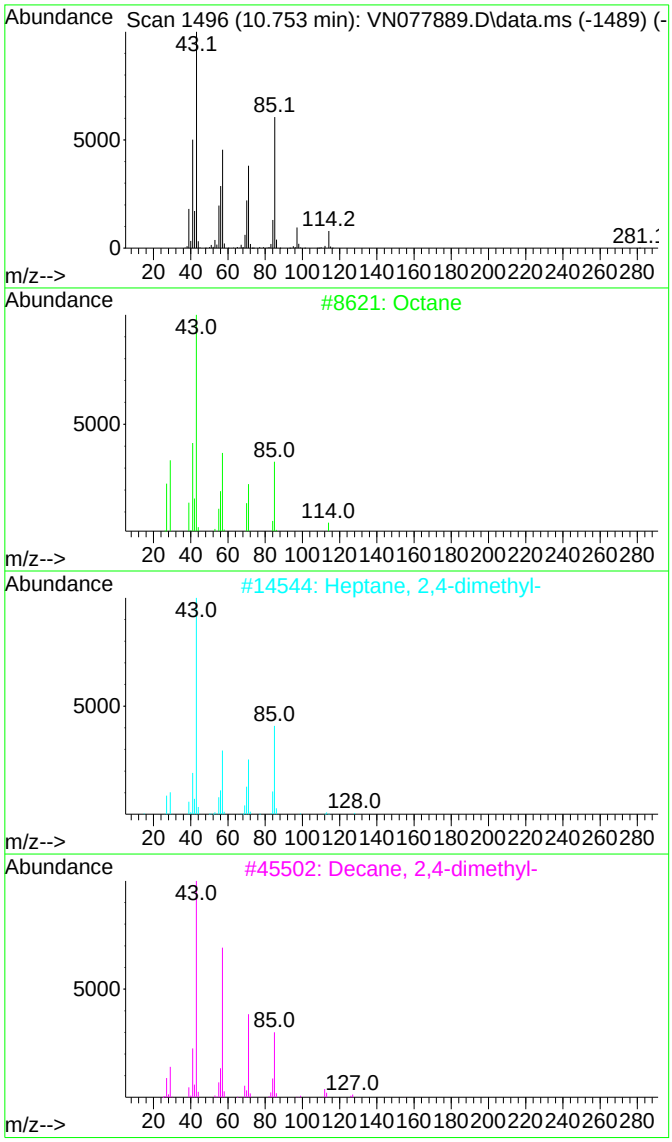
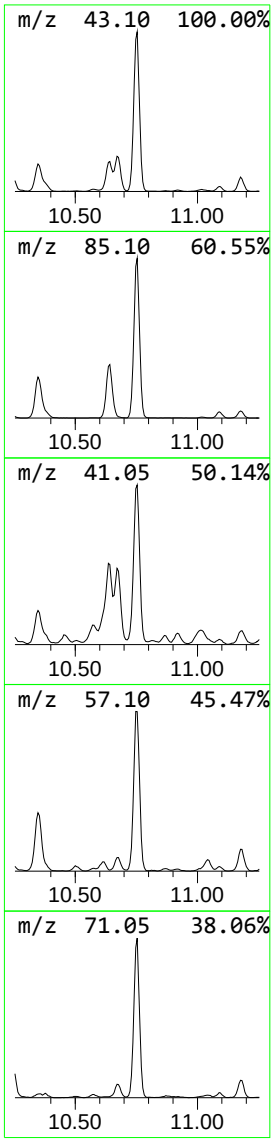
****

Peak Number 5 Octane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.753	198.34 ug/l	10841600	Chlorobenzene-d5	11.877

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	91
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
5	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	50





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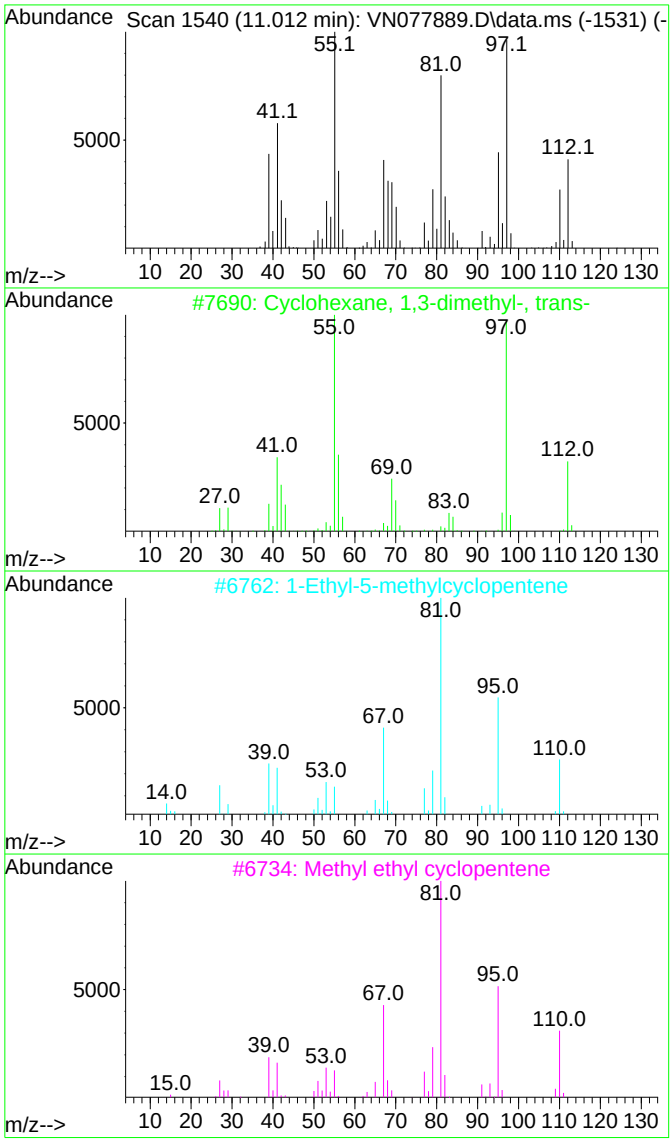
Quant Title : SW846 8260

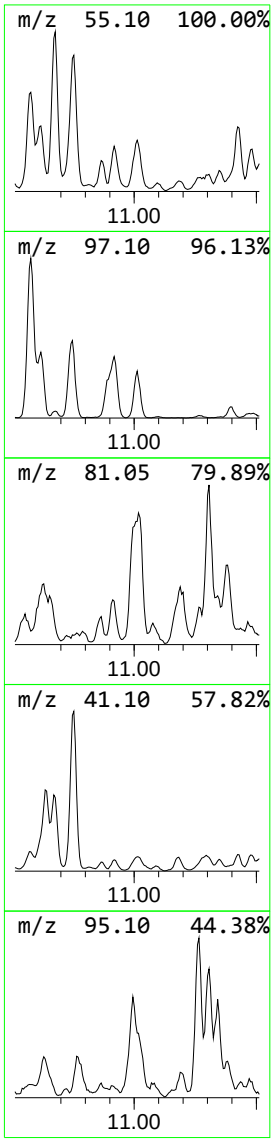
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.012	48.52 ug/l	2651940	Chlorobenzene-d5	11.877

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	74
2	1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	55
3	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	46
4	cis-1-Methyl-2-(2'-propenyl)cycl...	96	C7H12	076588-97-1	46
5	Cyclohexane, ethenyl-	110	C8H14	000695-12-5	43





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Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

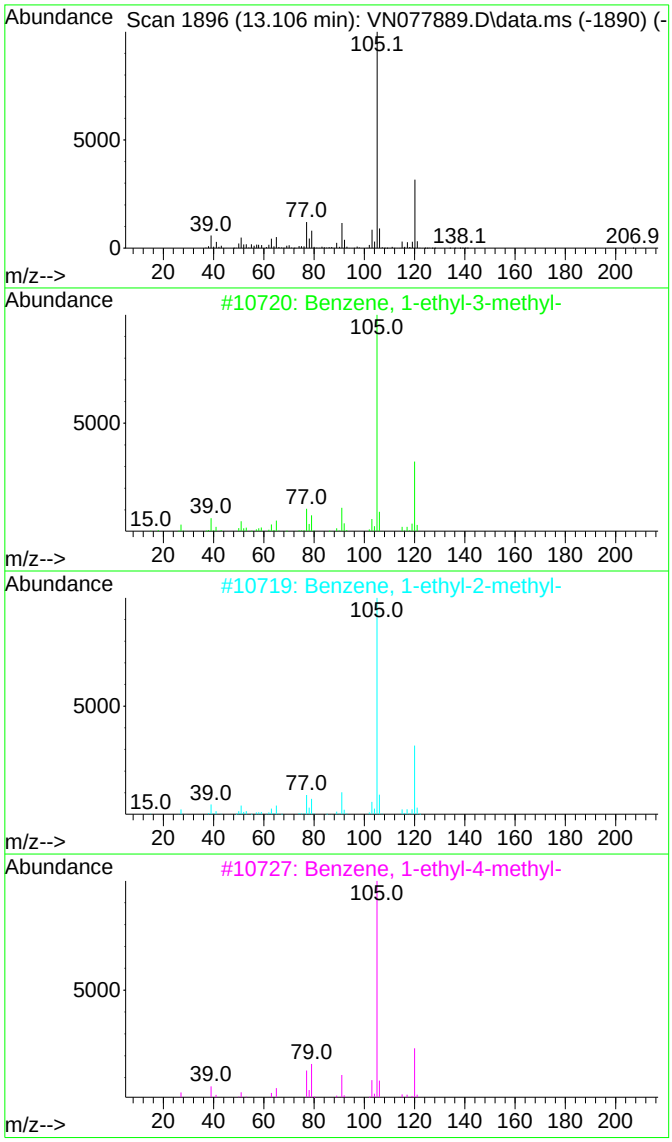
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

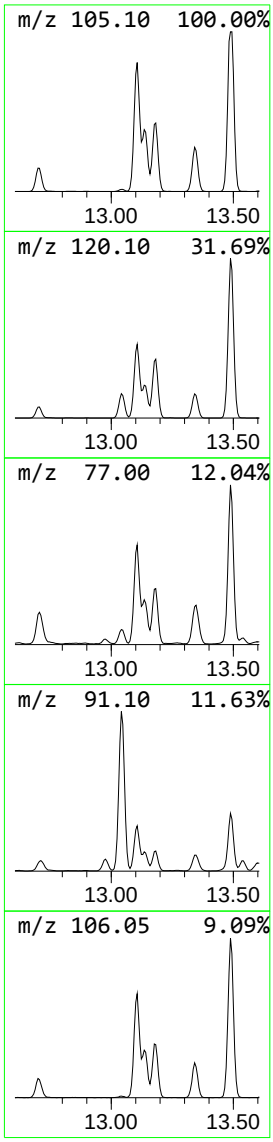
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	161.87 ug/l	45245000	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052423\
Data File : VN077889.D
Acq On : 25 May 2023 08:11
Operator : JC\MD
Sample : 02888-01
Misc : 4.99g/10mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

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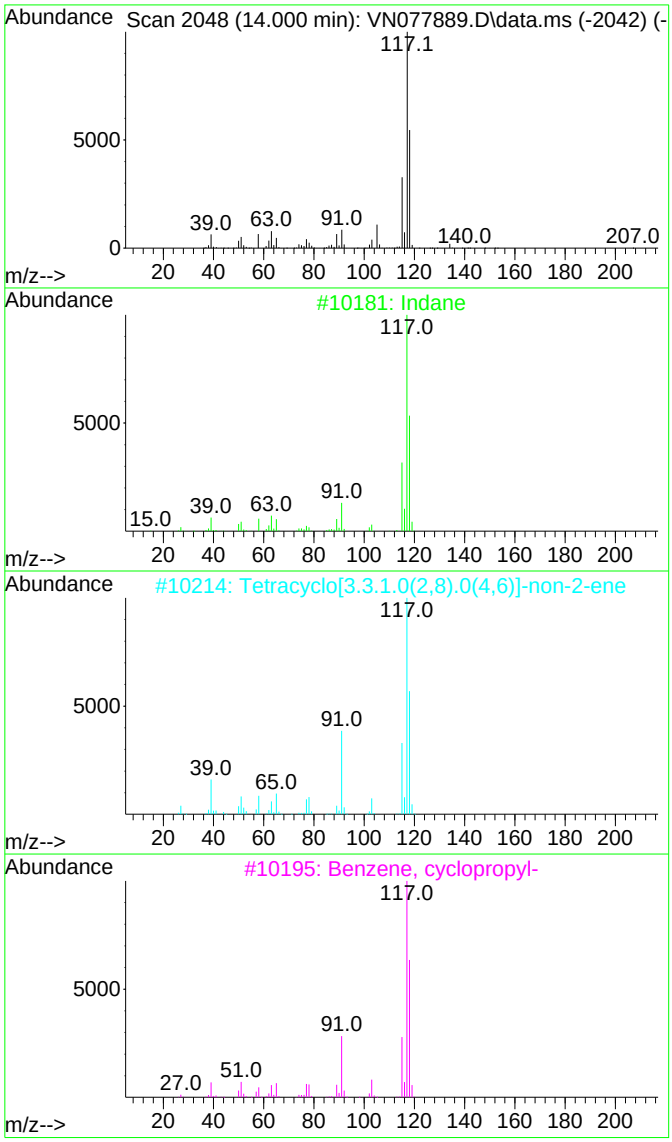
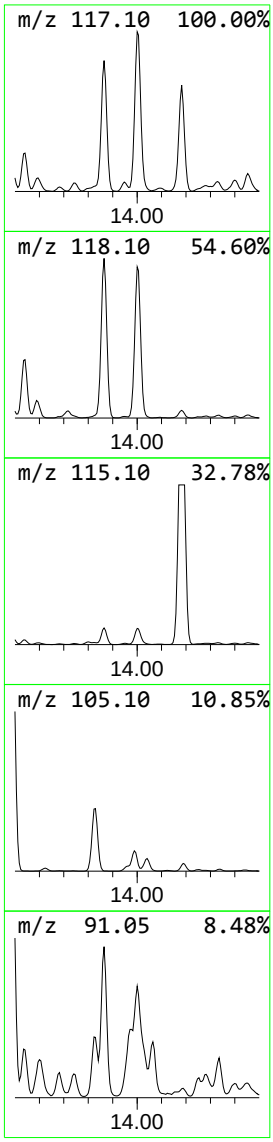
Peak Number 8 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	75.88 ug/l	21209900	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	68
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	47
5	Deltacyclene	118	C9H10	007785-10-6	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052423\
Data File : VN077889.D
Acq On : 25 May 2023 08:11
Operator : JC\MD
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ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

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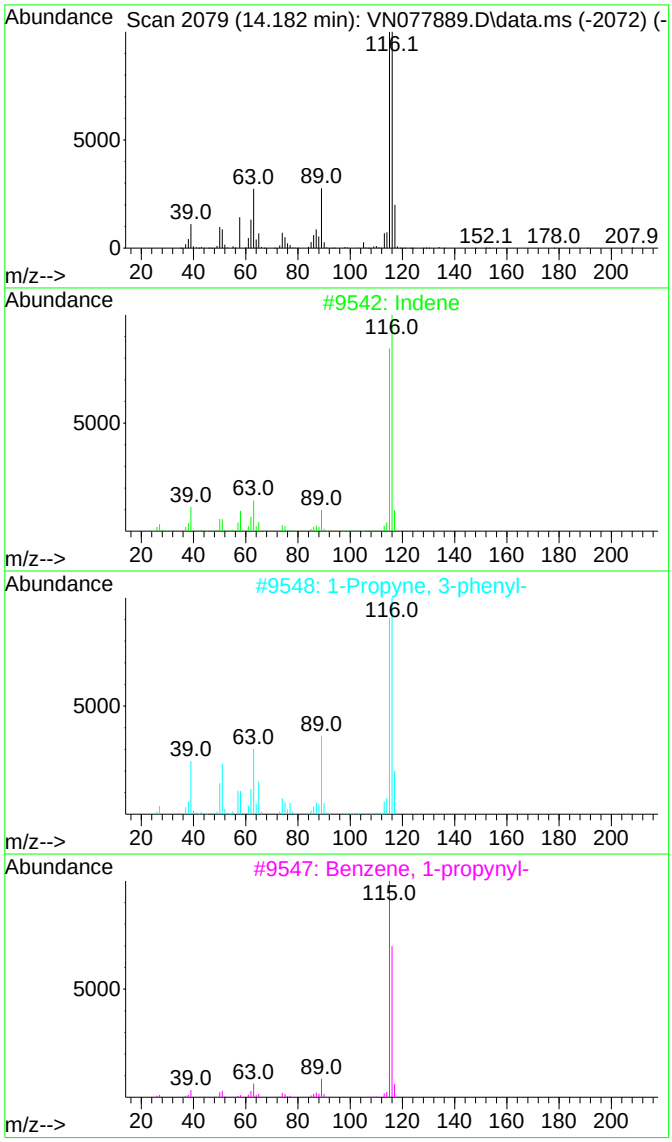
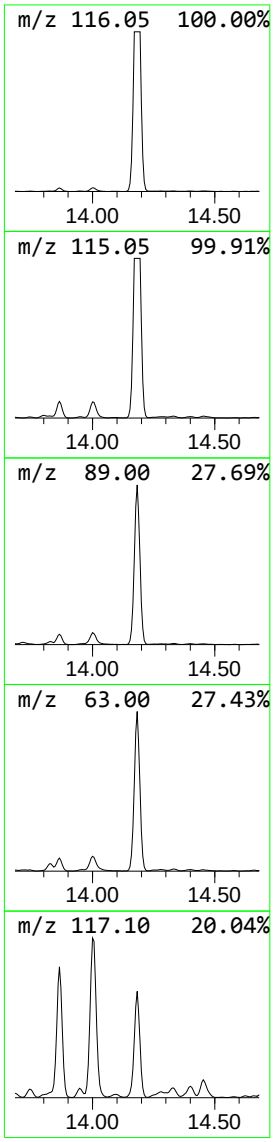
Peak Number 9 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	295.12 ug/l	82492900	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	94
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	86
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	56
5	3-Methylphenylacetylene	116	C9H8	000766-82-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052423\
Data File : VN077889.D
Acq On : 25 May 2023 08:11
Operator : JC\MD
Sample : 02888-01
Misc : 4.99g/10mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

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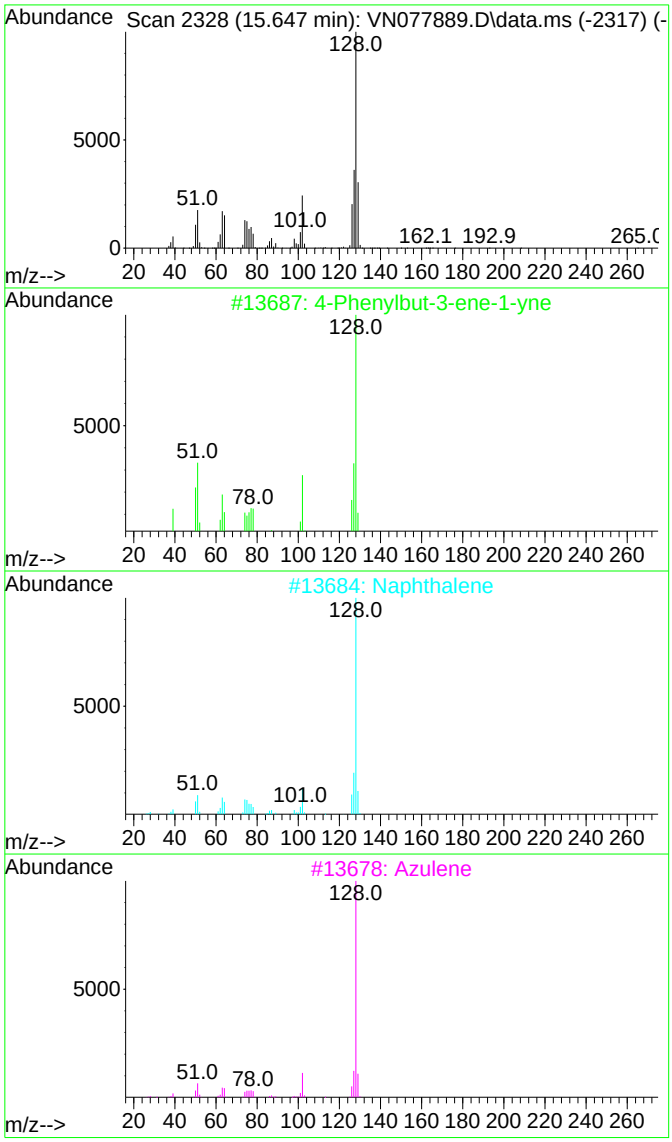
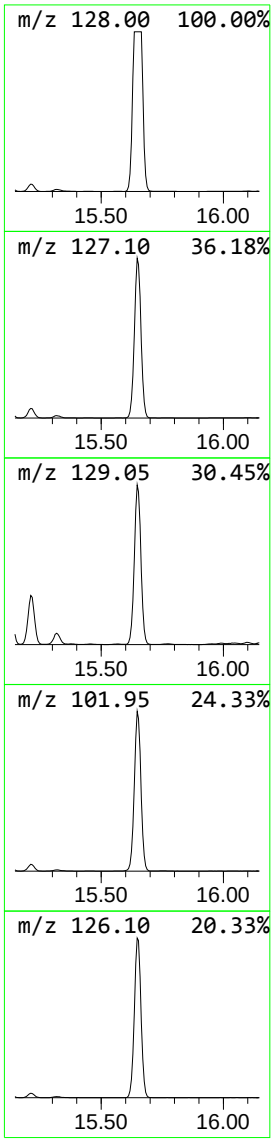
Peak Number 10 4-Phenylbut-3-ene-1-yne Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	294.50 ug/l	82317800	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	89
2	Naphthalene	128	C10H8	000091-20-3	81
3	Azulene	128	C10H8	000275-51-4	76
4	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	64
5	[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052423\
Data File : VN077889.D
Acq On : 25 May 2023 08:11
Operator : JC\MD
Sample : 02888-01
Misc : 4.99g/10mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
S-H4(BHF)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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
Isopropylcyclob...	8.859	60.6	ug/l	2828060	2	9.106	2334720	50.0
Heptane	8.971	156.1	ug/l	7288080	2	9.106	2334720	50.0
Heptane, 2-methyl-	10.212	85.2	ug/l	3978980	2	9.106	2334720	50.0
Heptane, 3-methyl-	10.347	64.2	ug/l	2998200	2	9.106	2334720	50.0
Octane	10.753	198.3	ug/l	10841600	3	11.877	2733080	50.0
Cyclohexane, 1,...	11.012	48.5	ug/l	2651940	3	11.877	2733080	50.0
Benzene, 1-ethy...	13.106	161.9	ug/l	45245000	4	13.800	13975900	50.0
Indane	14.000	75.9	ug/l	21209900	4	13.800	13975900	50.0
Indene	14.182	295.1	ug/l	82492900	4	13.800	13975900	50.0
4-Phenylbut-3-e...	15.647	294.5	ug/l	82317800	4	13.800	13975900	50.0