LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DCFH8

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-BP060723.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP015627.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.405	33	37	41	rBV	16747	21242	0.10%	0.035%
2	3.852	110	113	127	rBV	151888	266319	1.30%	0.442%
3	4.081	147	152	159	rVB3	13218	24852	0.12%	0.041%
4	7.246	683	690	704	rBV	351418	615693	3.00%	1.023%
5	7.405	710	717	731	rVB	285921	458274	2.23%	0.761%
6	7.610	746	752	761	rBV	381637	634361	3.09%	1.054%
7	8.081	824	832	845	rVB	451262	748434	3.65%	1.243%
8	8.805	948	955	966	rBV	363752	631823	3.08%	1.049%
9	9.263	1026	1033	1048	rBV	387262	672769	3.28%	1.117%
10	9.993	1148	1157	1170	rBV	329430	599087	2.92%	0.995%
11	10.540	1241	1250	1270	rBV	422328	868156	4.23%	1.442%
12	10.910	1306	1313	1320	rBV	693299	1131862	5.52%	1.880%
13	11.057	1330	1338	1354	rBV	262554	579226	2.82%	0.962%
14	12.275	1538	1545	1557	rVB7	18891	42564	0.21%	0.071%
15	13.610	1763	1772	1777	rVB	27087	48353	0.24%	0.080%
16	14.134	1852	1861	1868	rBV	973073	1354165	6.60%	2.249%
17	14.422	1903	1910	1927	rVB	1071432	1628173	7.94%	2.704%
18	14.728	1951	1962	1970	rVV	1113506	1616958	7.88%	2.686%
19	14.792	1970	1973	1981	rVB3	12527	22790	0.11%	0.038%
20	14.957	1994	2001	2024	rBV	208729	598935	2.92%	0.995%
21	15.128	2027	2030	2041	rVB10	19697	44437	0.22%	0.074%
22	15.722	2124	2131	2137	rBV	1378977	2005399	9.78%	3.331%
23	15.857	2148	2154	2162	rBV	380489	569817	2.78%	0.946%
24	16.086	2186	2193	2204	rBV	395951	582670	2.84%	0.968%
25	16.434	2246	2252	2257	rBV6	14946	30836	0.15%	0.051%
26	16.651	2283	2289	2296	rVB	91511	145943	0.71%	0.242%
27	16.863	2320	2325	2330	rBV5	17217	28360	0.14%	0.047%
28	17.216	2380	2385	2389	rBV3	17183	32718	0.16%	0.054%
29	17.357	2405	2409	2417	rVV2	55386	78305	0.38%	0.130%
30	17.422	2417	2420	2425	rBV4	34846	52140	0.25%	0.087%
31	17.486	2425	2431	2436	rVV	1505548	2086980	10.18%	3.466%
32	17.528	2436	2438	2443	rVV	106934	151425	0.74%	0.252%
33	17.586	2443	2448	2461	rVB	1508887	2143021	10.45%	3.560%
34	18.228	2554	2557	2562	rVB3	27860	38487	0.19%	0.064%
35	18.286	2562	2567	2572	rBV	191255	258519	1.26%	0.429%
36	18.345	2572	2577	2584	rBV	1146589	1493906	7.28%	2.481%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DCFH8

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-BP060723.MA.M
Title : SVOA CALIBRATION

37	18.622	2620	2624	2630	rBV6	34167	78154	0.38%	0.130%
38	18.686	2631	2635	2639	rVV5	33618	56220	0.27%	0.093%
39	19.222	2723	2726	2732	rVB2	49717	58288	0.28%	0.097%
40	19.427	2758	2761	2763	rBV	85144	104150	0.51%	0.173%
41	19.457	2763	2766	2767	rVV	106742	132542	0.65%	0.220%
42	19.480	2767	2770	2777	rVB	423982	565063	2.76%	0.939%
43	19.569	2781	2785	2792	rBV	356834	511002	2.49%	0.849%
44	19.810	2820	2826	2830	rBV	2146904	3077050	15.00%	5.111%
45	20.610	2960	2962	2968	rVB5	71507	87027	0.42%	0.145%
46	20.780	2988	2991	2995	rBV2	74782	97874	0.48%	0.163%
47	21.245	3065	3070	3075	rBV	564979	826369	4.03%	1.373%
48	21.569	3118	3125	3129	rBV	1777723	2766243	13.49%	4.595%
49	22.163	3224	3226	3229	rVB2	158296	162590	0.79%	0.270%
50	22.204	3230	3233	3243	rVB3	317439	502782	2.45%	0.835%
51	23.280	3411	3416	3421	rVB	660890	988728	4.82%	1.642%
52	23.951	3524	3530	3536	rBV2	1318988	2573037	12.55%	4.274%
53	24.115	3552	3558	3566	rBV	1007555	2028086	9.89%	3.369%
54	24.727	3657	3662	3673	rVB	611741	1314889	6.41%	2.184%
55	26.186	3905	3910	3921	rVB	551276	1457828	7.11%	2.421%
56	28.874	4354	4367	4384	rVB2	4902872	20510024	100.00%	34.067%

Sum of corrected areas: 60204945

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Data File : BP015627.D
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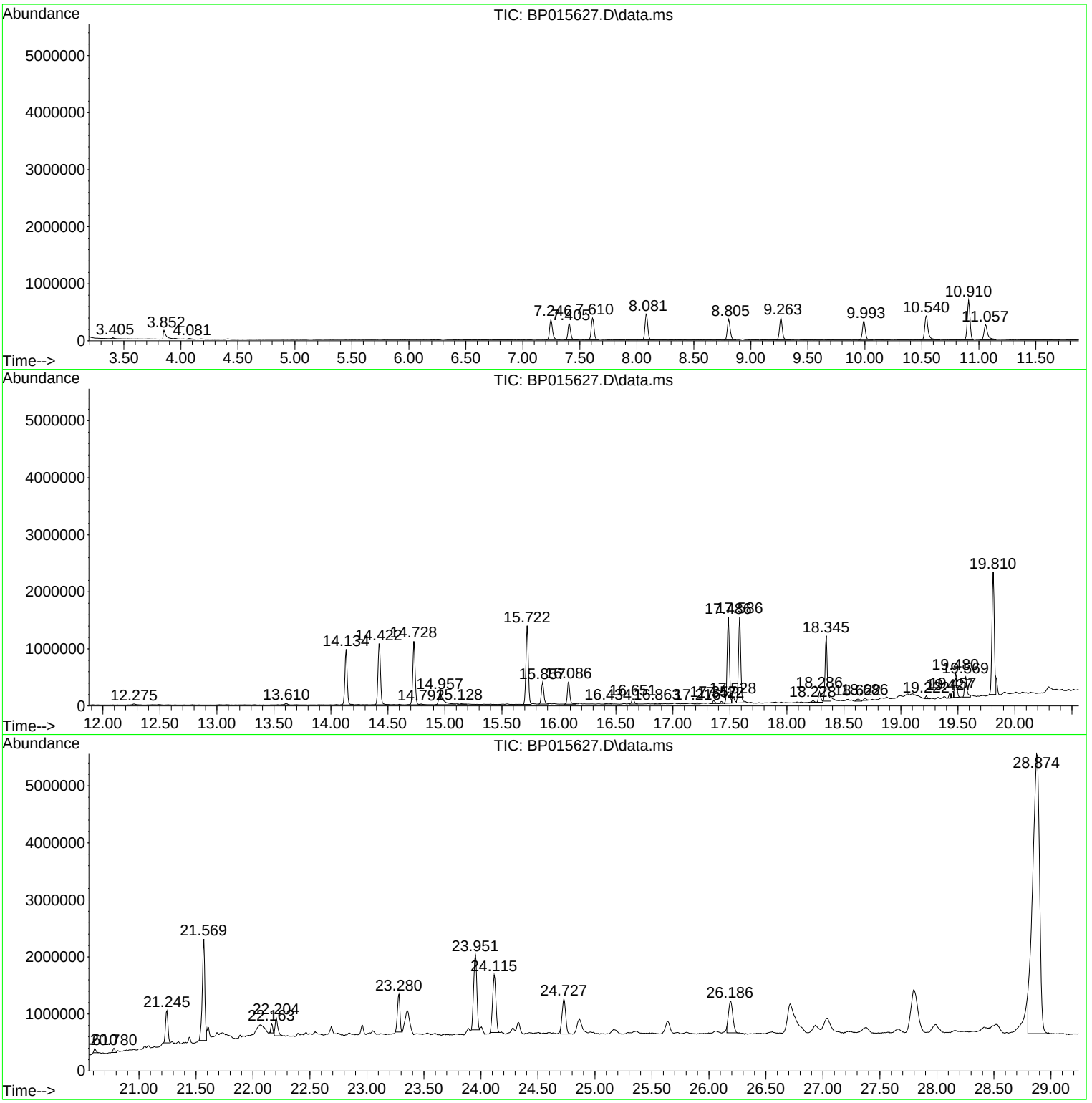
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.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\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
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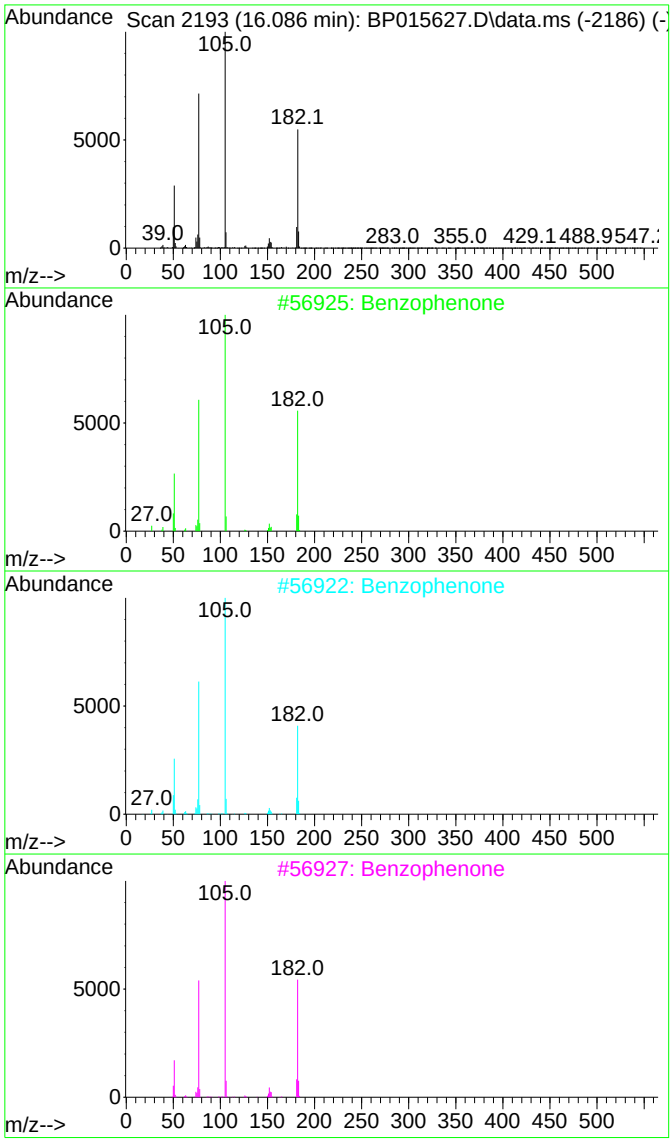
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

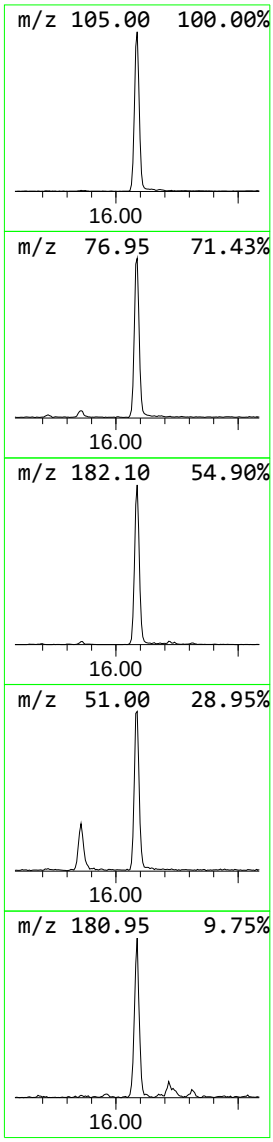
****

Peak Number 1 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.087	7.21 ng/ul	582670	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	95
5	Benzophenone	182	C13H10O	000119-61-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

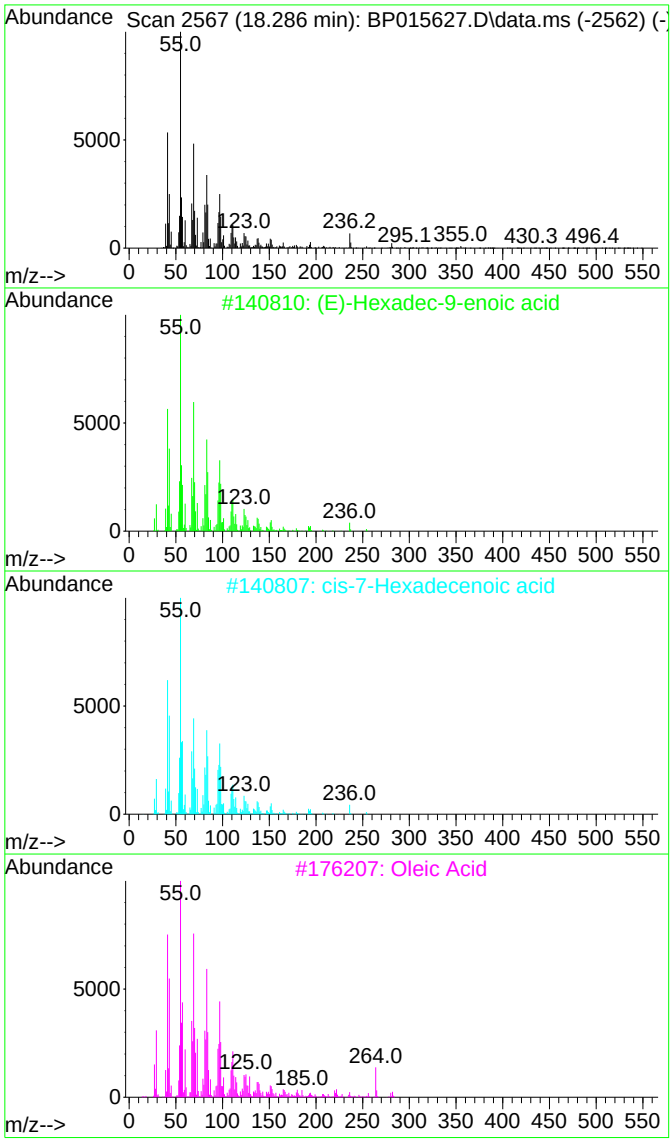
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

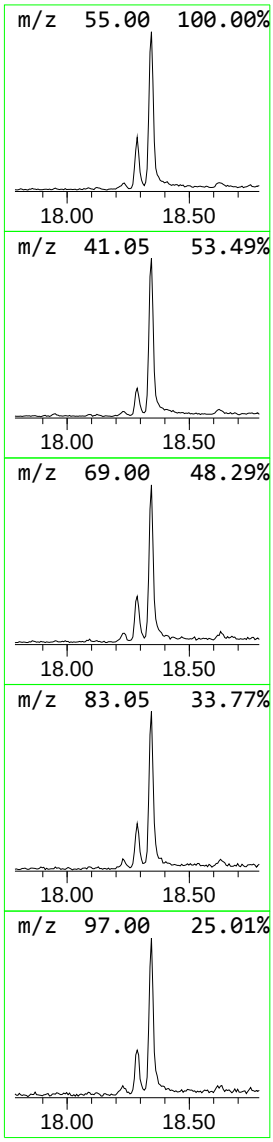
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	2.48 ng/ul	258519	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	98
3	Oleic Acid	282	C18H34O2	000112-80-1	94
4	Palmitoleic acid	254	C16H30O2	000373-49-9	93
5	Oleic Acid	282	C18H34O2	000112-80-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

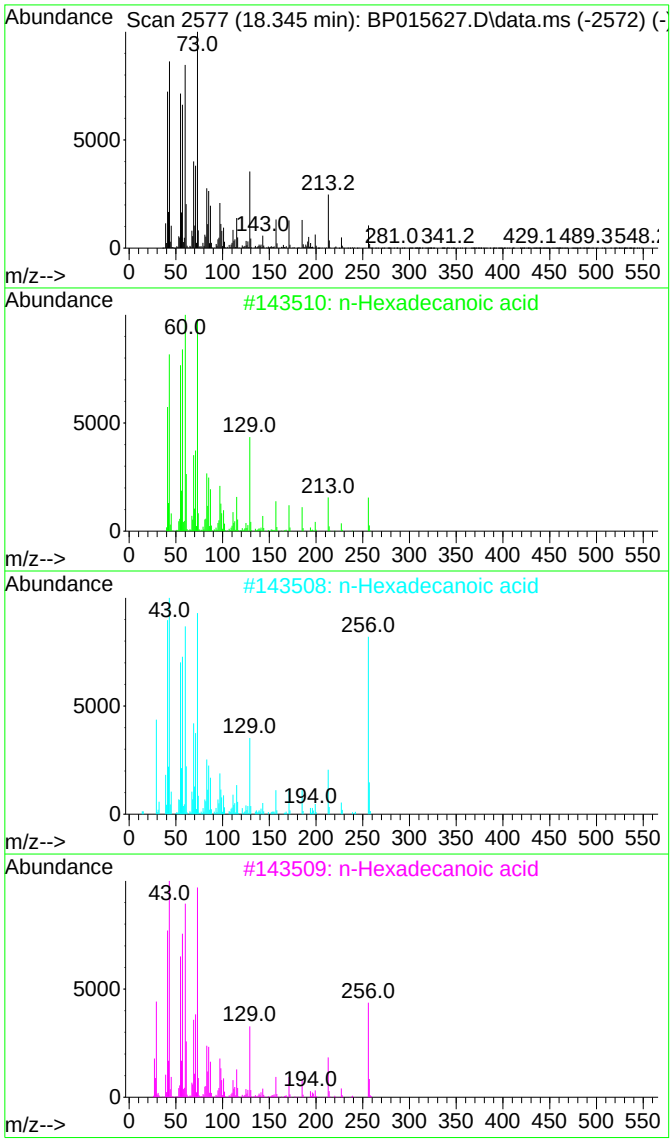
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

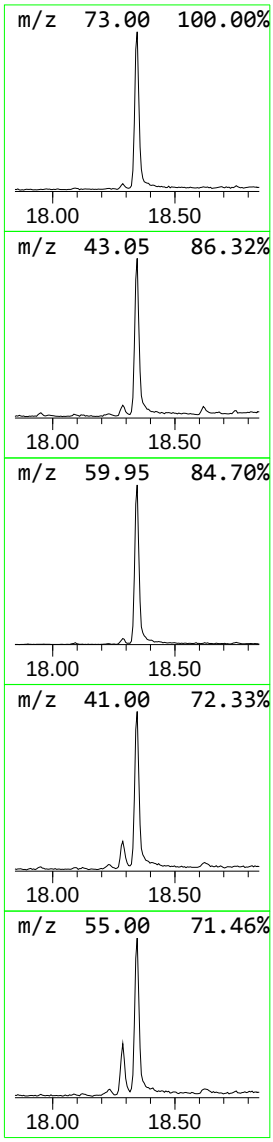
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	14.32 ng/ul	1493910	Phenanthrene-d10	17.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	Tridecanoic acid	214	C13H26O2	000638-53-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

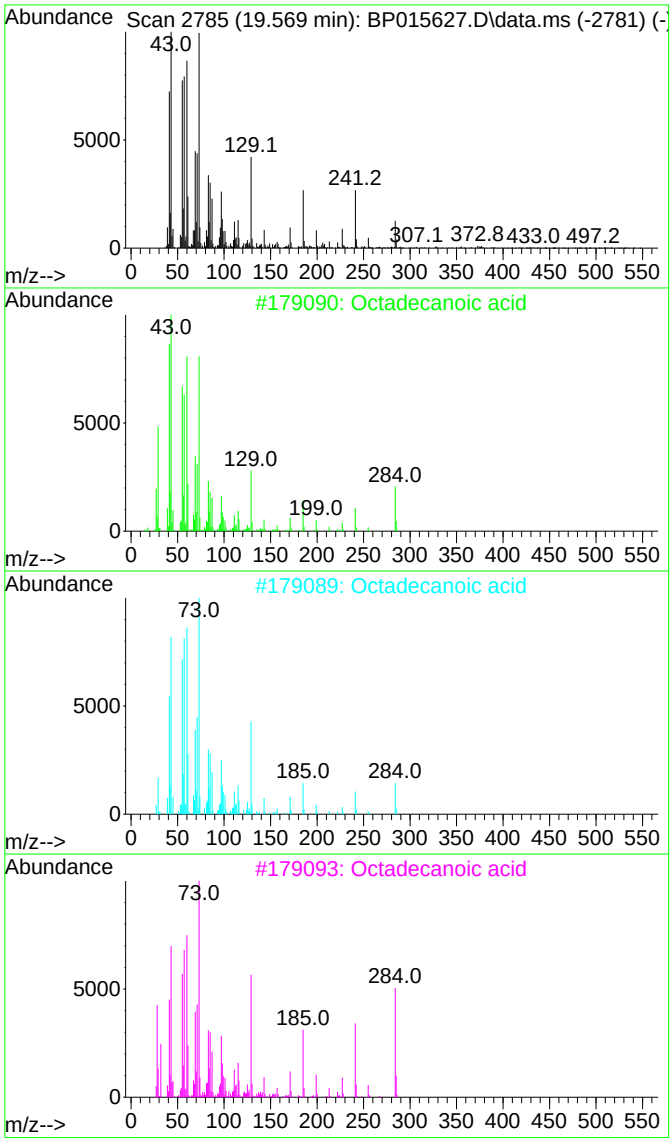
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

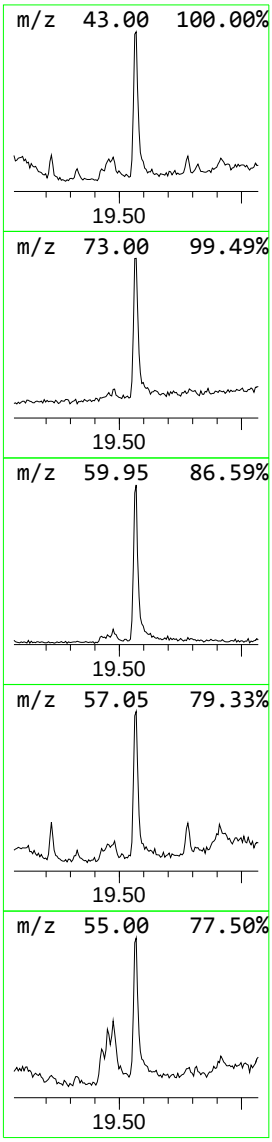
****

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.569	3.69 ng/ul	511002	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	95
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93





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Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

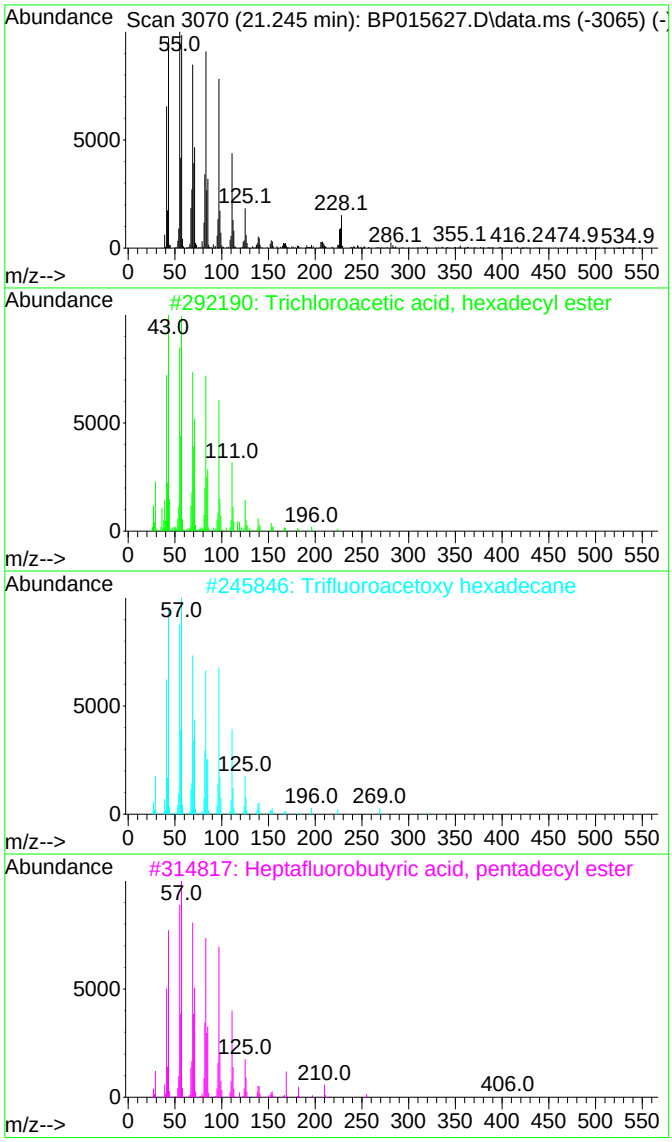
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

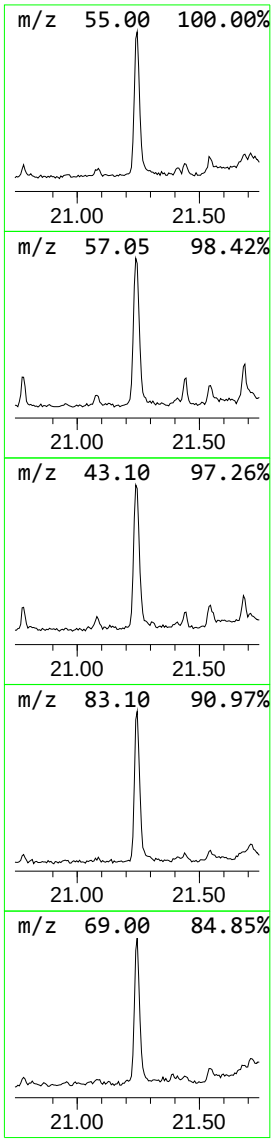
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	5.97 ng/ul	826369	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

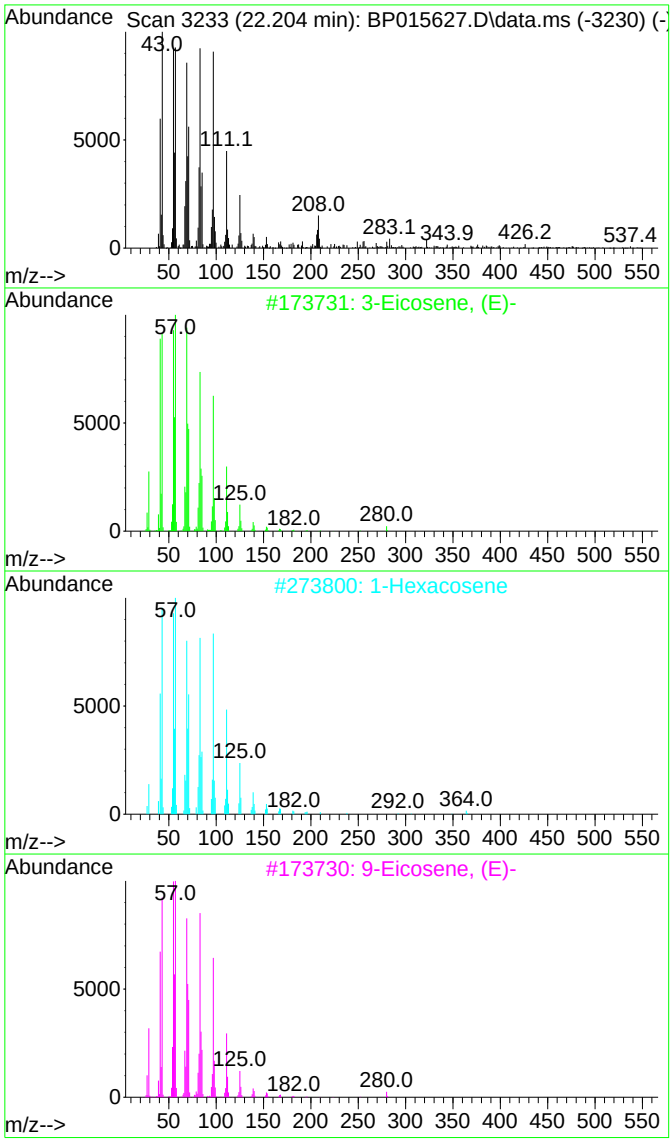
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

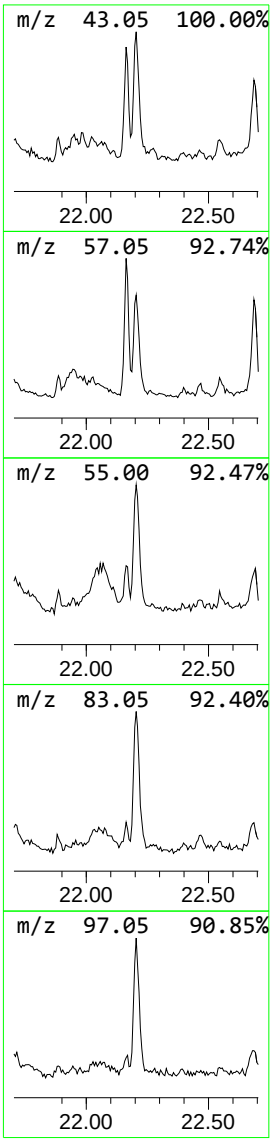
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.204	3.64 ng/ul	502782	Chrysene-d12	21.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	Nonacos-1-ene	406	C29H58	018835-35-3	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

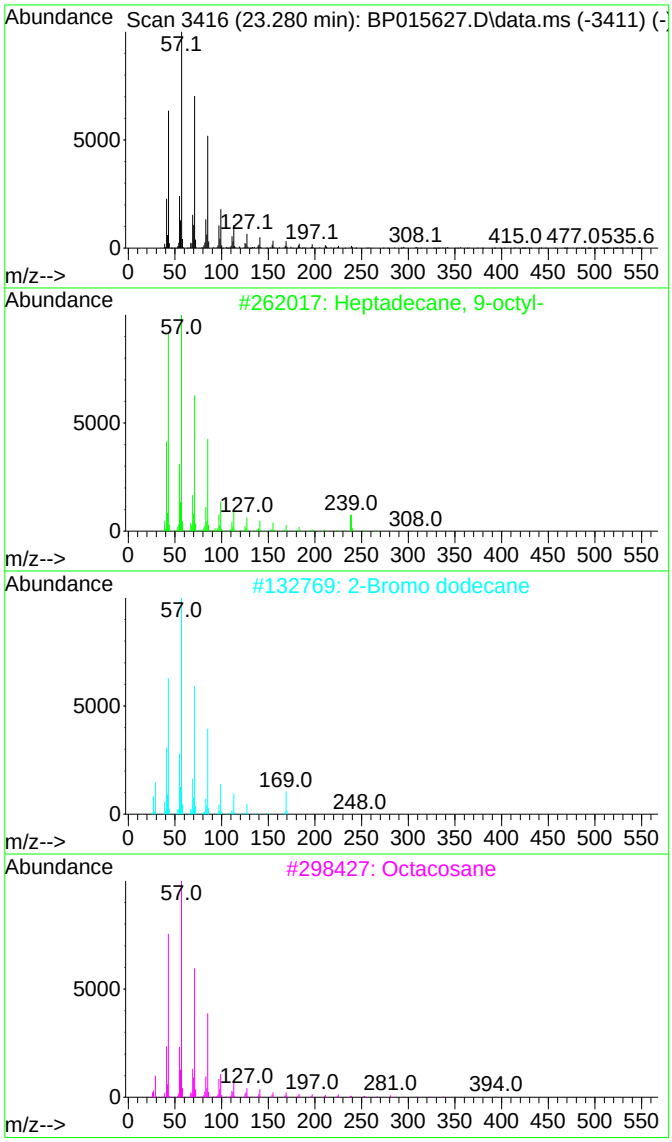
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

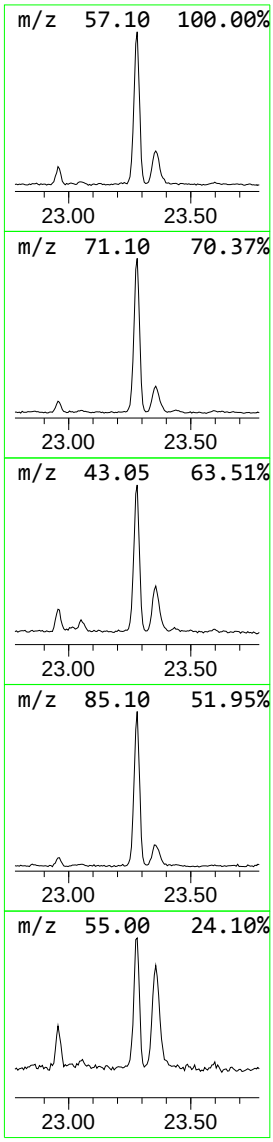
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.280	9.75 ng/ul	988728	Perylene-d12	24.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
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Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

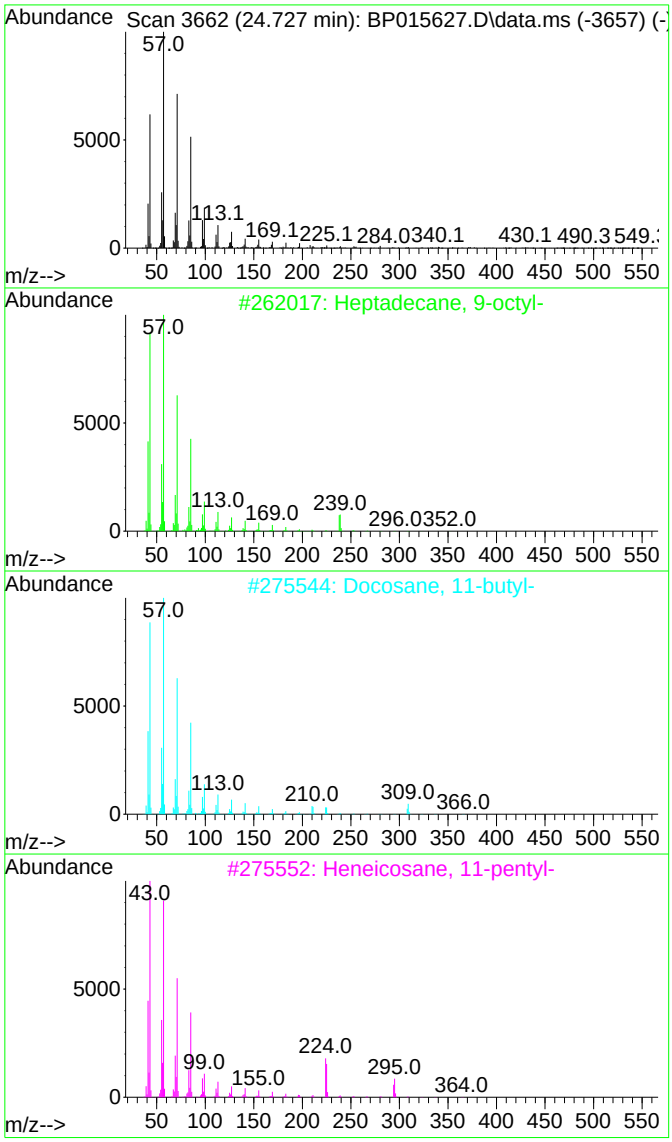
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

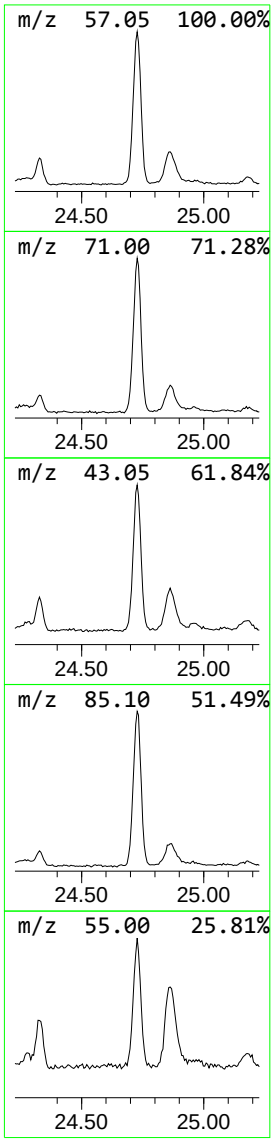
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.727	12.97 ng/ul	1314890	Perylene-d12	24.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
3	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





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Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

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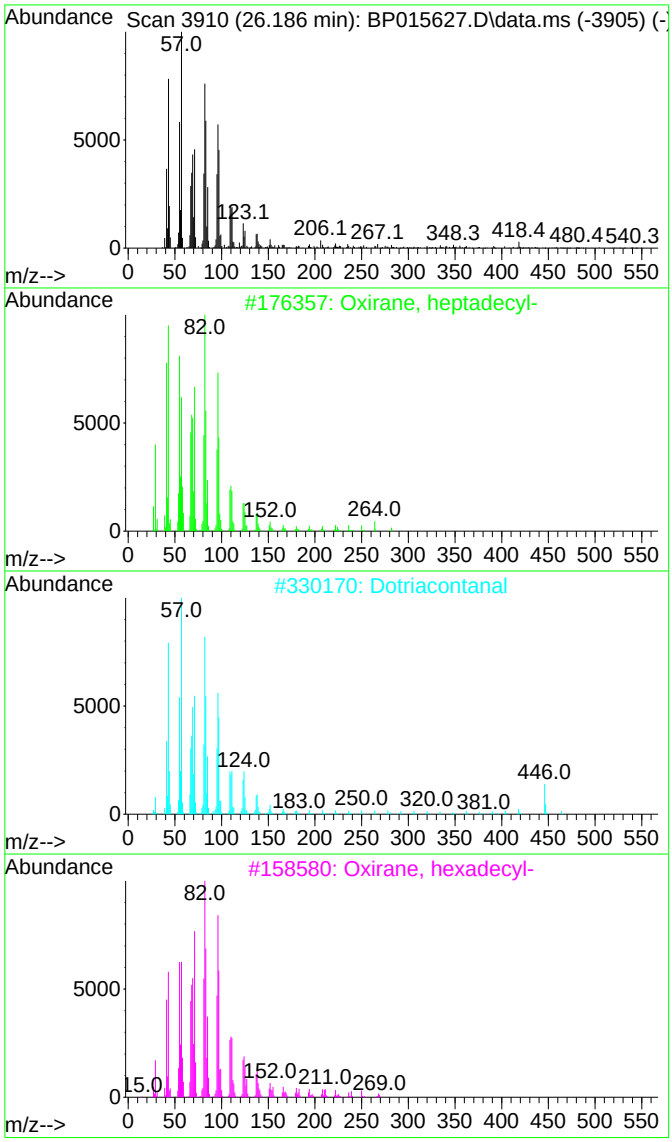
Quant Title : SVOA CALIBRATION

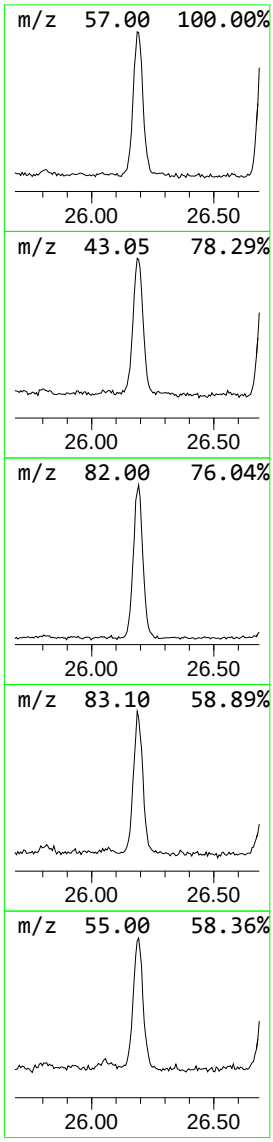
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Oxirane, heptadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.186	14.38 ng/ul	1457830	Perylene-d12	24.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Dotriacontanal	464	C32H64O	057878-00-9	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	Octacosanal	408	C28H56O	022725-64-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

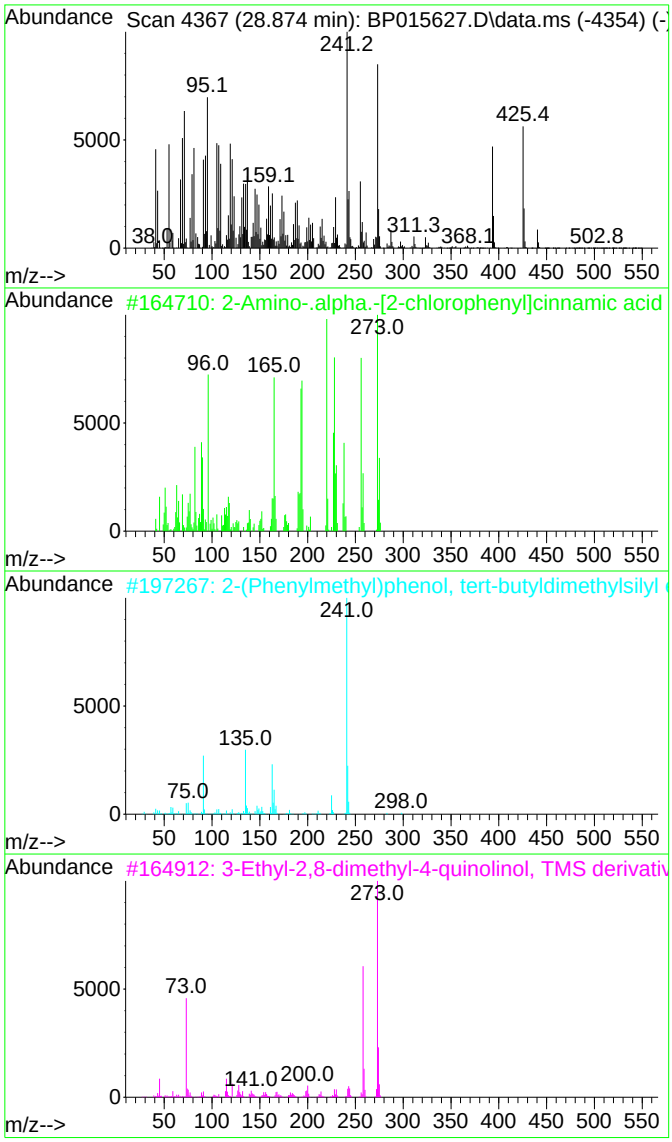
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

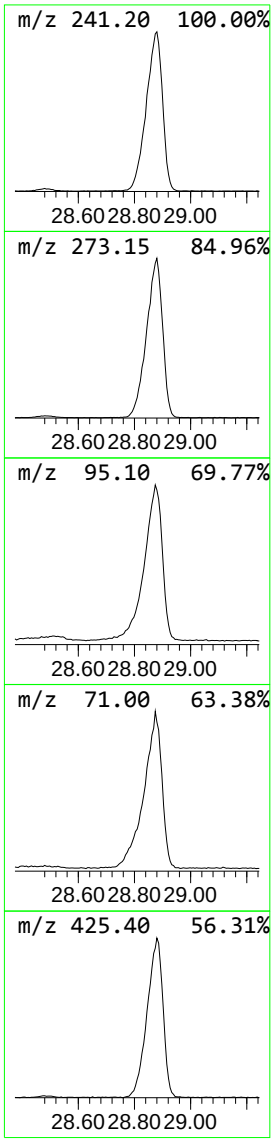
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.874	202.26 ng/ul	20510000	Perylene-d12	24.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2	2-(Phenylmethyl)phenol, tert-but...	298	C19H26OSi	1417315-87-7	25
3	3-Ethyl-2,8-dimethyl-4-quinolino...	273	C16H23NOSi	1000474-26-4	25
4	2-{[(4-Methyl-2-pyridinyl)amino]...	256	C13H16N4Si	1010494-07-4	15
5	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062023\
Data File : BP015627.D
Acq On : 20 Jun 2023 18:11
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.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
Benzophenone	16.087	7.2	ng/ul	582670	3	14.728	1616960	20.0
(E)-Hexadec-9-e...	18.286	2.5	ng/ul	258519	4	17.486	2086980	20.0
n-Hexadecanoic ...	18.345	14.3	ng/ul	1493910	4	17.486	2086980	20.0
Octadecanoic acid	19.569	3.7	ng/ul	511002	5	21.569	2766240	20.0
Trichloroacetic...	21.245	6.0	ng/ul	826369	5	21.569	2766240	20.0
(DEL) Alkane: S...	22.204	3.6	ng/ul	502782	5	21.569	2766240	20.0
(DEL) Alkane: S...	23.280	9.8	ng/ul	988728	6	24.116	2028090	20.0
(DEL) Alkane: S...	24.727	13.0	ng/ul	1314890	6	24.116	2028090	20.0
Oxirane, heptad...	26.186	14.4	ng/ul	1457830	6	24.116	2028090	20.0
2-Amino-.alpha....	28.874	202.3	ng/ul	20510000	6	24.116	2028090	20.0