LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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: BP015597.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	43	rVB	22686	32707	0.13%	0.040%
2	3.852	110	113	127	rBV	184614	331860	1.35%	0.409%
3	4.081	147	152	160	rVB2	17945	30866	0.13%	0.038%
4	7.240	681	689	705	rVB	439684	756509	3.08%	0.933%
5	7.405	709	717	728	rBV	371633	581188	2.36%	0.717%
6	7.611	745	752	762	rBV	482596	788286	3.21%	0.972%
7	8.081	824	832	845	rBV	629651	1004429	4.08%	1.239%
8	8.799	947	954	969	rBV	446979	793997	3.23%	0.979%
9	8.922	969	975	981	rVB2	15557	29043	0.12%	0.036%
10	9.257	1025	1032	1046	rBV	465798	831268	3.38%	1.025%
11	9.987	1148	1156	1166	rBV	428104	732412	2.98%	0.903%
12	10.534	1241	1249	1270	rBV	536749	1083397	4.41%	1.336%
13	10.910	1305	1313	1320	rBV	918477	1546668	6.29%	1.908%
14	11.057	1330	1338	1352	rBV	301093	657988	2.68%	0.812%
15	12.269	1538	1544	1548	rBV4	23890	42393	0.17%	0.052%
16	13.610	1766	1772	1778	rVV2	31451	54958	0.22%	0.068%
17	14.134	1853	1861	1868	rBV	1215625	1708835	6.95%	2.108%
18	14.422	1903	1910	1926	rVB	1363765	1976164	8.04%	2.438%
19	14.728	1952	1962	1969	rBV	1447165	2159104	8.78%	2.663%
20	14.945	1993	1999	2022	rBV	241097	684371	2.78%	0.844%
21	15.128	2026	2030	2039	rVB9	23073	53688	0.22%	0.066%
22	15.716	2124	2130	2137	rBV	1612304	2440661	9.92%	3.011%
23	15.845	2147	2152	2162	rBV	484681	742071	3.02%	0.915%
24	16.081	2186	2192	2201	rBV	481750	681042	2.77%	0.840%
25	16.434	2250	2252	2260	rVB9	21414	34044	0.14%	0.042%
26	16.645	2284	2288	2299	rVB	116370	170437	0.69%	0.210%
27	16.857	2321	2324	2330	rVB5	20512	28855	0.12%	0.036%
28	17.210	2380	2384	2389	rBV4	23646	37740	0.15%	0.047%
29	17.357	2405	2409	2416	rBV	61558	90018	0.37%	0.111%
30	17.422	2416	2420	2424	rBV3	45091	63796	0.26%	0.079%
31	17.481	2424	2430	2435	rBV	1791364	2623794	10.67%	3.236%
32	17.522	2435	2437	2441	rVV	108209	140943	0.57%	0.174%
33	17.581	2441	2447	2455	rVB2	1700405	2414670	9.82%	2.979%
34	18.228	2553	2557	2562	rBV5	33925	46288	0.19%	0.057%
35	18.286	2562	2567	2572	rBV	236416	315314	1.28%	0.389%
36	18.345	2572	2577	2583	rBV	1539667	1912904	7.78%	2.360%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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	rBV3	47587	99212	0.40%	0.122%
38	18.675	2630	2633	2638	rVV6	24673	44856	0.18%	0.055%
39	18.828	2655	2659	2663	rBV5	34848	82169	0.33%	0.101%
40	18.980	2683	2685	2690	rBV5	34711	52704	0.21%	0.065%
41	19.222	2723	2726	2730	rVB2	54930	55983	0.23%	0.069%
42	19.428	2758	2761	2763	rBV2	116541	144723	0.59%	0.179%
43	19.451	2763	2765	2766	rVV	146059	135810	0.55%	0.168%
44	19.480	2766	2770	2776	rVB	492435	680374	2.77%	0.839%
45	19.563	2780	2784	2791	rBV	484685	681791	2.77%	0.841%
46	19.804	2819	2825	2835	rBV2	2531952	3802302	15.46%	4.690%
47	20.610	2959	2962	2967	rBV5	105393	139983	0.57%	0.173%
48	20.780	2988	2991	2994	rBV2	88973	105371	0.43%	0.130%
49	21.245	3065	3070	3082	rVB3	659659	1142262	4.64%	1.409%
50	21.439	3101	3103	3109	rVB2	136546	160542	0.65%	0.198%
51	21.563	3118	3124	3129	rBV	2216726	3484925	14.17%	4.299%
52	22.163	3224	3226	3229	rVV	168201	181915	0.74%	0.224%
53	22.204	3230	3233	3242	rVB2	336959	615589	2.50%	0.759%
54	22.963	3359	3362	3366	rVB	197608	249842	1.02%	0.308%
55	23.280	3411	3416	3421	rBV	799271	1230996	5.01%	1.518%
56	23.945	3522	3529	3535	rBV2	1514084	3047226	12.39%	3.759%
57	24.110	3550	3557	3564	rBV	1253124	2669379	10.85%	3.293%
58	24.727	3657	3662	3673	rVB	710137	1549382	6.30%	1.911%
59	26.192	3905	3911	3925	rVB2	672170	1852650	7.53%	2.285%
60	26.715	3994	4000	4024	rVB2	596674	2831512	11.51%	3.493%
61	27.798	4175	4184	4204	rVB3	847565	3812295	15.50%	4.703%
62	28.868	4351	4366	4383	rVB2	5596792	24592813	100.00%	30.336%

Sum of corrected areas: 81069314

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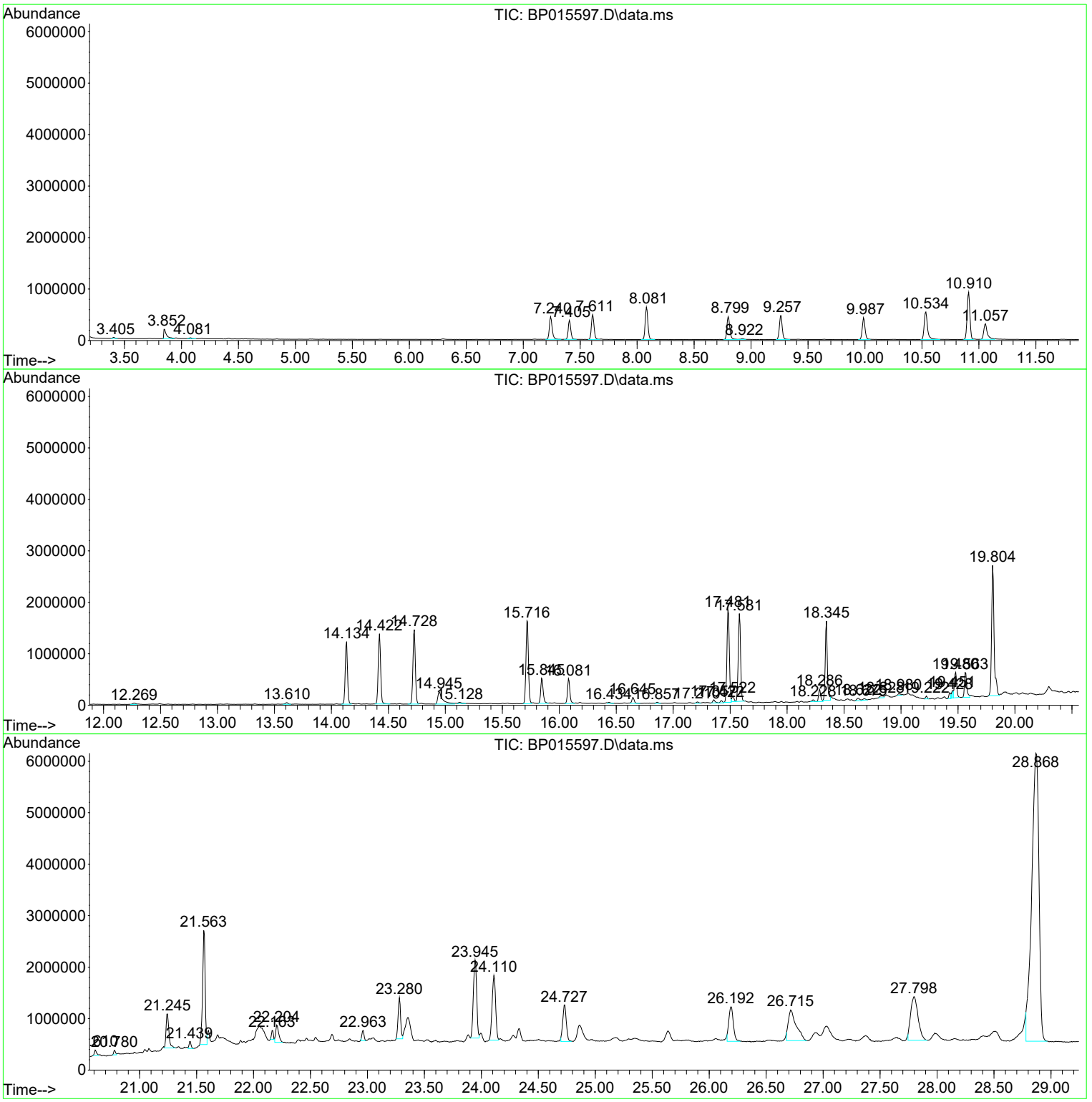
Misc :
ALS Vial : 28 Sample Multiplier: 1

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\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

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

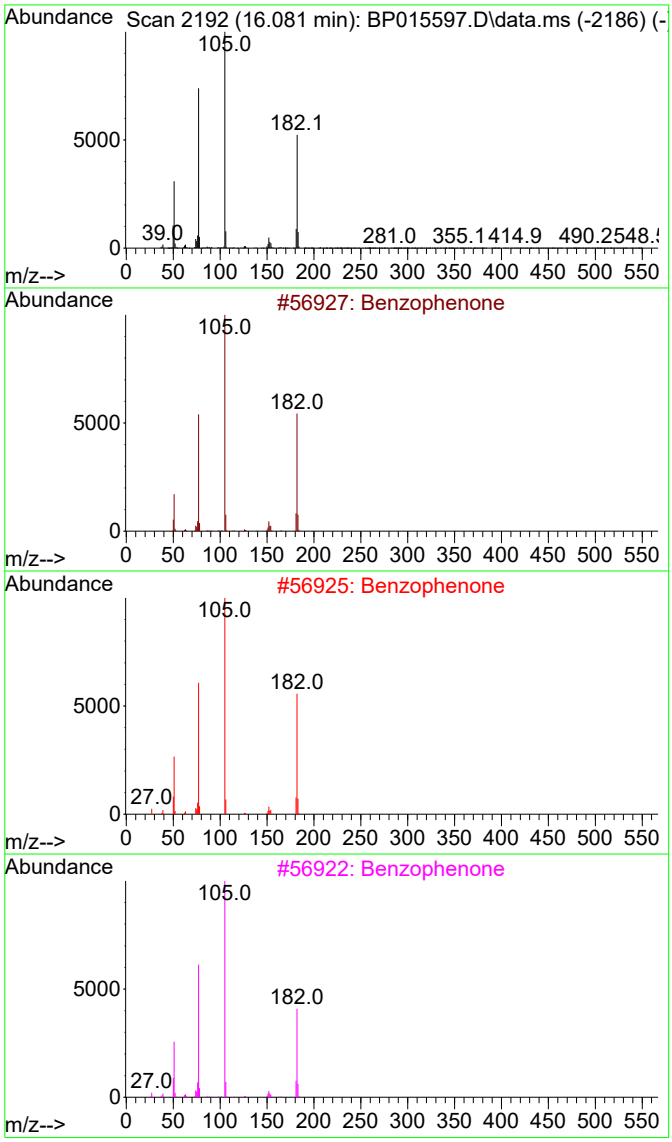
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

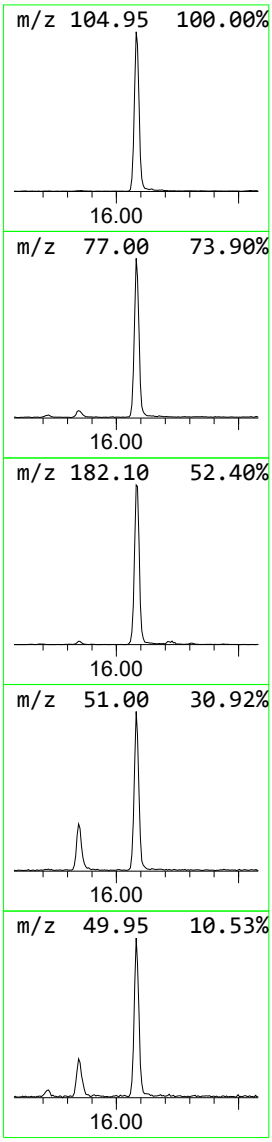
****

Peak Number 1 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.081	6.31 ng/ul	681042	Acenaphthene-d10	14.728

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	91
5	Benzophenone	182	C13H10O	000119-61-9	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

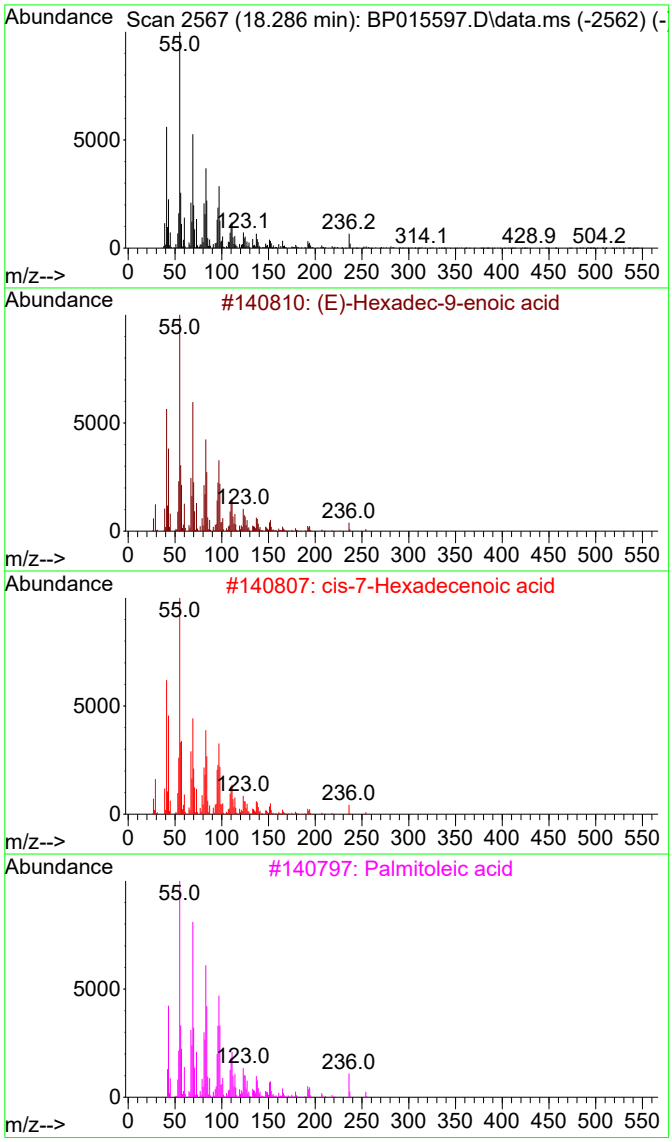
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

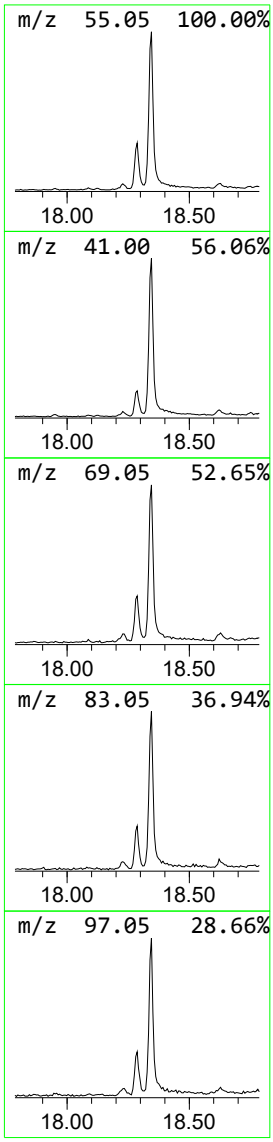
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	2.40 ng/ul	315314	Phenanthrene-d10	17.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	98
2	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	97
3	Palmitoleic acid	254	C16H30O2	000373-49-9	94
4	Erucic acid	338	C22H42O2	000112-86-7	93
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

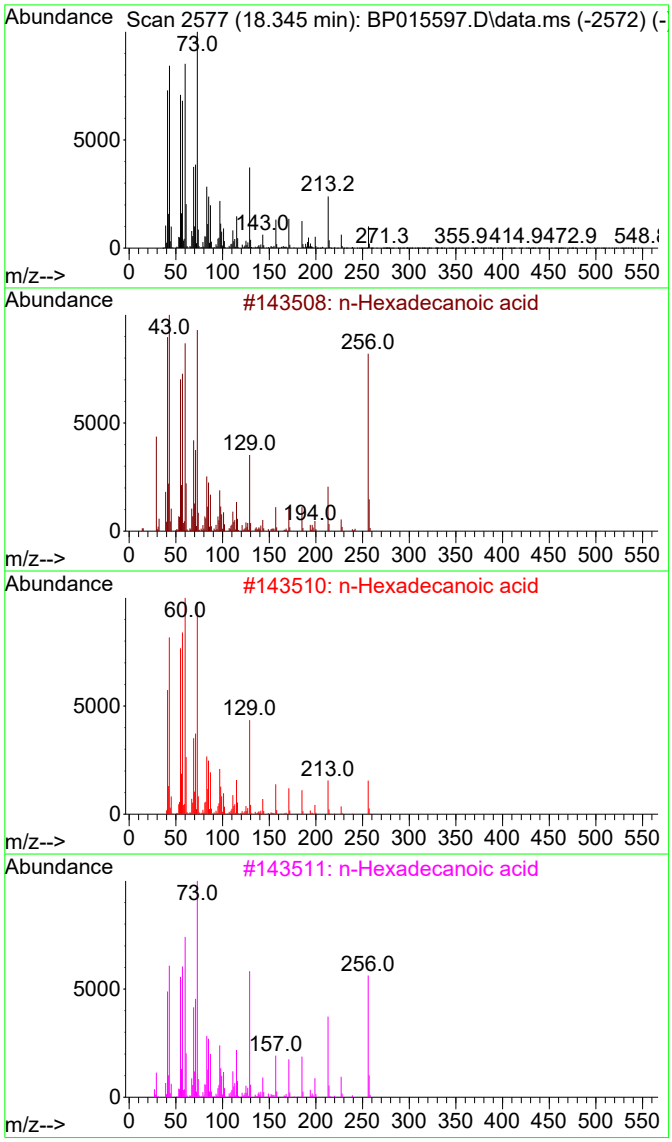
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

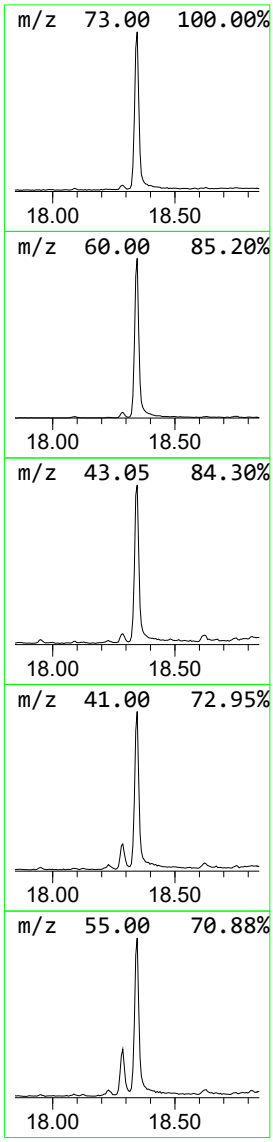
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	14.58 ng/ul	1912900	Phenanthrene-d10	17.481

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	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

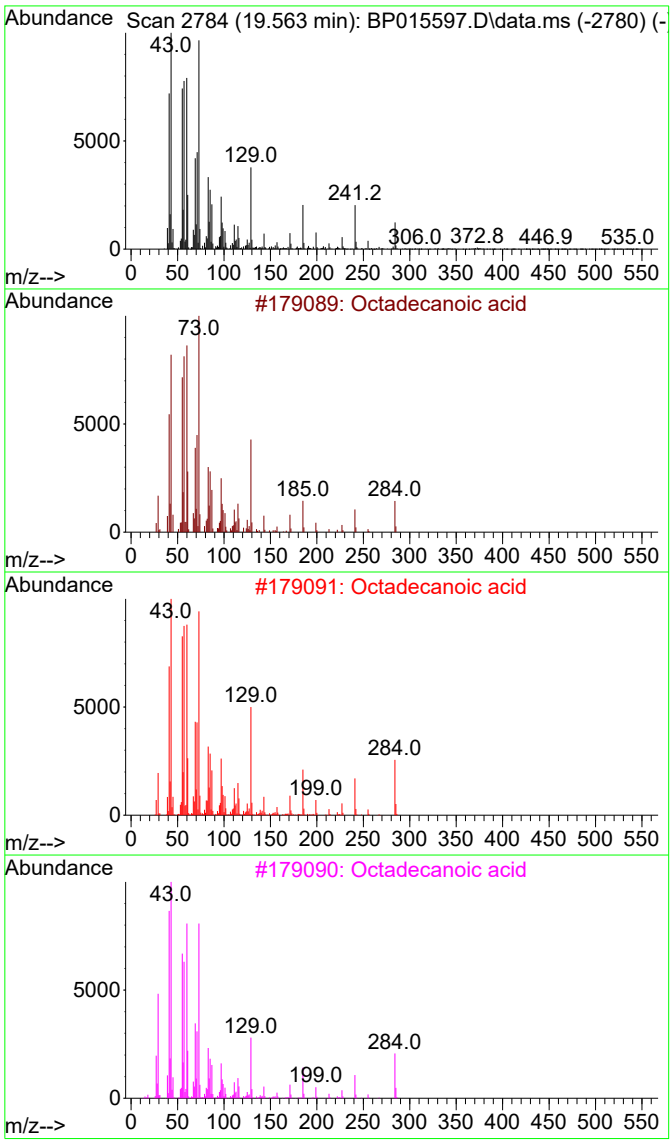
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

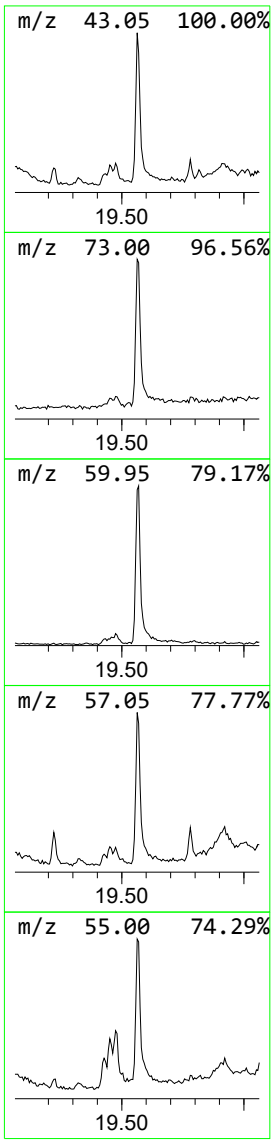
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.563	3.91 ng/ul	681791	Chrysene-d12	21.563

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

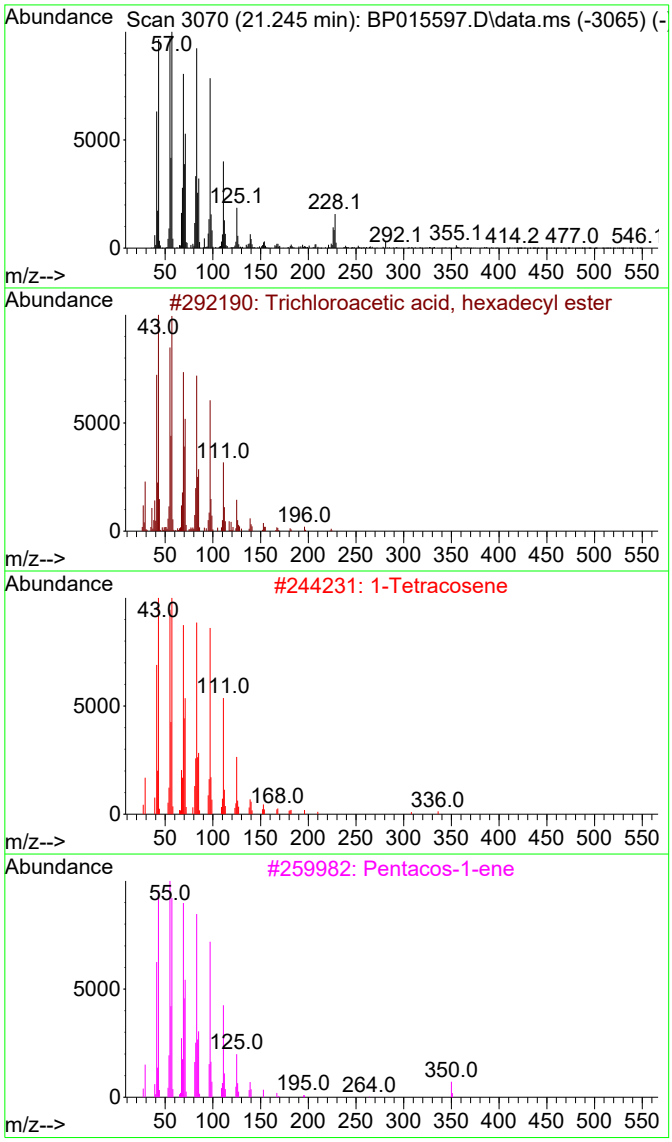
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

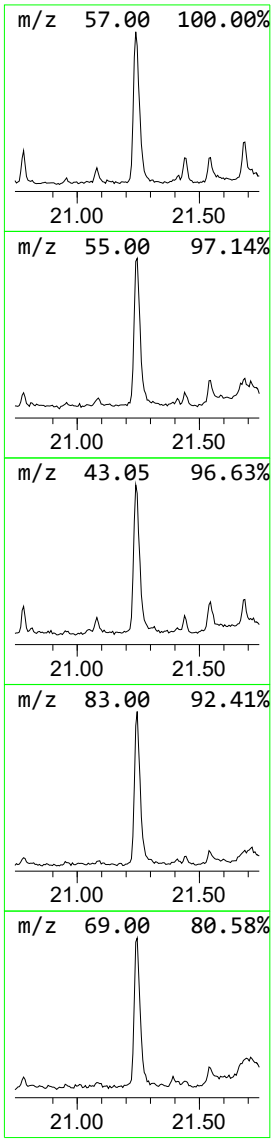
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	6.56 ng/ul	1142260	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Tetracosene	336	C24H48	010192-32-2	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	Heptacos-1-ene	378	C27H54	015306-27-1	94
5	1-Tricosene	322	C23H46	018835-32-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

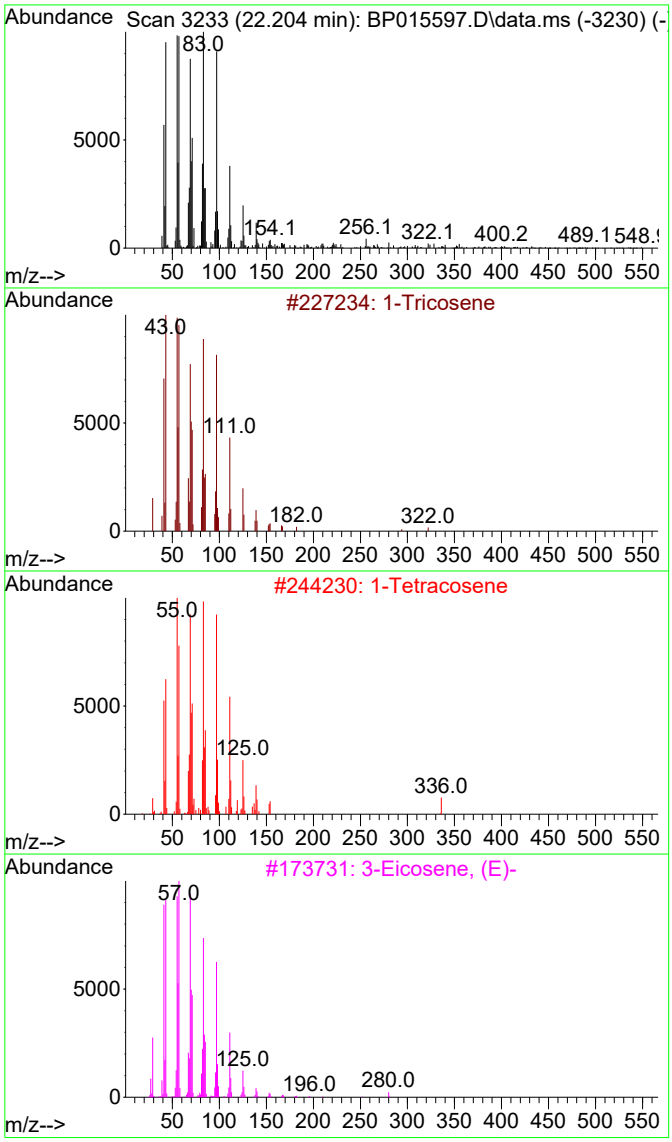
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

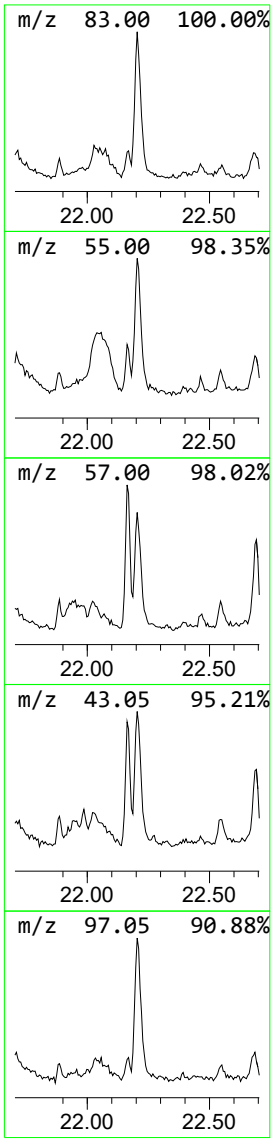
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.204	3.53 ng/ul	615589	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	99
2	1-Tetracosene	336	C24H48	010192-32-2	99
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
4	1-Docosene	308	C22H44	001599-67-3	96
5	Cyclohexadecane	224	C16H32	000295-65-8	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFH8

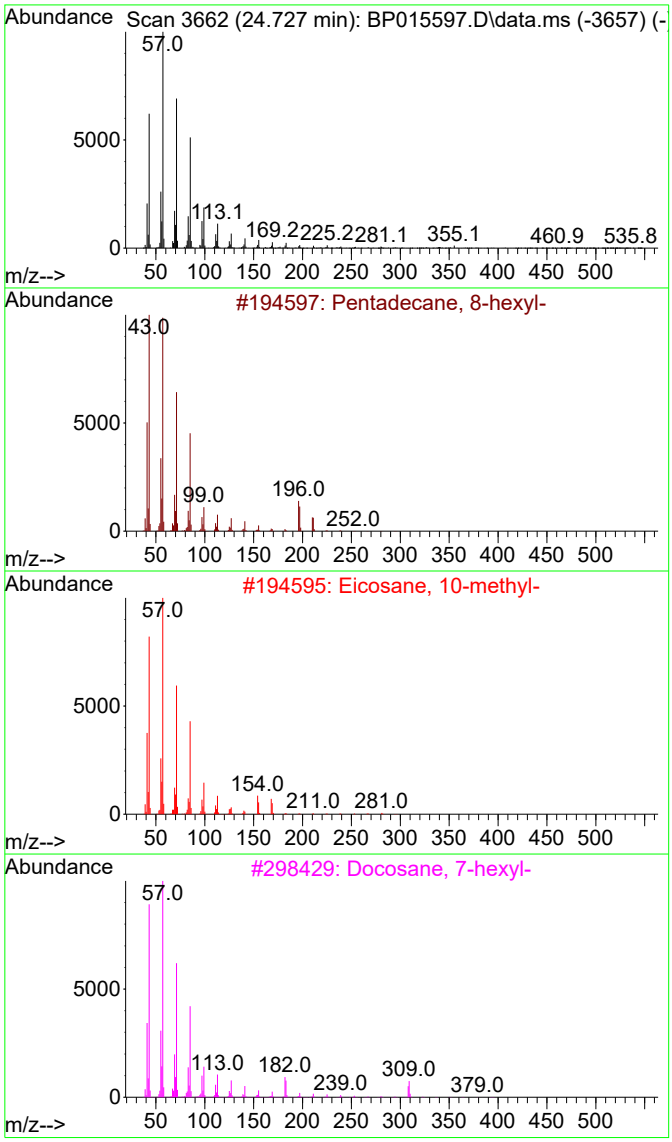
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

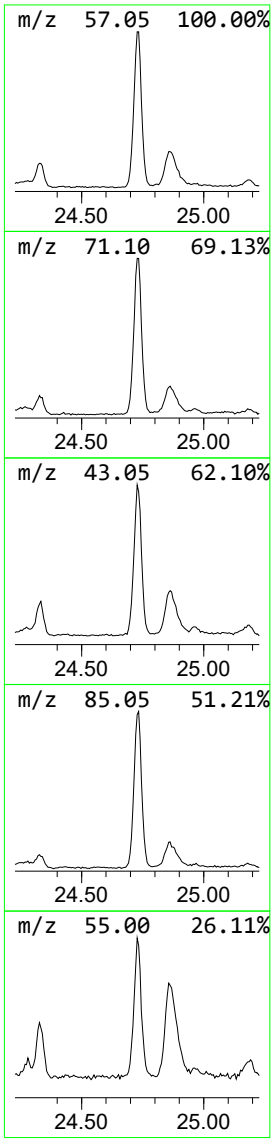
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.727	11.61 ng/ul	1549380	Perylene-d12	24.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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

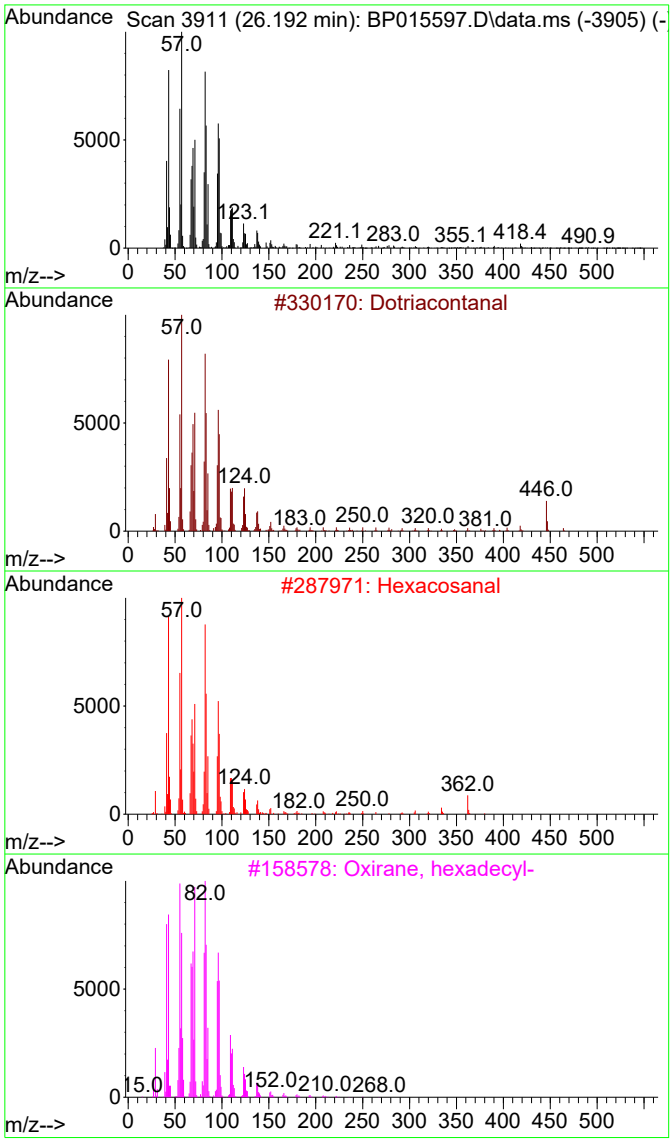
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

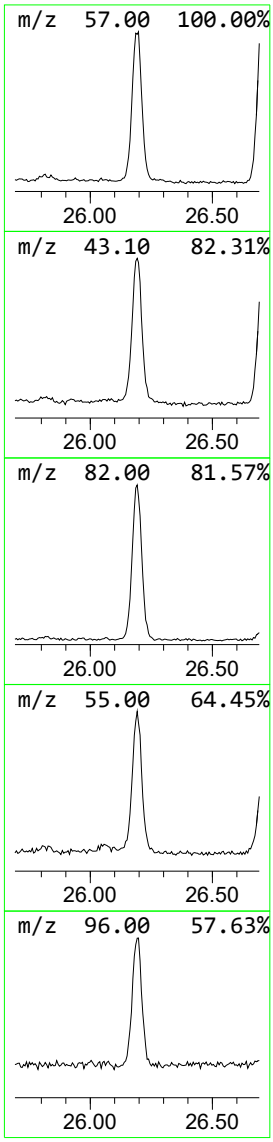
****

Peak Number 8 Dotriacontanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.192	13.88 ng/ul	1852650	Perylene-d12	24.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontanal	464	C32H64O	057878-00-9	91
2	Hexacosanal	380	C26H52O	026627-85-0	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90





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Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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

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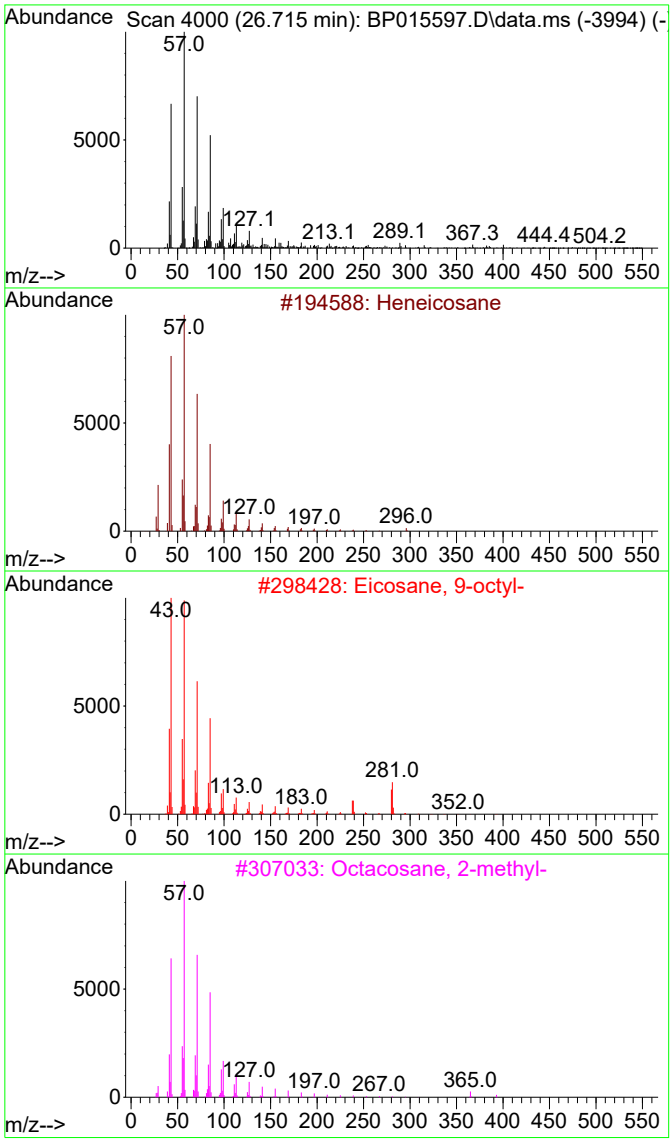
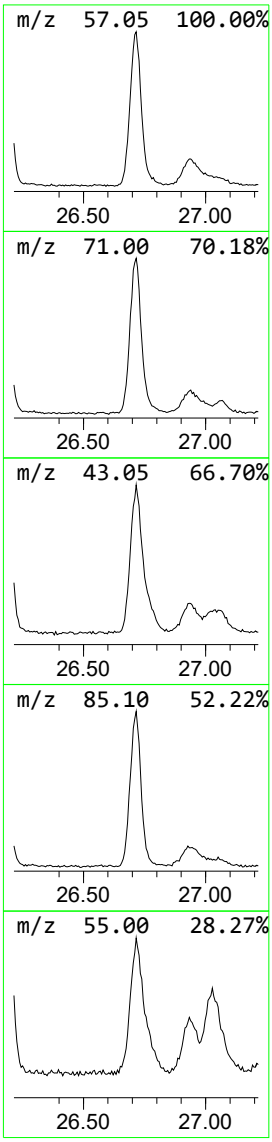
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.715	21.21 ng/ul	2831510	Perylene-d12	24.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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

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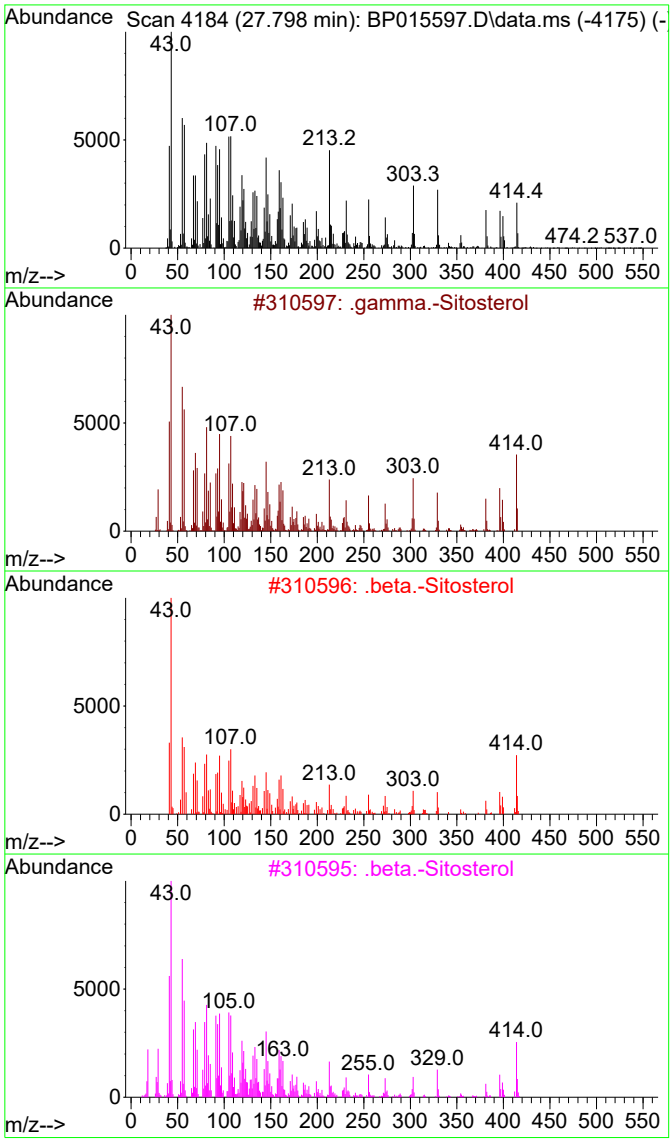
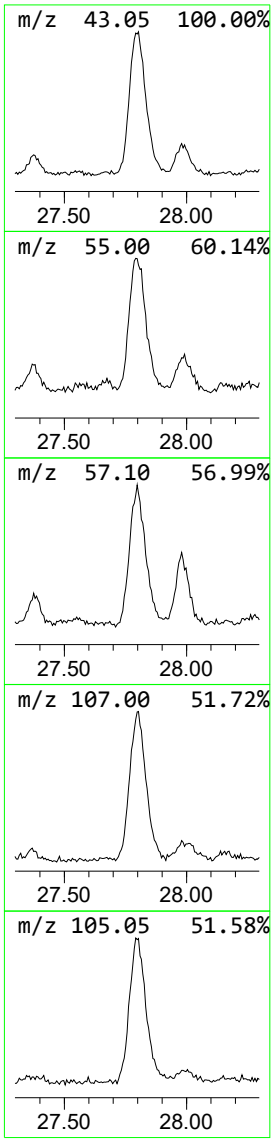
Peak Number 10 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.798	28.56 ng/ul	3812300	Perylene-d12	24.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	93
4	Campesterol	400	C28H48O	000474-62-4	49
5	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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

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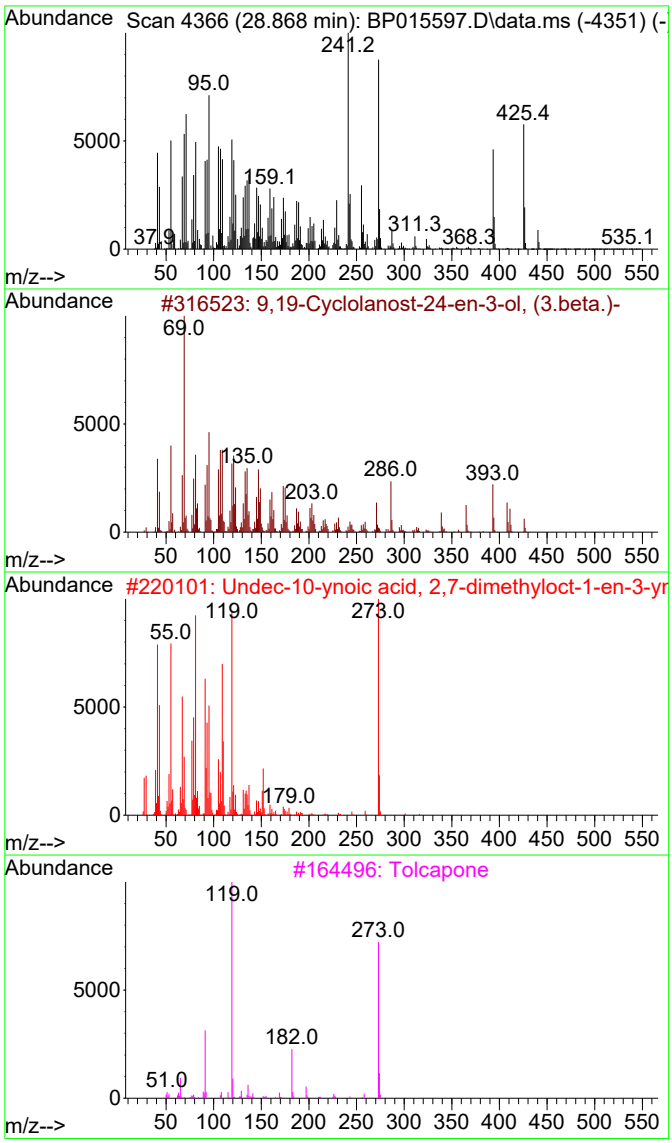
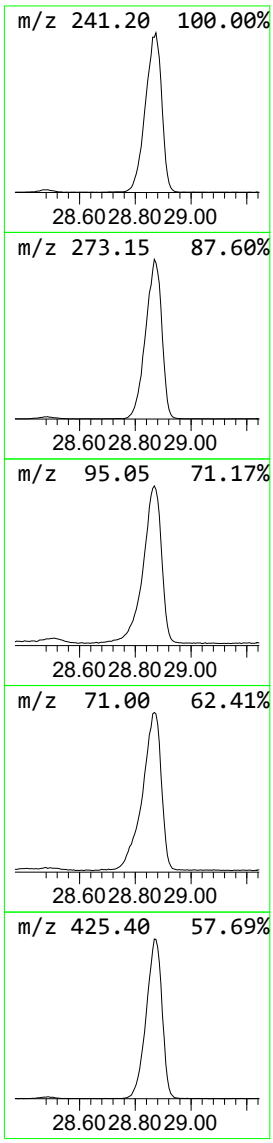
Peak Number 11 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.868	184.26 ng/ul	24592800	Perylene-d12	24.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3....	426	C30H50O	000469-38-5	25
2	Undec-10-ynoic acid, 2,7-dimethy...	316	C21H32O2	1000406-96-7	22
3	Tolcapone	273	C14H11NO5	134308-13-7	15
4	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	15
5	3-Bromo-4-hydroxy-5-methoxypheny...	241	C9H8BrNO2	081038-44-0	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061623\
Data File : BP015597.D
Acq On : 17 Jun 2023 00:49
Operator : MA/JU
Sample : 03080-09
Misc :
ALS Vial : 28 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	16.081	6.3	ng/ul	681042	3	14.728	2159100	20.0
(E)-Hexadec-9-e...	18.286	2.4	ng/ul	315314	4	17.481	2623790	20.0
n-Hexadecanoic ...	18.345	14.6	ng/ul	1912900	4	17.481	2623790	20.0
Octadecanoic acid	19.563	3.9	ng/ul	681791	5	21.563	3484930	20.0
Trichloroacetic...	21.245	6.6	ng/ul	1142260	5	21.563	3484930	20.0
(DEL) Alkane: S...	22.204	3.5	ng/ul	615589	5	21.563	3484930	20.0
(DEL) Alkane: S...	24.727	11.6	ng/ul	1549380	6	24.110	2669380	20.0
Dotriacontanal	26.192	13.9	ng/ul	1852650	6	24.110	2669380	20.0
(DEL) Alkane: S...	26.715	21.2	ng/ul	2831510	6	24.110	2669380	20.0
.gamma.-Sitosterol	27.798	28.6	ng/ul	3812300	6	24.110	2669380	20.0
unknown-01	28.868	184.3	ng/ul	24592800	6	24.110	2669380	20.0