LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP015045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.446	6	10	22	rVB	99107	144463	1.89%	0.267%
2	3.887	83	85	99	rBV	361568	583400	7.64%	1.077%
3	4.134	123	127	131	rVB4	8751	13331	0.17%	0.025%
4	4.464	181	183	192	rVB4	11014	14834	0.19%	0.027%
5	4.646	207	214	222	rBV7	16586	59822	0.78%	0.110%
6	5.193	303	307	312	rVB	22601	33647	0.44%	0.062%
7	5.411	339	344	346	rBV5	5500	9282	0.12%	0.017%
8	7.252	653	657	658	rBV4	9852	11680	0.15%	0.022%
9	7.293	658	664	674	rVB	242736	388393	5.09%	0.717%
10	7.463	686	693	704	rBV	811405	1255451	16.44%	2.318%
11	7.669	721	728	736	rBV	758875	1217186	15.94%	2.248%
12	7.728	736	738	751	rVB9	11320	29782	0.39%	0.055%
13	7.928	766	772	779	rVB2	30650	53631	0.70%	0.099%
14	8.146	801	809	816	rBV	312033	504531	6.61%	0.932%
15	8.852	921	929	941	rBV	648742	1102232	14.43%	2.035%
16	9.322	1002	1009	1021	rBV	898432	1463960	19.17%	2.703%
17	9.722	1071	1077	1084	rBV	56856	86025	1.13%	0.159%
18	9.775	1084	1086	1093	rVB8	5033	9961	0.13%	0.018%
19	10.052	1125	1133	1144	rBV2	687603	1237813	16.21%	2.286%
20	10.146	1144	1149	1155	rVB2	53319	87516	1.15%	0.162%
21	10.363	1181	1186	1198	rVB2	25833	47554	0.62%	0.088%
22	10.593	1217	1225	1239	rBV	1095509	1861691	24.38%	3.438%
23	10.887	1270	1275	1281	rVB10	4012	9185	0.12%	0.017%
24	10.981	1283	1291	1298	rVV	453685	766365	10.03%	1.415%
25	11.116	1306	1314	1328	rBV	1017390	1803852	23.62%	3.331%
26	12.216	1496	1501	1507	rBV	38674	57164	0.75%	0.106%
27	12.563	1554	1560	1578	rBV4	28802	83054	1.09%	0.153%
28	13.310	1685	1687	1695	rVB9	4318	8330	0.11%	0.015%
29	13.604	1729	1737	1741	rBV8	9770	18244	0.24%	0.034%
30	13.675	1743	1749	1755	rVV	29160	47068	0.62%	0.087%
31	14.192	1829	1837	1845	rBV	2484257	3596264	47.09%	6.641%
32	14.251	1845	1847	1851	rVB5	9284	11287	0.15%	0.021%
33	14.304	1851	1856	1863	rBV5	8623	16497	0.22%	0.030%
34	14.363	1863	1866	1870	rVB6	5231	8040	0.11%	0.015%
35	14.481	1880	1886	1898	rVV2	2533244	3924153	51.38%	7.247%
36	14.663	1914	1917	1924	rVB6	7353	10826	0.14%	0.020%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Title : SVOA CALIBRATION

37	14.787	1932	1938	1947	rVB	752048	1101002	14.42%	2.033%
38	14.975	1964	1970	1977	rBV	88700	165582	2.17%	0.306%
39	15.187	2002	2006	2016	rVB	13014	29468	0.39%	0.054%
40	15.592	2065	2075	2077	rBV6	17807	35334	0.46%	0.065%
41	15.781	2100	2107	2118	rBV	3797702	5392574	70.61%	9.958%
42	15.892	2120	2126	2139	rVV	355215	505569	6.62%	0.934%
43	16.022	2140	2148	2154	rVB5	27364	58802	0.77%	0.109%
44	16.139	2162	2168	2176	rBV	752676	988568	12.94%	1.826%
45	16.345	2201	2203	2209	rVB7	8139	13241	0.17%	0.024%
46	16.481	2222	2226	2227	rBV3	11886	14193	0.19%	0.026%
47	16.710	2261	2265	2271	rVB	25026	37398	0.49%	0.069%
48	16.922	2298	2301	2307	rVB8	13563	24205	0.32%	0.045%
49	17.281	2358	2362	2367	rBV4	19185	25956	0.34%	0.048%
50	17.333	2367	2371	2374	rVV2	14209	19575	0.26%	0.036%
51	17.539	2400	2406	2414	rBV	983760	1407554	18.43%	2.599%
52	17.639	2417	2423	2439	rVV2	4312118	6385143	83.61%	11.791%
53	17.810	2450	2452	2454	rBV3	9015	10285	0.13%	0.019%
54	18.286	2529	2533	2541	rVB9	25974	43793	0.57%	0.081%
55	18.398	2547	2552	2562	rBV	311486	514655	6.74%	0.950%
56	18.804	2617	2621	2625	rVB	108132	117336	1.54%	0.217%
57	19.222	2688	2692	2697	rBV2	59141	98220	1.29%	0.181%
58	19.439	2725	2729	2733	rVB	69702	91567	1.20%	0.169%
59	19.510	2736	2741	2750	rVB	85923	154997	2.03%	0.286%
60	19.622	2756	2760	2767	rBV2	105004	165692	2.17%	0.306%
61	19.863	2795	2801	2813	rBV	5707592	7637237	100.00%	14.104%
62	21.292	3041	3044	3054	rBV	339959	462369	6.05%	0.854%
63	21.621	3095	3100	3109	rBV	964168	1320055	17.28%	2.438%
64	24.033	3503	3510	3527	rVB2	2644864	5694819	74.57%	10.517%
65	24.204	3533	3539	3548	rVB	489674	1059005	13.87%	1.956%

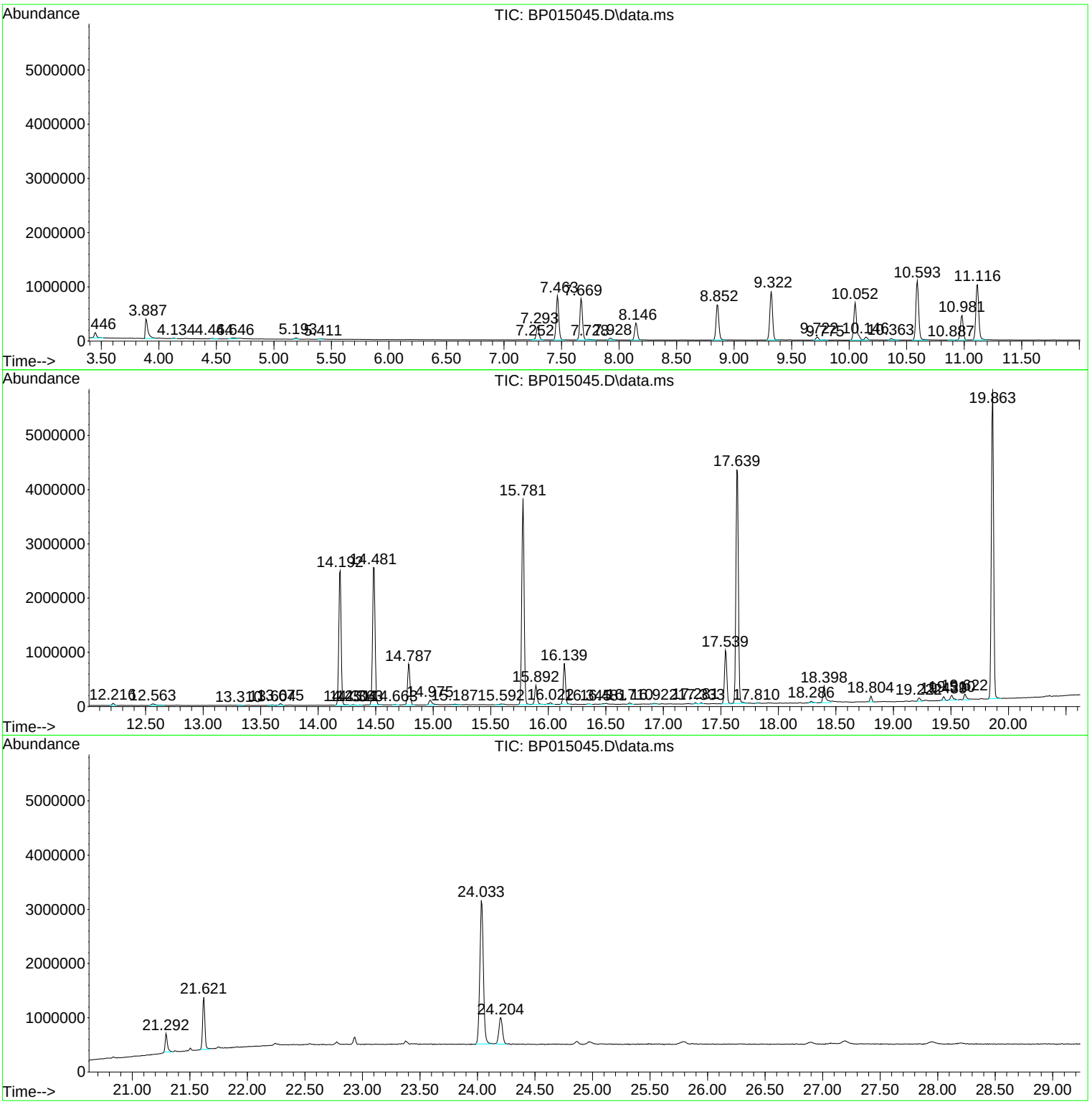
Sum of corrected areas: 54150708

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

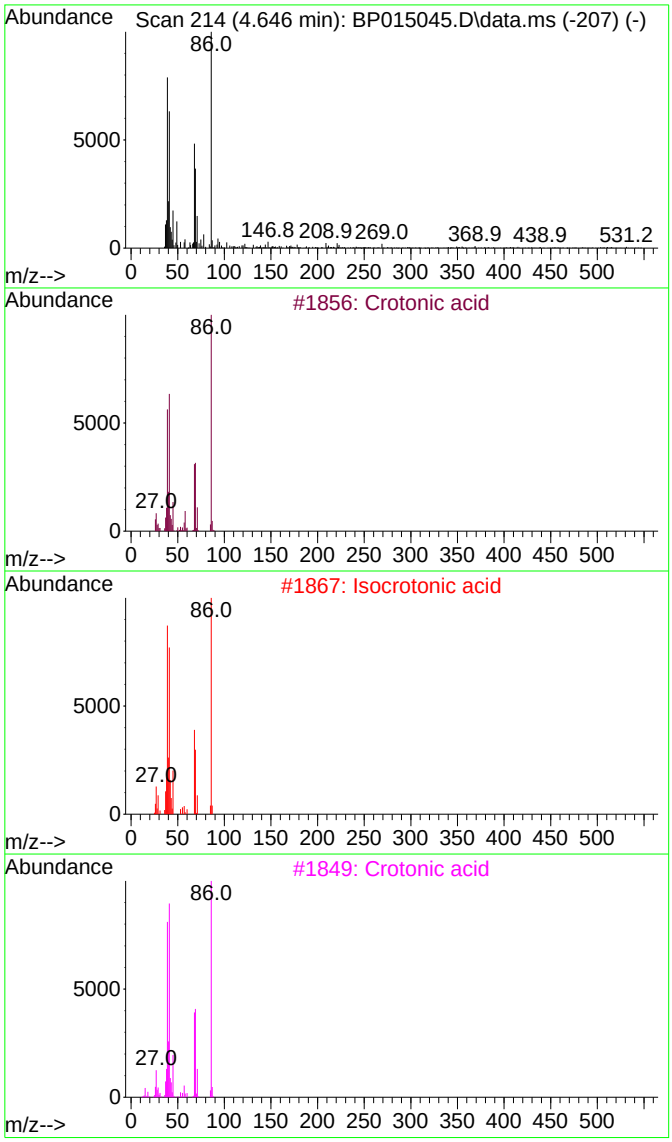
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

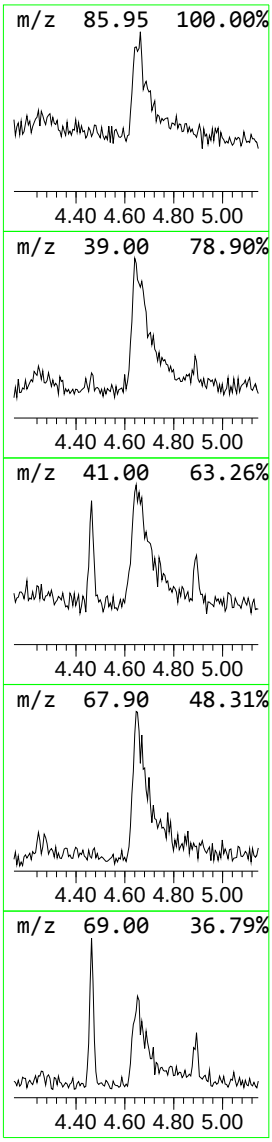
****

Peak Number 1 Crotonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.646	2.37 ng/ul	59822	1,4-Dichlorobenzene-d4	8.146

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crotonic acid	86	C4H6O2	003724-65-0	91
2	Isocrotonic acid	86	C4H6O2	000503-64-0	91
3	Crotonic acid	86	C4H6O2	003724-65-0	90
4	2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	90
5	Crotonic acid	86	C4H6O2	003724-65-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

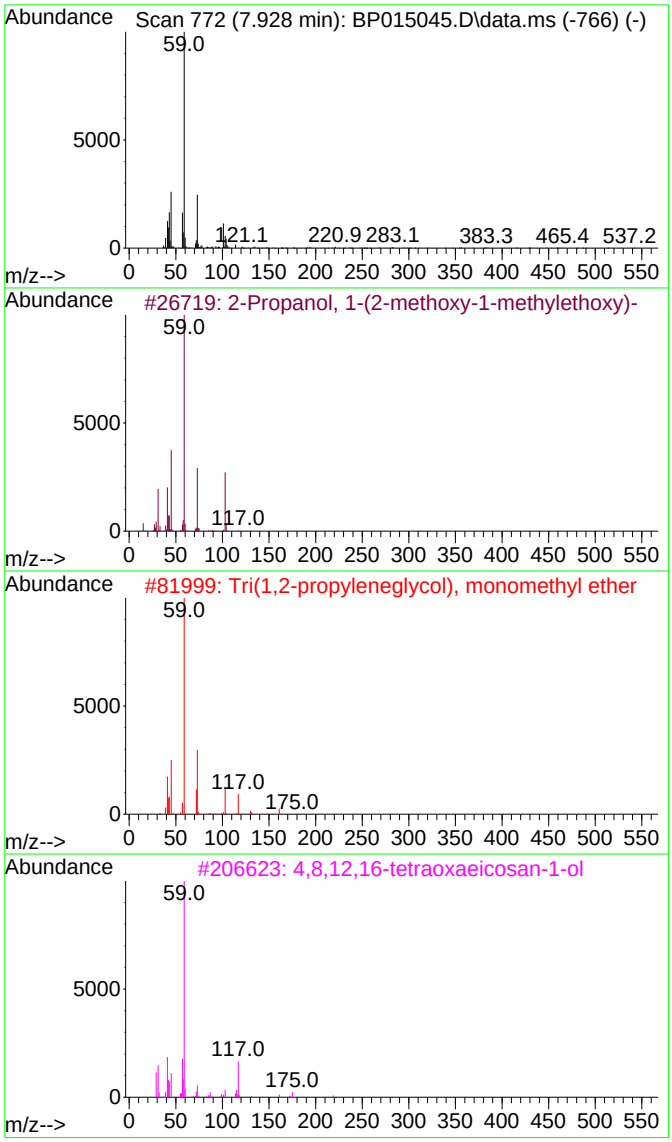
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

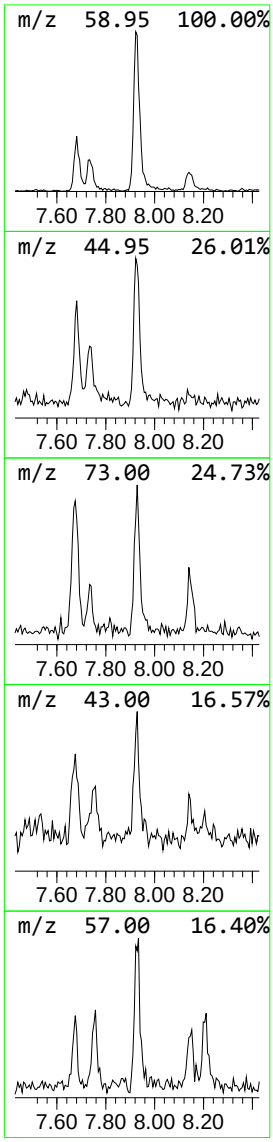
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	2.13 ng/ul	53631	1,4-Dichlorobenzene-d4	8.146

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	64
3	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	59
4	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	56
5	Hexylene glycol	118	C6H14O2	000107-41-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

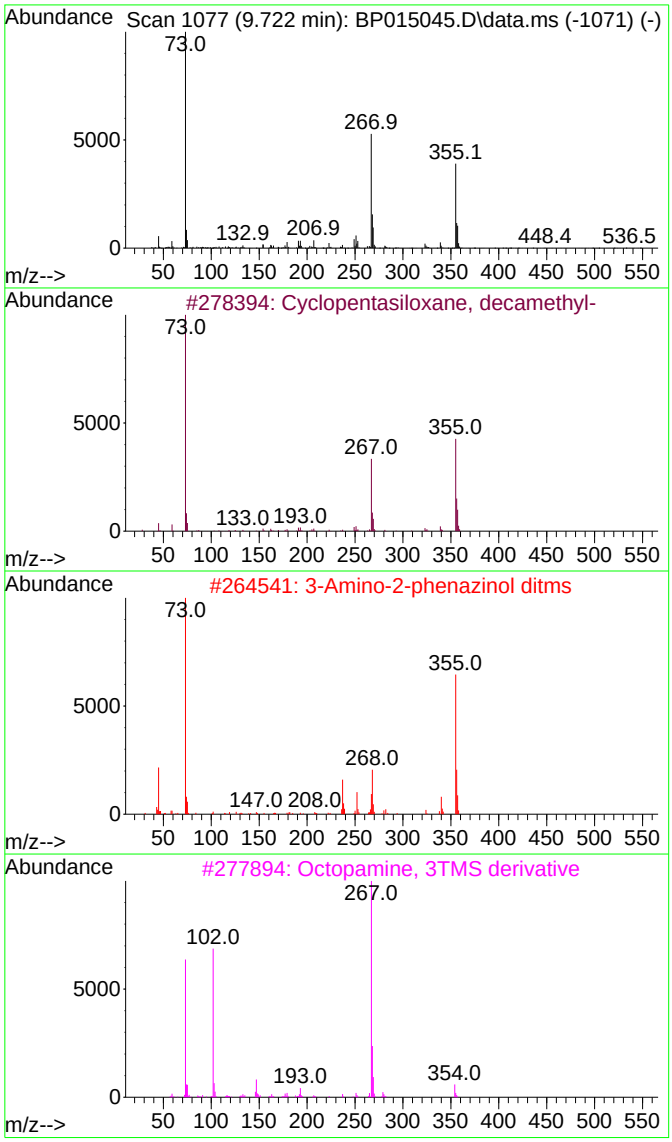
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

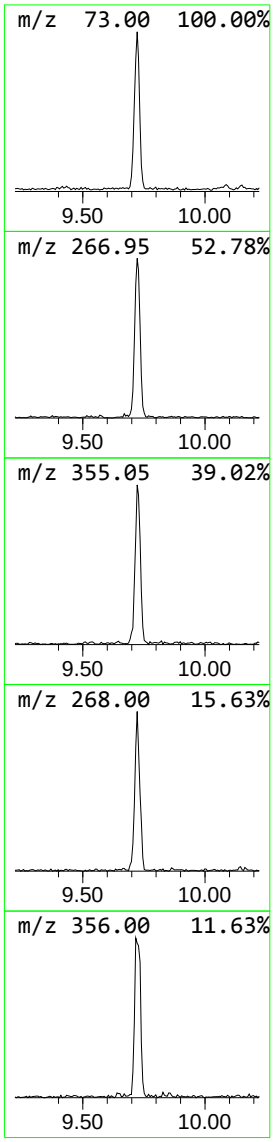
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentasiloxane, decamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	2.25 ng/ul	86025	Naphthalene-d8	10.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	91
2	3-Amino-2-phenazinol ditms	355	C18H25N3OSi2	1000332-15-5	47
3	Octopamine, 3TMS derivative	369	C17H35NO2Si3	068595-60-8	43
4	Benzeneethanamine, N-[(pentafluo...	563	C24H34F5NO3Si3	055429-13-5	43
5	Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

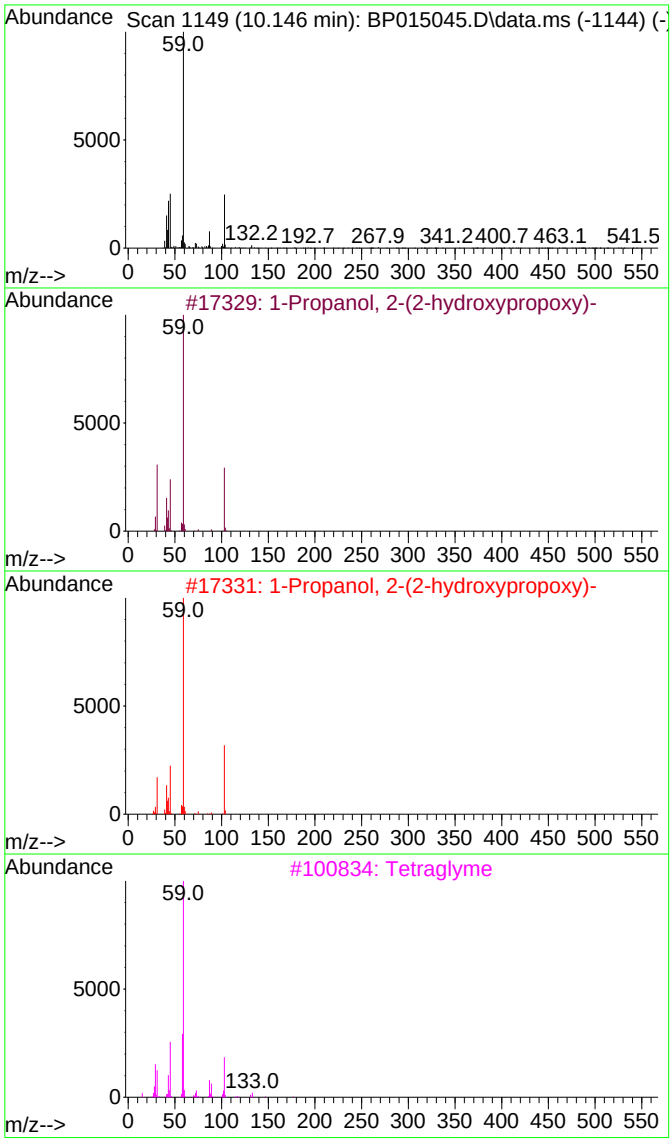
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

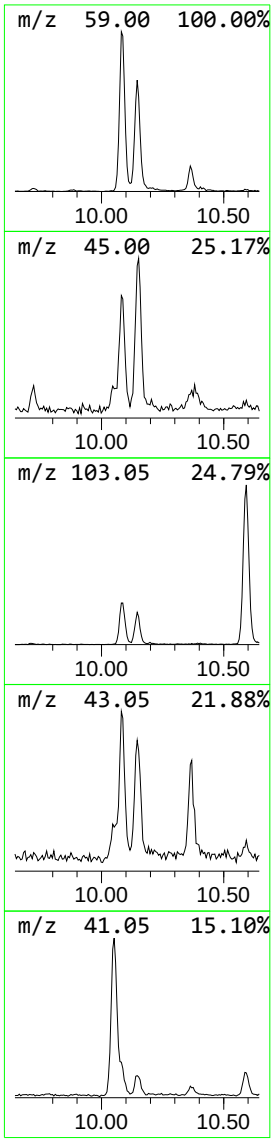
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.146	2.28 ng/ul	87516	Naphthalene-d8	10.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
3	Tetraglyme	222	C10H22O5	000143-24-8	64
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5	Methane, diethoxy-	104	C5H12O2	000462-95-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

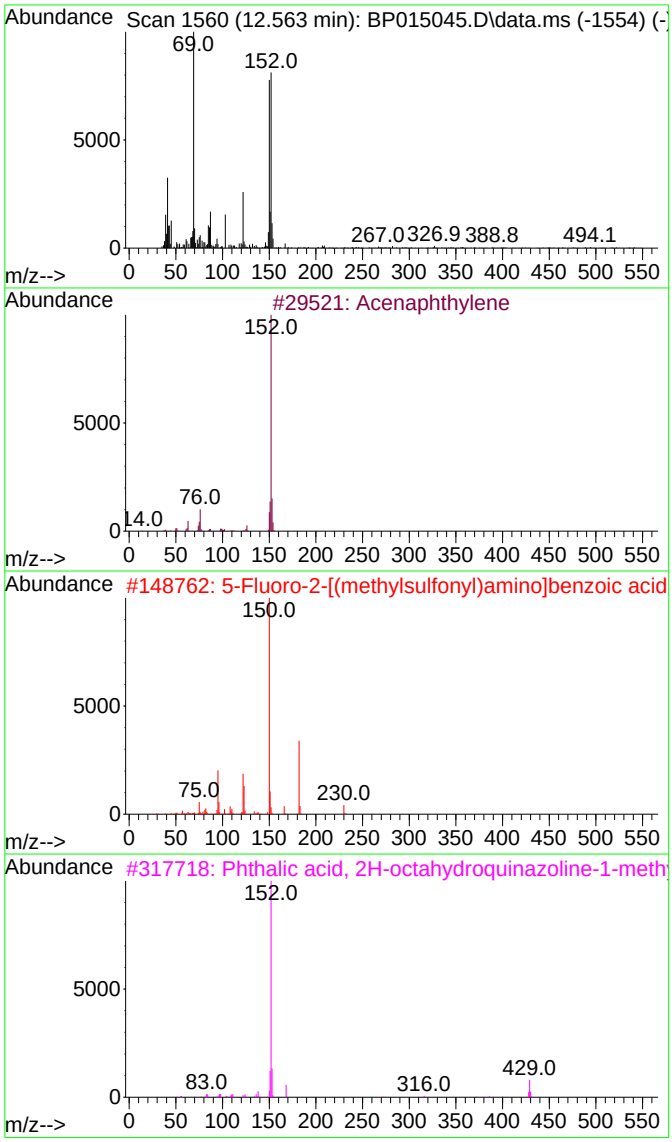
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

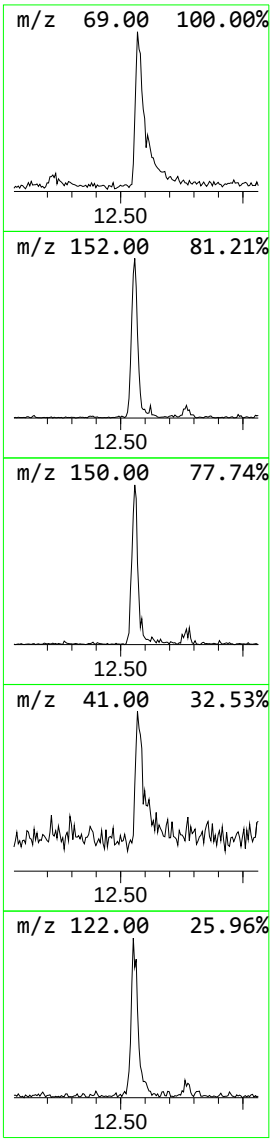
****

Peak Number 5 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	2.17 ng/ul	83054	Naphthalene-d8	10.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthylene	152	C12H8	000208-96-8	25
2	5-Fluoro-2-[(methylsulfonyl)amin...	261	C10H12FNO4S	1000499-76-6	22
3	Phthalic acid, 2H-octahydroquina...	429	C26H39NO4	1000322-80-9	22
4	[1,2,4]Triazolo[1,5-a]pyrimidin-...	150	C6H6N4O	002503-56-2	22
5	5-Fluoro-1-methyl-1H-benzimidazole	150	C8H7FN2	1365271-95-9	22





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JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

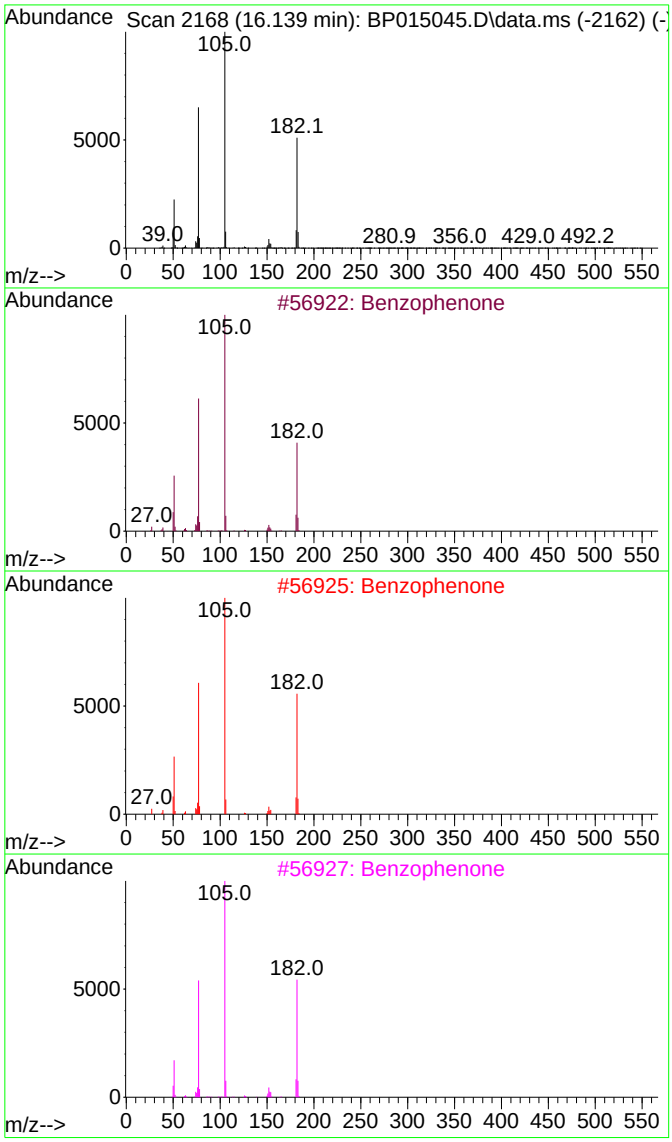
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

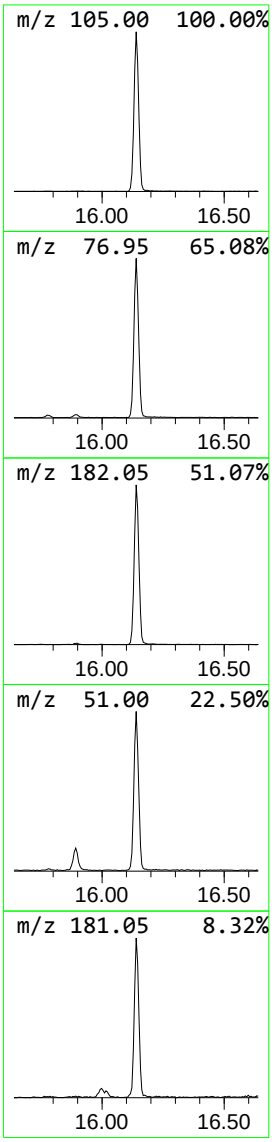
****

Peak Number 6 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	17.96 ng/ul	988568	Acenaphthene-d10	14.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	93
5	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

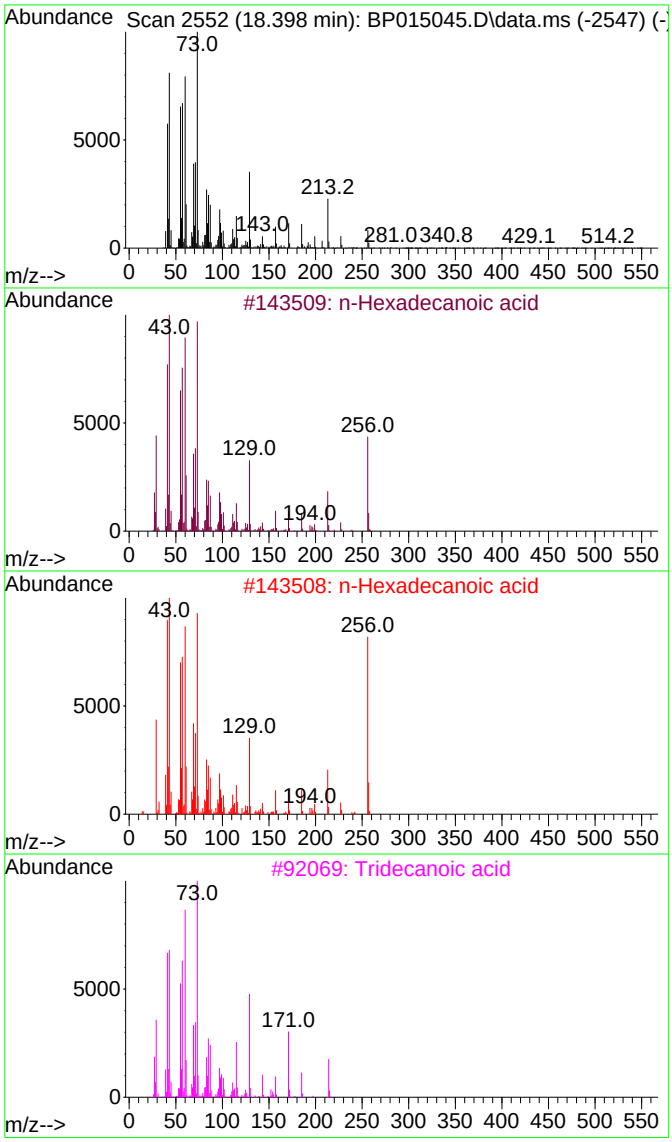
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

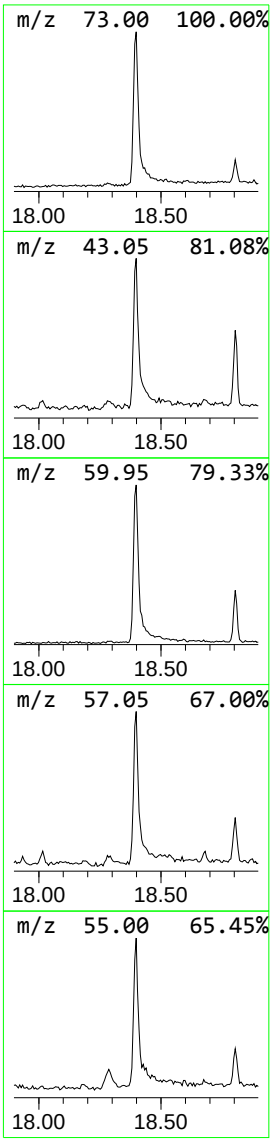
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	7.31 ng/ul	514655	Phenanthrene-d10	17.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tridecanoic acid	214	C13H26O2	000638-53-9	96
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95





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Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

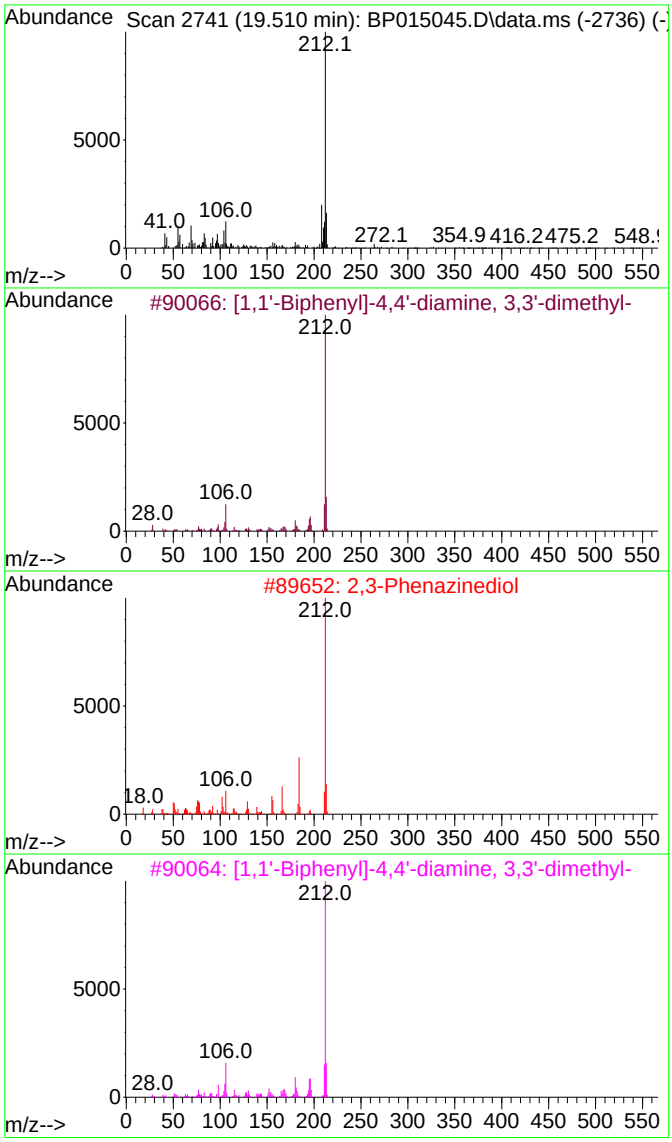
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

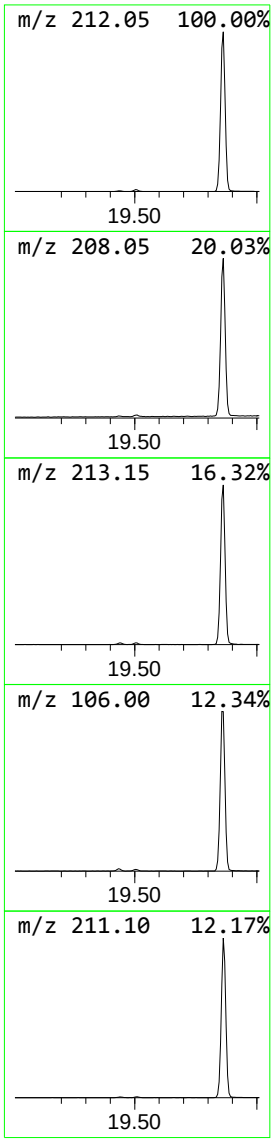
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 [1,1'-Biphenyl]-4,4'-diamin... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	2.20 ng/ul	154997	Phenanthrene-d10	17.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,1'-Biphenyl]-4,4'-diamine, 3,...	212	C14H16N2	000119-93-7	64
2	2,3-Phenazinediol	212	C12H8N2O2	019220-18-9	59
3	[1,1'-Biphenyl]-4,4'-diamine, 3,...	212	C14H16N2	000119-93-7	59
4	Harmine	212	C13H12N2O	000442-51-3	59
5	[1,1'-biphenyl]-4,4'-diamine, 2,...	212	C14H16N2	1000400-65-3	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

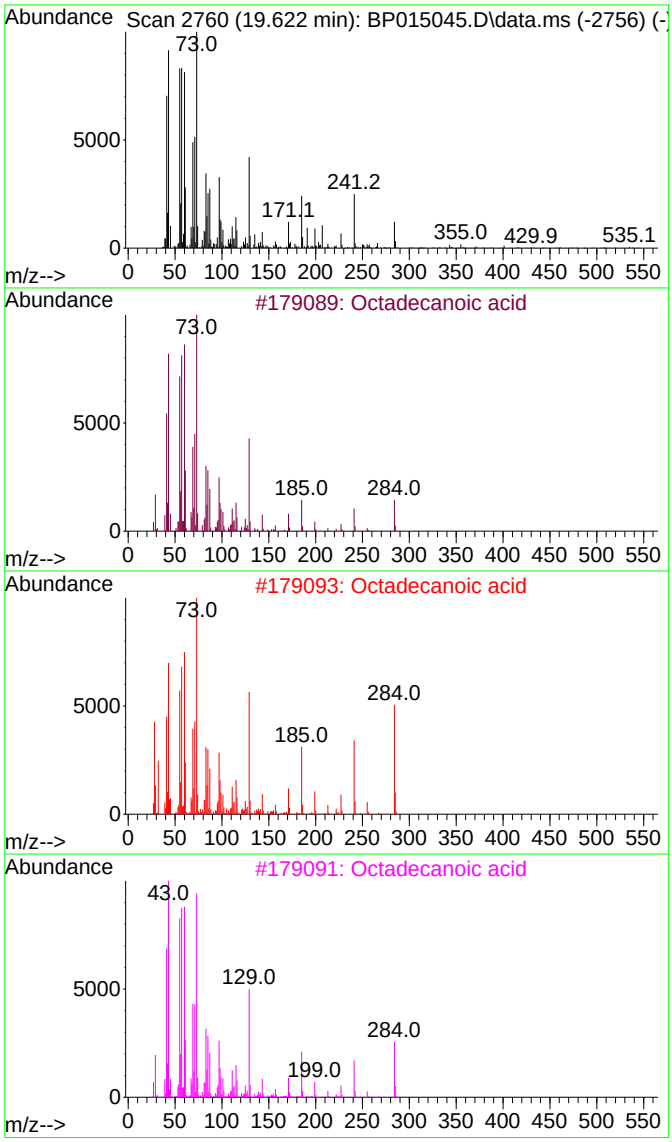
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

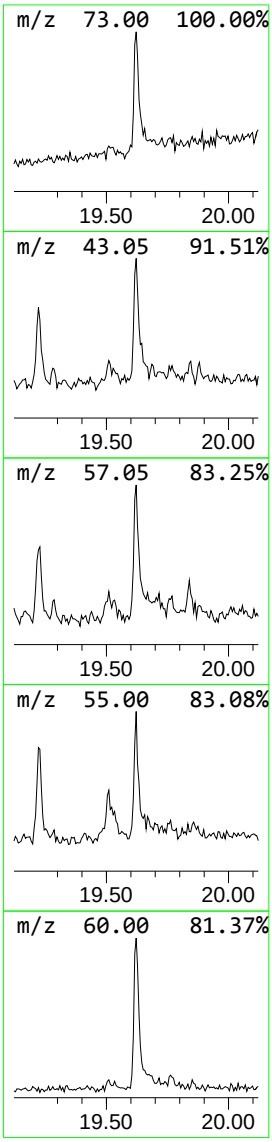
****

Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.622	2.51 ng/ul	165692	Chrysene-d12	21.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	97
4	Octadecanoic acid	284	C18H36O2	000057-11-4	95
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

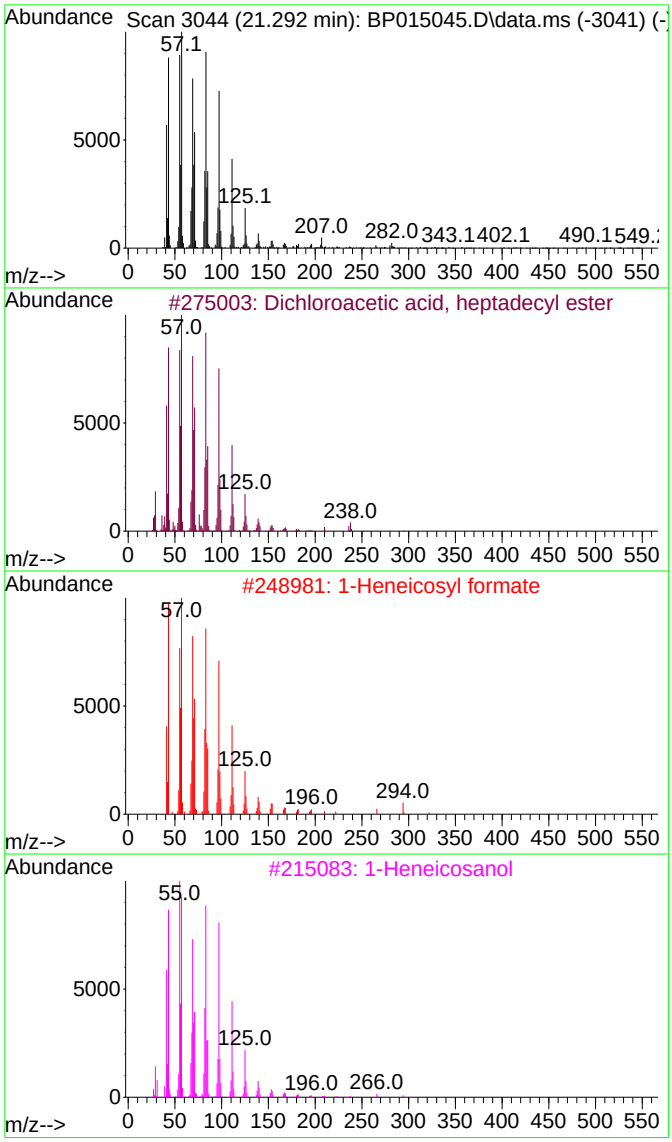
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

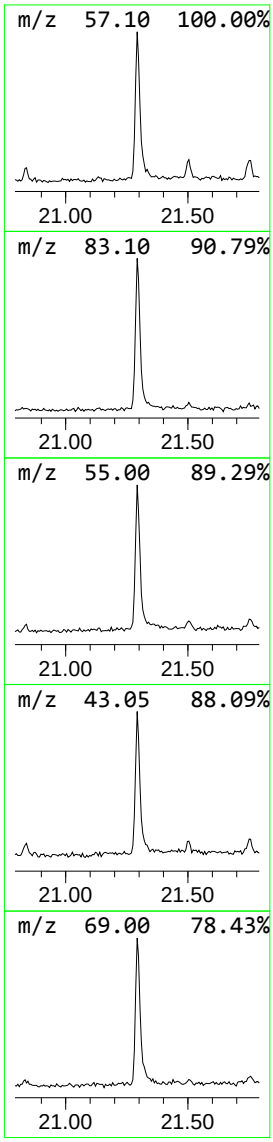
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.292	7.01 ng/ul	462369	Chrysene-d12	21.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015045.D
Acq On : 10 May 2023 16:36
Operator : CG/JU
Sample : 02694-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREQ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Crotonic acid	4.646	2.4	ng/ul	59822	1	8.146	504531	20.0
2-Propanol, 1-(...	7.928	2.1	ng/ul	53631	1	8.146	504531	20.0
Cyclopentasilox...	9.722	2.3	ng/ul	86025	2	10.981	766365	20.0
1-Propanol, 2-(...	10.146	2.3	ng/ul	87516	2	10.981	766365	20.0
unknown-01	12.563	2.2	ng/ul	83054	2	10.981	766365	20.0
Benzophenone	16.139	18.0	ng/ul	988568	3	14.787	1101000	20.0
n-Hexadecanoic ...	18.398	7.3	ng/ul	514655	4	17.539	1407550	20.0
[1,1'-Biphenyl]...	19.510	2.2	ng/ul	154997	4	17.539	1407550	20.0
Octadecanoic acid	19.622	2.5	ng/ul	165692	5	21.622	1320060	20.0
Dichloroacetic ...	21.292	7.0	ng/ul	462369	5	21.622	1320060	20.0