LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

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\82X100124W.M
Title : SW846 8260

Signal : TIC: VX043374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	69	80	82	rBV7	4865	13254	2.83%	0.288%
2	2.941	296	304	323	rVB	6300	16482	3.52%	0.358%
3	4.611	568	578	594	rBB3	1168	4968	1.06%	0.108%
4	5.379	694	704	720	rBV3	54574	161318	34.47%	3.500%
5	5.544	721	731	746	rVV	88328	251220	53.68%	5.450%
6	5.952	789	798	816	rBV	62750	171644	36.67%	3.724%
7	6.757	920	930	952	rBV	145990	353748	75.58%	7.674%
8	8.647	1233	1240	1254	rBV	290796	468017	100.00%	10.153%
9	10.049	1465	1470	1487	rBV	278248	406861	86.93%	8.827%
10	11.079	1634	1639	1654	rBV	231326	309867	66.21%	6.722%
11	11.756	1746	1750	1759	rVB6	3762	7774	1.66%	0.169%
12	12.018	1788	1793	1804	rBV	281908	380491	81.30%	8.255%
13	12.311	1837	1841	1849	rVV6	8122	16599	3.55%	0.360%
14	12.555	1875	1881	1884	rBV4	3897	7818	1.67%	0.170%
15	12.658	1895	1898	1903	rBV5	2355	4742	1.01%	0.103%
16	12.725	1905	1909	1912	rVV5	4032	7051	1.51%	0.153%
17	12.756	1912	1914	1919	rVV4	3706	5140	1.10%	0.112%
18	12.817	1919	1924	1931	rVB3	20252	30130	6.44%	0.654%
19	12.890	1932	1936	1938	rBV3	3697	6127	1.31%	0.133%
20	12.920	1938	1941	1945	rVV	8713	13074	2.79%	0.284%
21	12.981	1947	1951	1956	rVV5	14506	22364	4.78%	0.485%
22	13.042	1956	1961	1964	rVB6	7431	11126	2.38%	0.241%
23	13.292	1996	2002	2007	rVB4	25626	42038	8.98%	0.912%
24	13.341	2007	2010	2013	rBV3	3889	5275	1.13%	0.114%
25	13.414	2015	2022	2025	rBV5	28761	59755	12.77%	1.296%
26	13.506	2033	2037	2042	rVB4	8684	15031	3.21%	0.326%
27	13.591	2047	2051	2054	rBV5	11027	17842	3.81%	0.387%
28	13.676	2061	2065	2067	rBV5	12579	17693	3.78%	0.384%
29	13.737	2072	2075	2077	rVV2	9916	12983	2.77%	0.282%
30	13.768	2077	2080	2082	rVV2	12533	16015	3.42%	0.347%
31	13.798	2082	2085	2089	rVV3	23337	32405	6.92%	0.703%
32	13.847	2089	2093	2100	rVV5	23870	47568	10.16%	1.032%
33	13.914	2100	2104	2109	rVV6	10740	22071	4.72%	0.479%
34	14.067	2125	2129	2132	rBV3	18396	24407	5.21%	0.530%
35	14.170	2143	2146	2150	rBV5	11169	14894	3.18%	0.323%
36	14.225	2150	2155	2160	rBV6	29045	57981	12.39%	1.258%

LSC Area Percent Report

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Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Title : SW846 8260

37	14.481	2193	2197	2206	rBV7	27291	70791	15.13%	1.536%
38	14.554	2206	2209	2210	rBV3	11770	13715	2.93%	0.298%
39	14.615	2215	2219	2225	rBV	112618	159410	34.06%	3.458%
40	14.670	2225	2228	2232	rBV2	57247	72964	15.59%	1.583%
41	14.755	2239	2242	2245	rBV4	35164	40502	8.65%	0.879%
42	14.792	2245	2248	2250	rVV4	23942	27273	5.83%	0.592%
43	14.823	2250	2253	2254	rVV	25878	29359	6.27%	0.637%
44	14.847	2254	2257	2261	rVB2	64973	79634	17.02%	1.728%
45	15.182	2308	2312	2314	rBV4	66300	91313	19.51%	1.981%
46	15.213	2314	2317	2320	rVB2	57148	65866	14.07%	1.429%
47	15.249	2320	2323	2326	rBV	28146	33393	7.13%	0.724%
48	15.414	2347	2350	2355	rVB	76865	105309	22.50%	2.285%
49	15.493	2358	2363	2364	rBV3	45511	74332	15.88%	1.613%
50	15.743	2401	2404	2412	rVB5	89464	136382	29.14%	2.959%
51	15.859	2418	2423	2429	rBV6	41002	99984	21.36%	2.169%
52	16.097	2457	2462	2467	rBV3	98489	194024	41.46%	4.209%
53	16.280	2487	2492	2503	rVB4	77695	259407	55.43%	5.628%

Sum of corrected areas: 4609431

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
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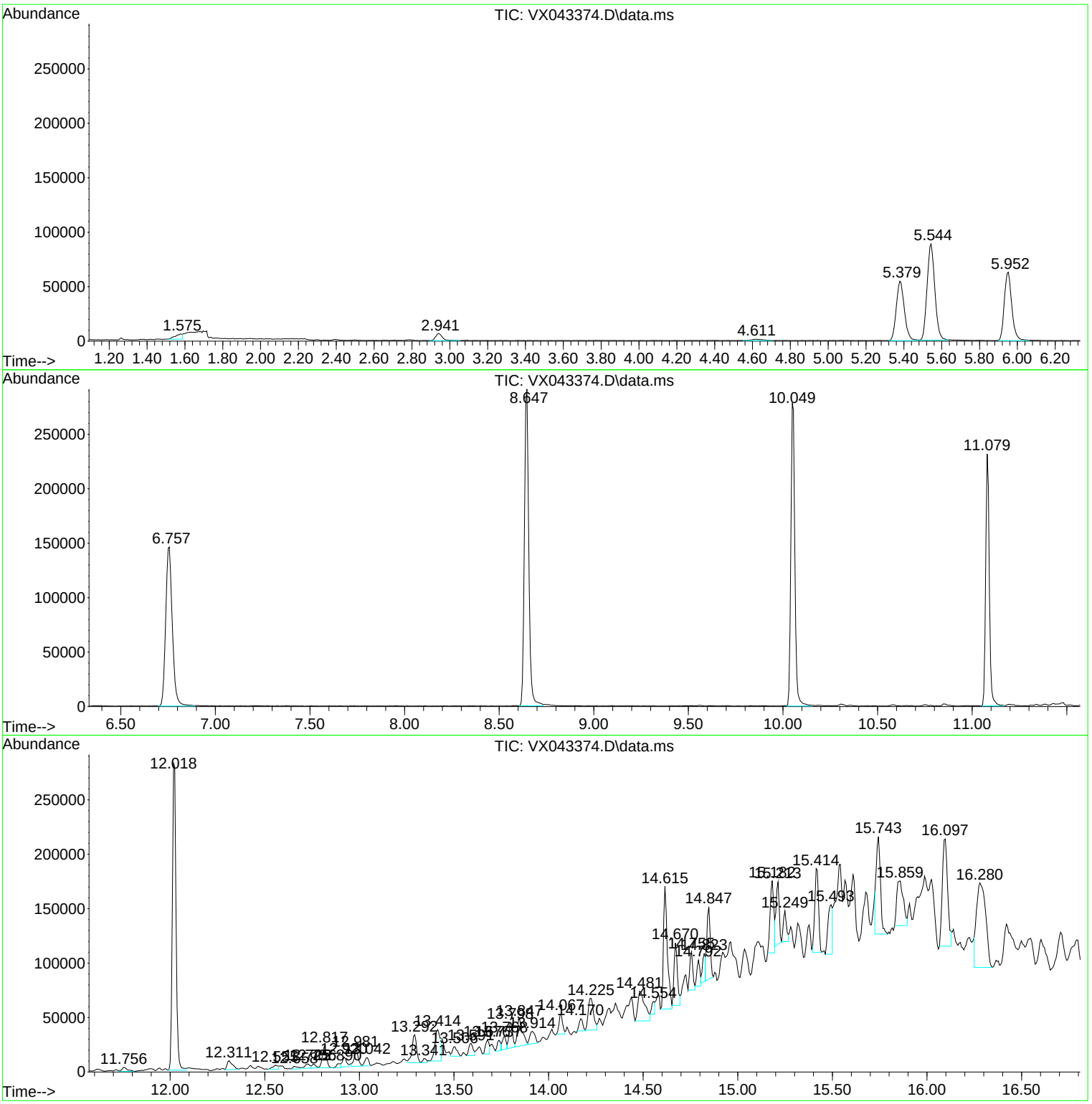
Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

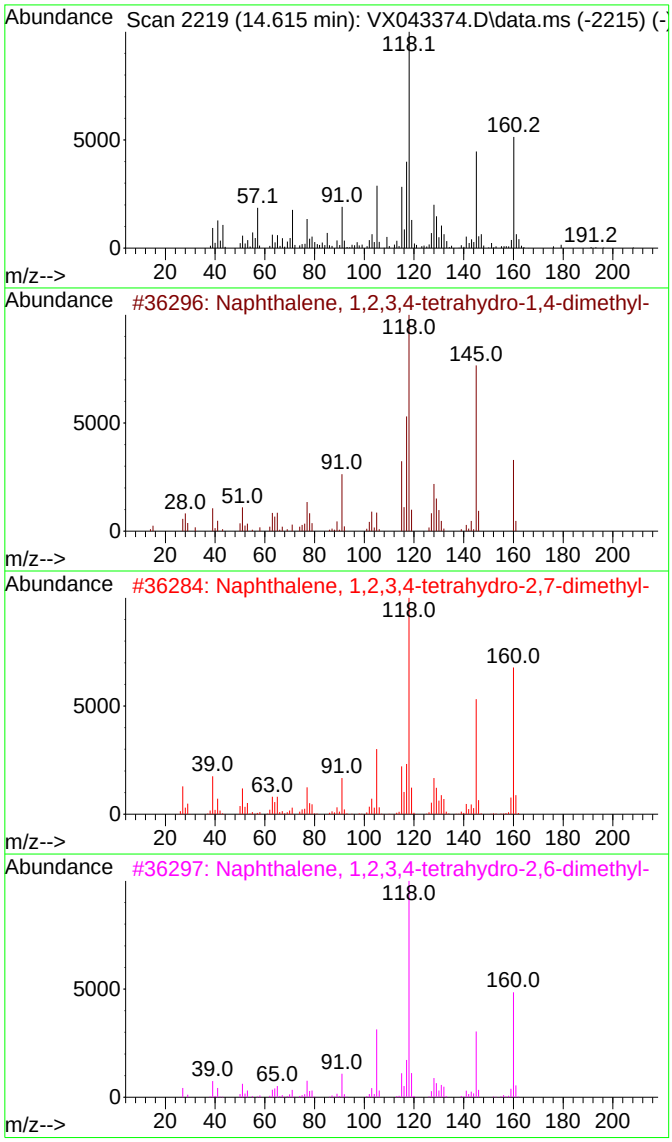
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

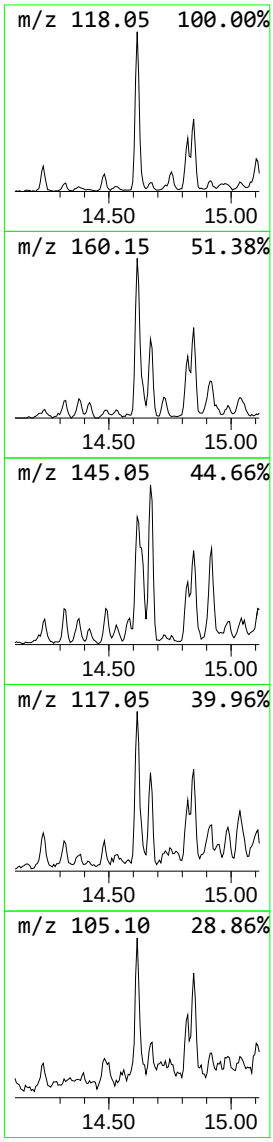
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	20.95 ug/l	159410	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	81
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	64
5	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

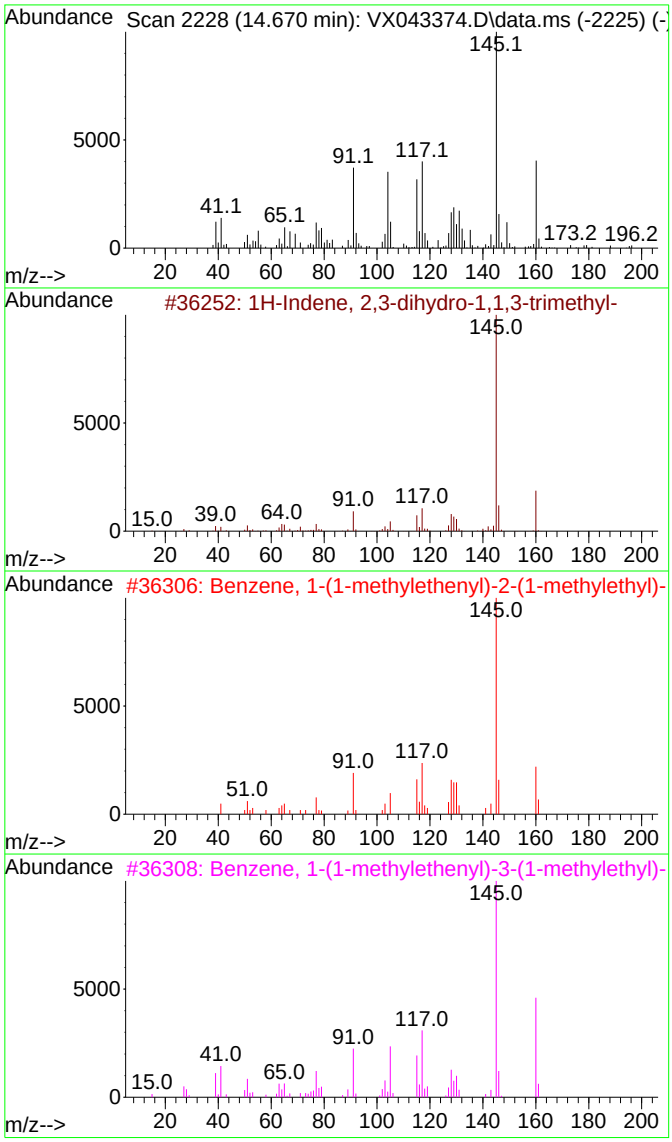
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

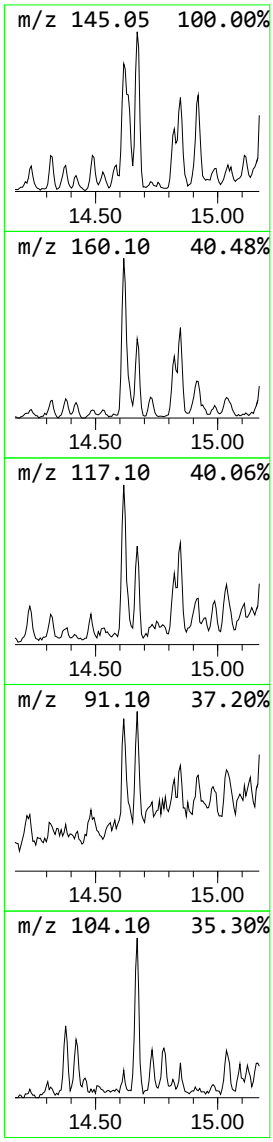
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	9.59 ug/l	72964	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	81
2	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	76
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	74
4	Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	72
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

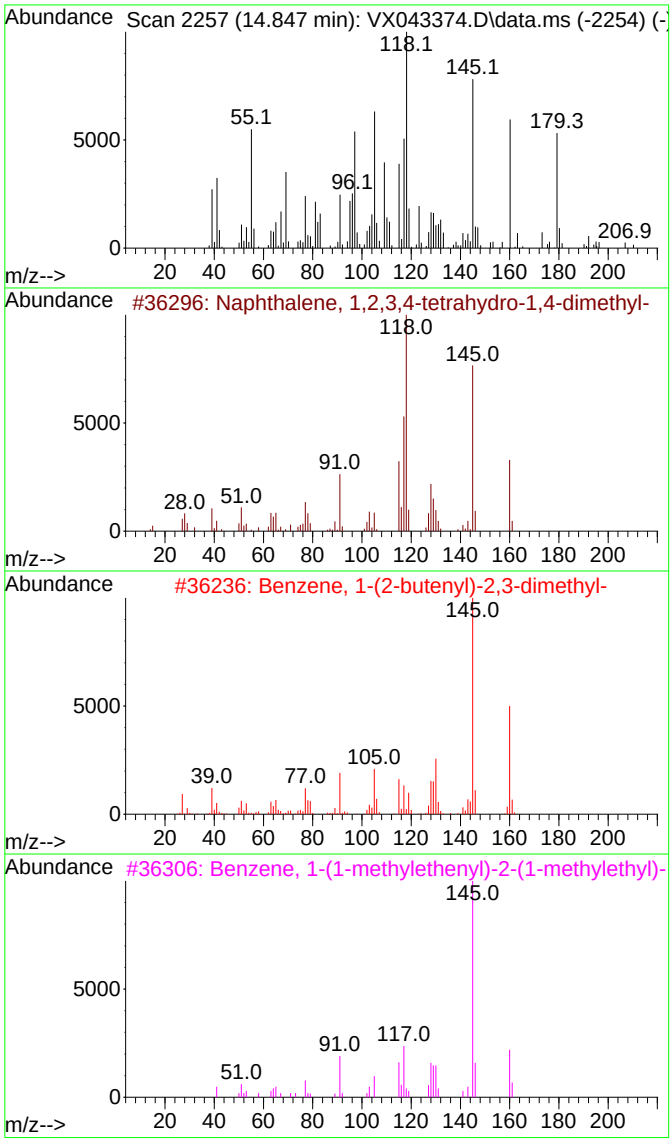
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

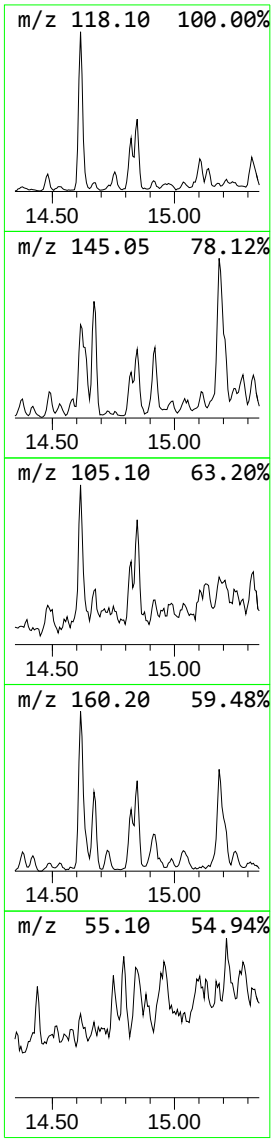
****

Peak Number 3 unknown14.847 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	10.46 ug/l	79634	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	78
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	47
3	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	46
4	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	46
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
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Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

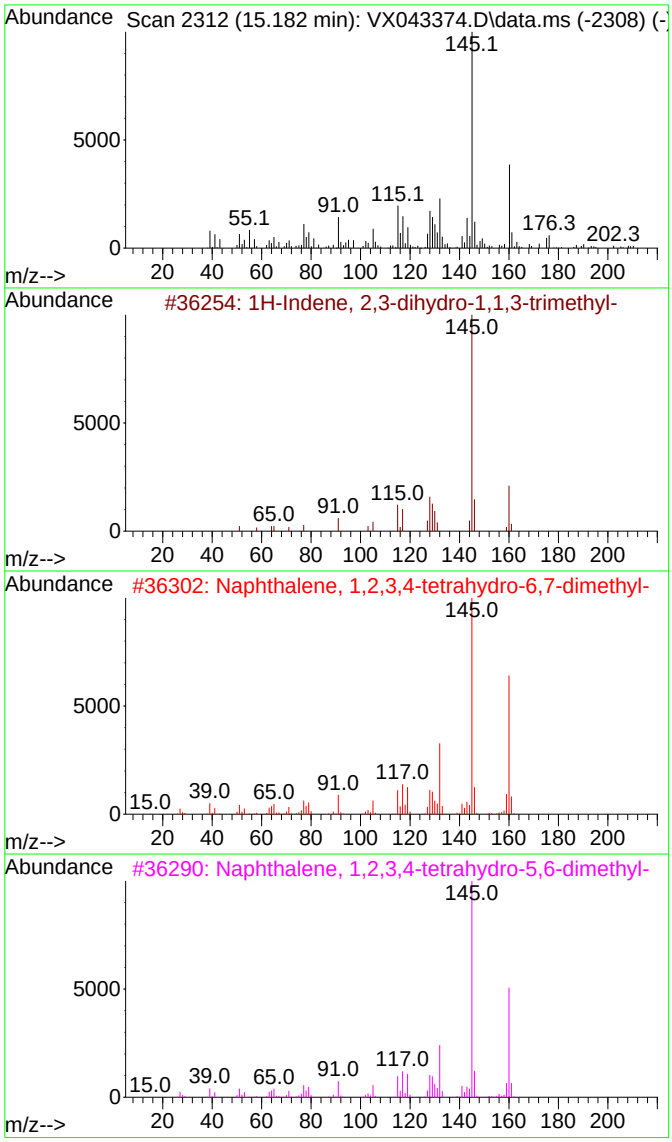
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

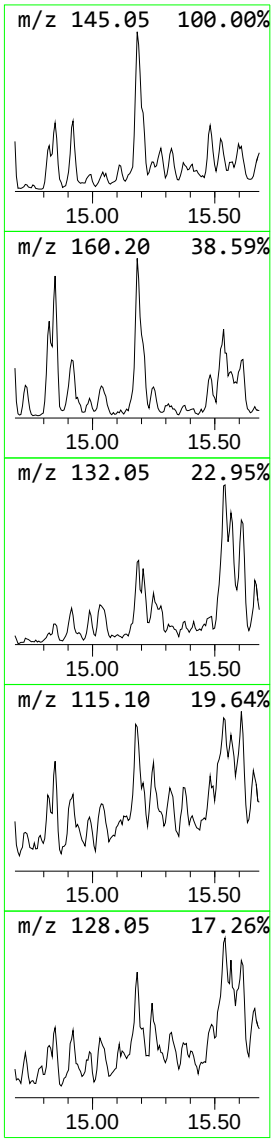
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	12.00 ug/l	91313	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	93
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	93
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91
5	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	90





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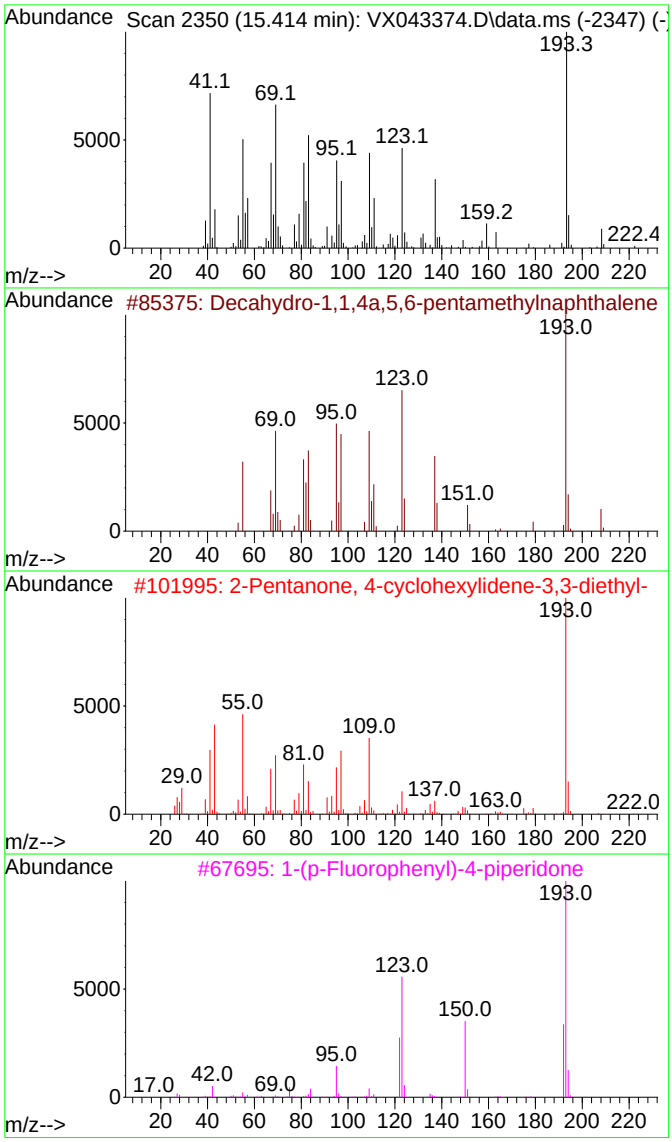
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

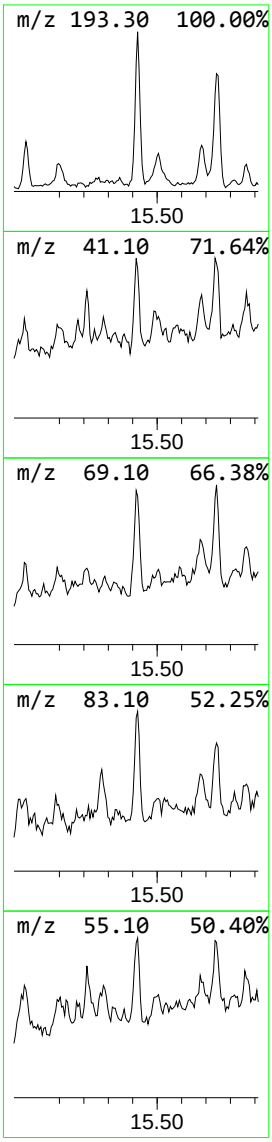
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	13.84 ug/l	105309	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	93
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	18
5	N-(4-Fluorophenyl)piperidin-4-amine	194	C11H15FN2	038043-08-2	15





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Quant Title : SW846 8260

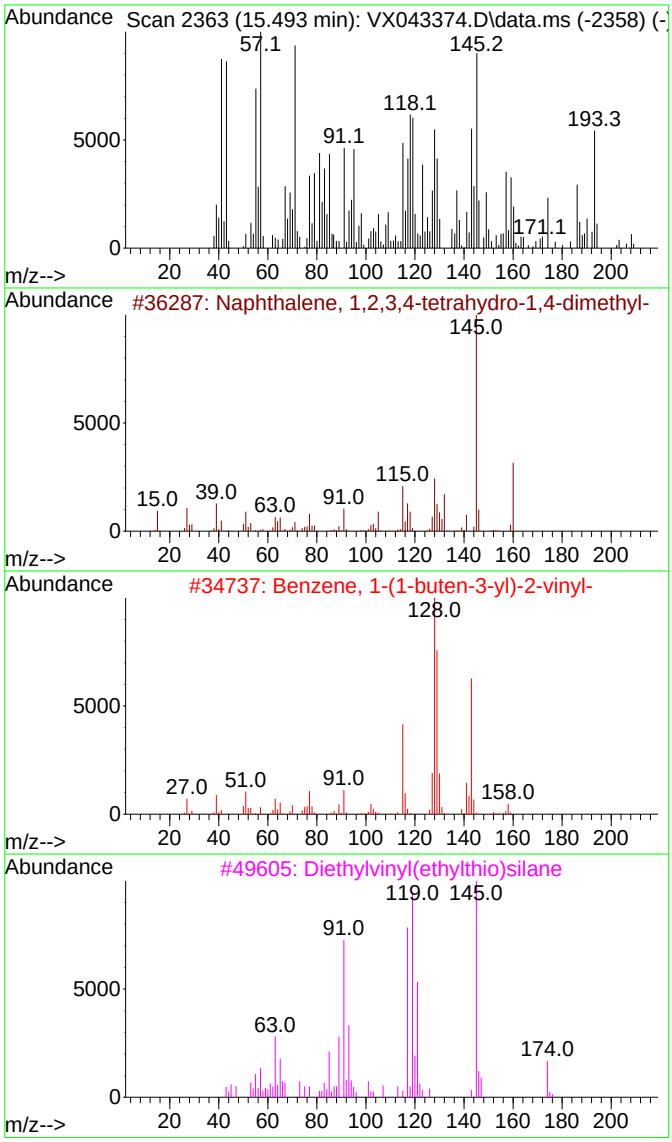
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

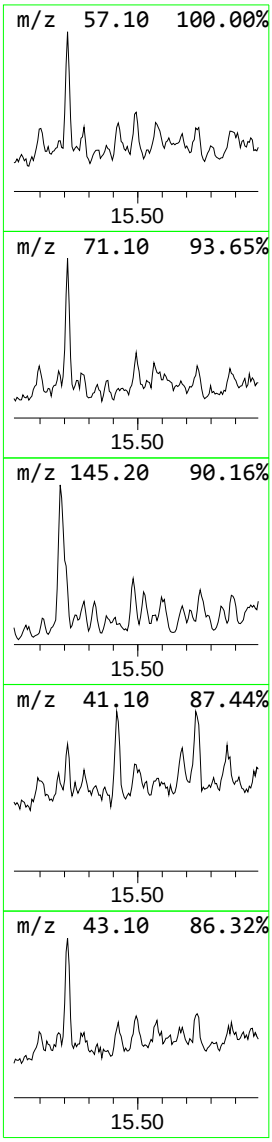
****

Peak Number 6 unknown15.493 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	9.77 ug/l	74332	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	38
2	Benzene, 1-(1-buten-3-yl)-2-vinyl-	158	C12H14	1000162-74-4	25
3	Diethylvinyl(ethylthio)silane	174	C8H18SSi	078859-24-2	25
4	Isoquinoline, 2-oxide	145	C9H7NO	001532-72-5	22
5	Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	18





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

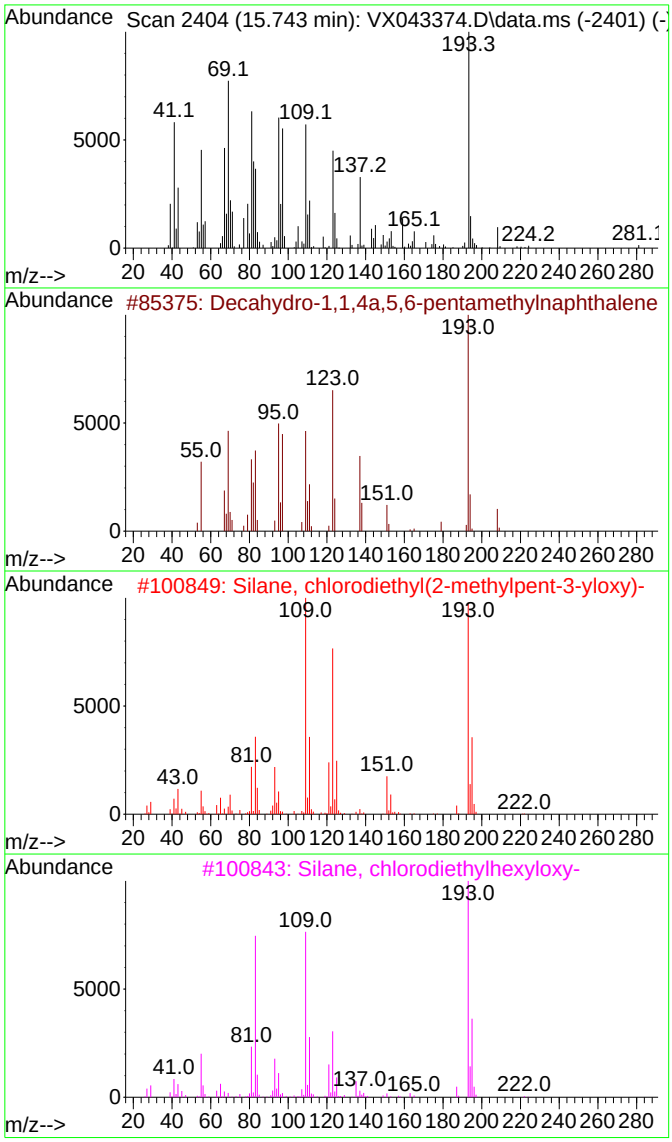
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

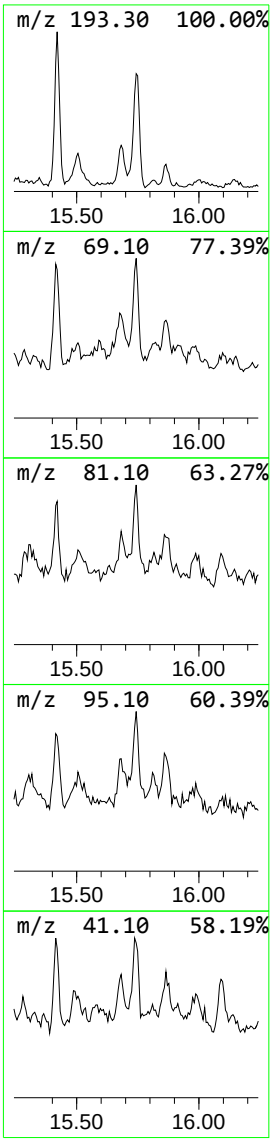
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown15.743 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	17.92 ug/l	136382	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	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	43
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35
4	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	22
5	7-Ethyl-2-undecen-6-one	196	C13H24O	1000374-14-9	18





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

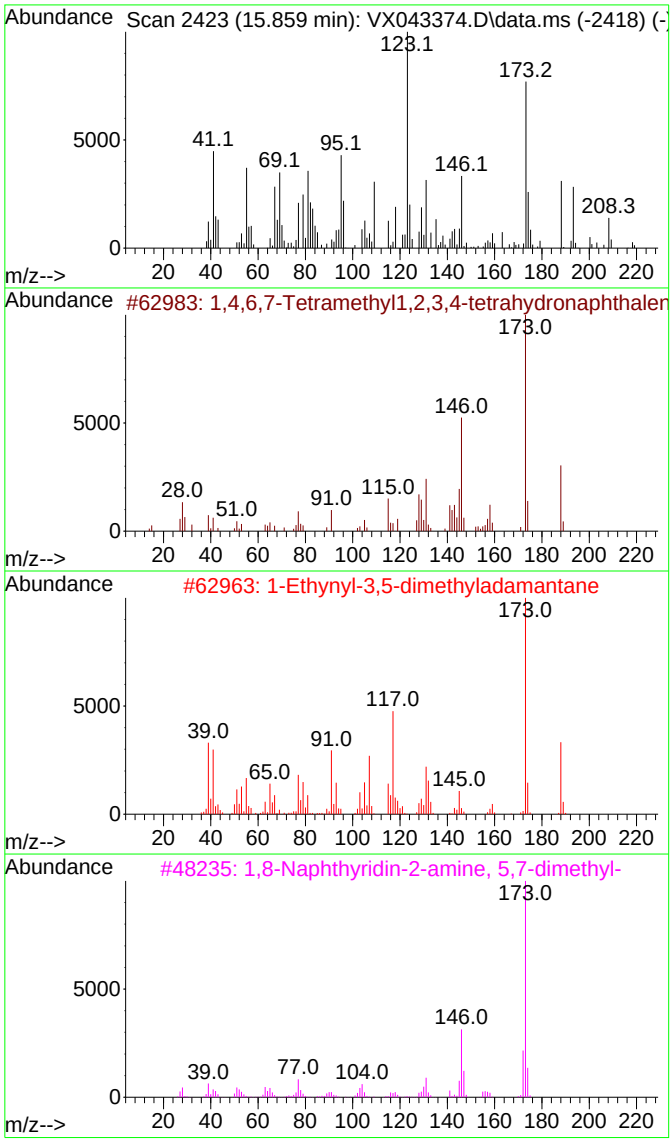
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

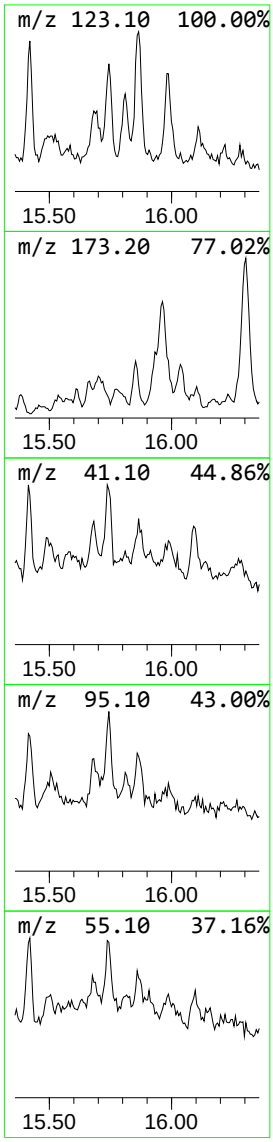
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown15.859 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.859	13.14 ug/l	99984	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,6,7-Tetramethyl1,2,3,4-tetra...	188	C14H20	1000113-61-3	30
2	1-Ethynyl-3,5-dimethyladamantane	188	C14H20	1000245-73-3	25
3	1,8-Naphthyridin-2-amine, 5,7-di...	173	C10H11N3	039565-07-6	25
4	1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	054789-22-9	22
5	Benzamide, 4-fluoro-N-(6-bromoqu...	344	C16H10BrFN2O	327991-32-2	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
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Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

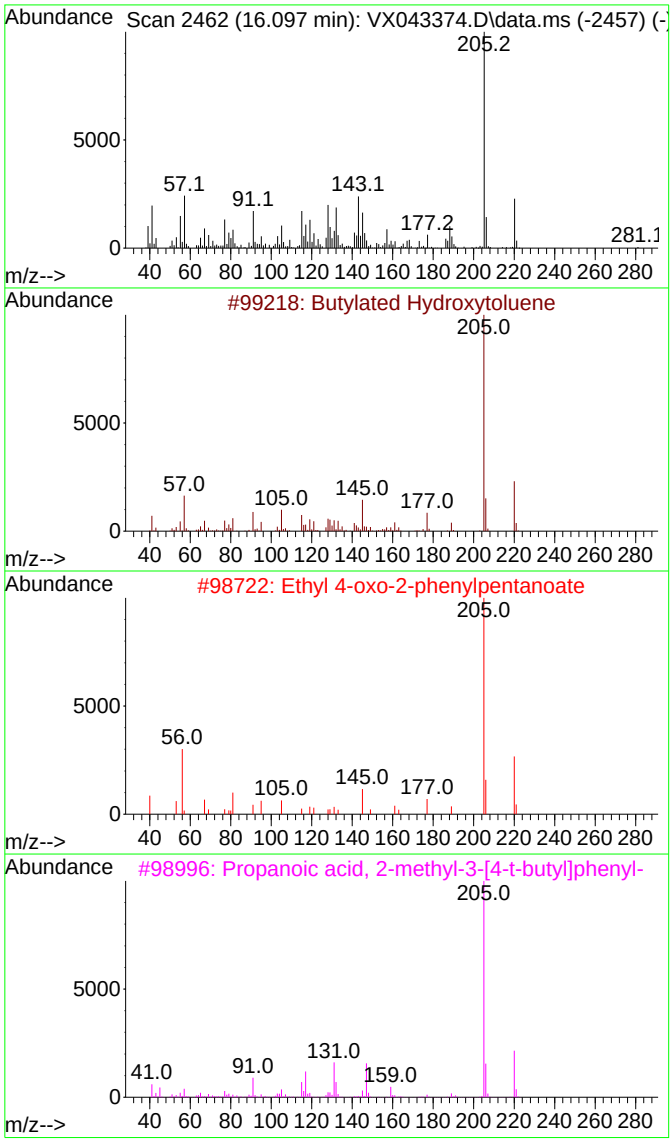
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

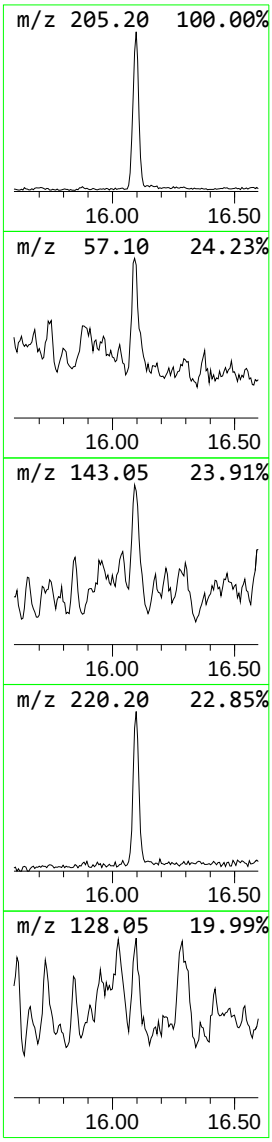
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.097	25.50 ug/l	194024	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	86
2	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	64
3	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	47
4	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	46
5	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
Acq On : 14 Oct 2024 11:49
Operator : JC/MD
Sample : P4393-01 20X
Misc : 1.31g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

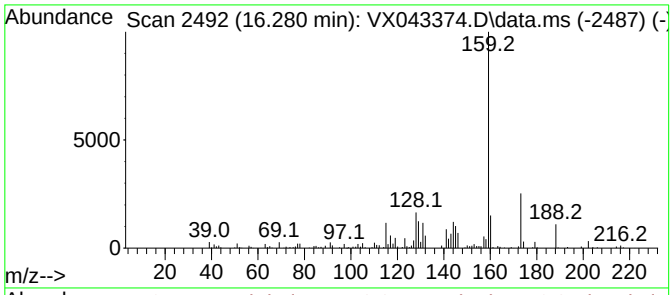
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

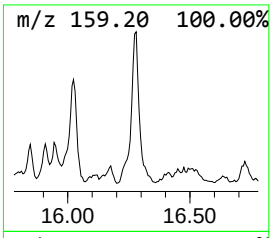
****

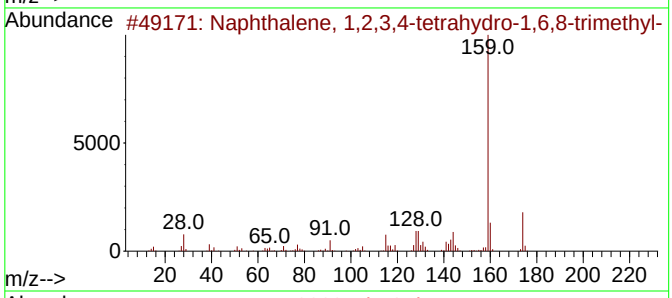
Peak Number 10 cis-Calamenene Concentration Rank 1

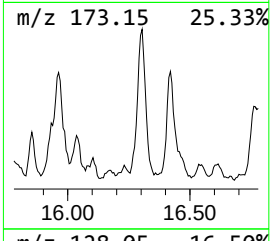
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	34.09 ug/l	259407	1,4-Dichlorobenzene-d4	12.024

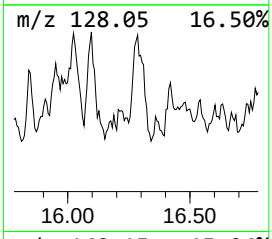
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	76
2	cis-Calamenene	202	C15H22	072937-55-4	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-55-0	76
4	trans-Calamenene	202	C15H22	073209-42-4	76
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	76

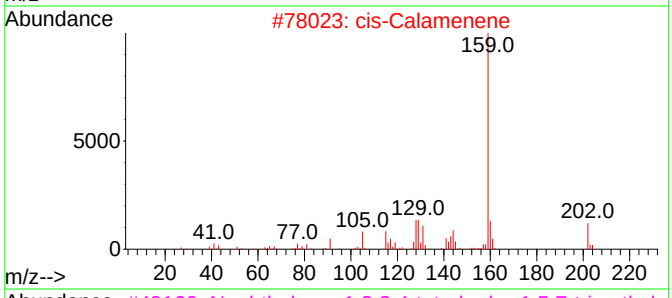


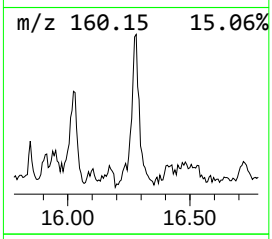


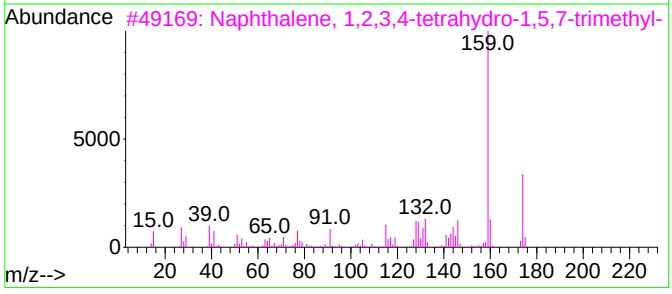


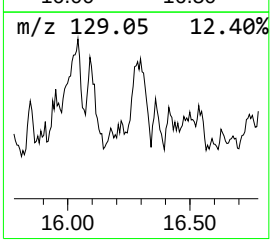












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043374.D
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUST-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.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, 1,...	14.615	20.9	ug/l	159410	4	12.024	380491	50.0
1H-Indene, 2,3-...	14.670	9.6	ug/l	72964	4	12.024	380491	50.0
unknown14.847	14.847	10.5	ug/l	79634	4	12.024	380491	50.0
Naphthalene, 1,...	15.182	12.0	ug/l	91313	4	12.024	380491	50.0
Decahydro-1,1,4...	15.414	13.8	ug/l	105309	4	12.024	380491	50.0
unknown15.493	15.493	9.8	ug/l	74332	4	12.024	380491	50.0
unknown15.743	15.743	17.9	ug/l	136382	4	12.024	380491	50.0
unknown15.859	15.859	13.1	ug/l	99984	4	12.024	380491	50.0
Butylated Hydro...	16.097	25.5	ug/l	194024	4	12.024	380491	50.0
cis-Calamenene	16.280	34.1	ug/l	259407	4	12.024	380491	50.0