LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXW3

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-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	21	25	35	rVB	121592	165458	0.39%	0.101%
2	3.764	95	98	113	rBV	918464	1306334	3.09%	0.800%
3	4.087	149	153	159	rVB	41209	56751	0.13%	0.035%
4	5.040	309	315	322	rVB2	55329	94906	0.22%	0.058%
5	5.264	348	353	359	rVB	26001	47516	0.11%	0.029%
6	7.105	659	666	676	rVB	1746077	2754664	6.51%	1.688%
7	7.269	688	694	703	rBV	1439836	2257519	5.33%	1.383%
8	7.475	722	729	738	rBV	1895124	2902921	6.86%	1.779%
9	7.946	801	809	816	rBV	2271002	3529283	8.34%	2.162%
10	8.658	922	930	939	rBV	1913173	3062681	7.24%	1.876%
11	9.111	1000	1007	1017	rBV	1678285	2763387	6.53%	1.693%
12	9.510	1071	1075	1082	rVB	45843	74751	0.18%	0.046%
13	9.840	1123	1131	1146	rBV	1356160	2320062	5.48%	1.421%
14	10.375	1215	1222	1235	rBV	2030072	3504622	8.28%	2.147%
15	10.757	1278	1287	1295	rBV	2930343	4886302	11.55%	2.994%
16	10.899	1304	1311	1323	rBV	1532237	2744917	6.49%	1.682%
17	12.340	1552	1556	1560	rBV	34704	49804	0.12%	0.031%
18	13.404	1728	1737	1742	rBV3	55328	101371	0.24%	0.062%
19	13.993	1829	1837	1846	rBV	3256092	4481339	10.59%	2.746%
20	14.110	1852	1857	1863	rBV7	31545	50284	0.12%	0.031%
21	14.175	1863	1868	1872	rBV	41606	60137	0.14%	0.037%
22	14.281	1879	1886	1898	rVV	3815233	5535841	13.08%	3.392%
23	14.475	1915	1919	1925	rVB	32809	46713	0.11%	0.029%
24	14.587	1931	1938	1945	rBV	3856805	5696932	13.46%	3.490%
25	14.793	1967	1973	1991	rBV	730590	1300711	3.07%	0.797%
26	14.993	2002	2007	2012	rVB4	45622	73030	0.17%	0.045%
27	15.581	2100	2107	2114	rBV	4659213	6523551	15.42%	3.997%
28	15.704	2121	2128	2139	rBV	789153	1149521	2.72%	0.704%
29	15.945	2158	2169	2179	rBV	3182019	4225237	9.98%	2.589%
30	16.451	2248	2255	2260	rBV10	24538	65006	0.15%	0.040%
31	16.516	2261	2266	2274	rVV	169124	249990	0.59%	0.153%
32	16.728	2298	2302	2309	rBV7	54540	95684	0.23%	0.059%
33	17.228	2383	2387	2391	rBV3	65826	98335	0.23%	0.060%
34	17.345	2401	2407	2417	rVV	4251307	6059488	14.32%	3.712%
35	17.445	2417	2424	2432	rVV	4247687	5952595	14.07%	3.647%
36	17.698	2464	2467	2469	rBV4	40162	51625	0.12%	0.032%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

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-BP120722.M
Title : SVOA CALIBRATION

37	17.863	2492	2495	2500	rVB3	46356	60608	0.14%	0.037%
38	18.104	2533	2536	2540	rVB3	46175	48148	0.11%	0.029%
39	18.157	2541	2545	2550	rBV	217654	314146	0.74%	0.192%
40	18.216	2550	2555	2570	rVV	1361579	1995146	4.71%	1.222%
41	18.498	2600	2603	2607	rBV5	52803	86613	0.20%	0.053%
42	18.551	2608	2612	2616	rVV2	89890	144411	0.34%	0.088%
43	18.628	2622	2625	2629	rBV5	47636	93989	0.22%	0.058%
44	19.351	2738	2748	2753	rBV2	314799	805079	1.90%	0.493%
45	19.445	2761	2764	2772	rBV2	203847	292477	0.69%	0.179%
46	19.675	2798	2803	2815	rBV	5504091	7753906	18.32%	4.751%
47	21.128	3046	3050	3060	rBV	1373099	2038512	4.82%	1.249%
48	21.433	3097	3102	3107	rBV	5285720	6855072	16.20%	4.200%
49	23.751	3490	3496	3512	rVB2	4376427	9682120	22.88%	5.932%
50	23.916	3517	3524	3533	rVB2	3677461	7464456	17.64%	4.573%
51	24.527	3624	3628	3639	rVB	890340	1833816	4.33%	1.124%
52	27.462	4120	4127	4145	rVB2	1969473	7098706	16.78%	4.349%
53	28.509	4293	4305	4323	rVB2	10645763	42316277	100.00%	25.925%

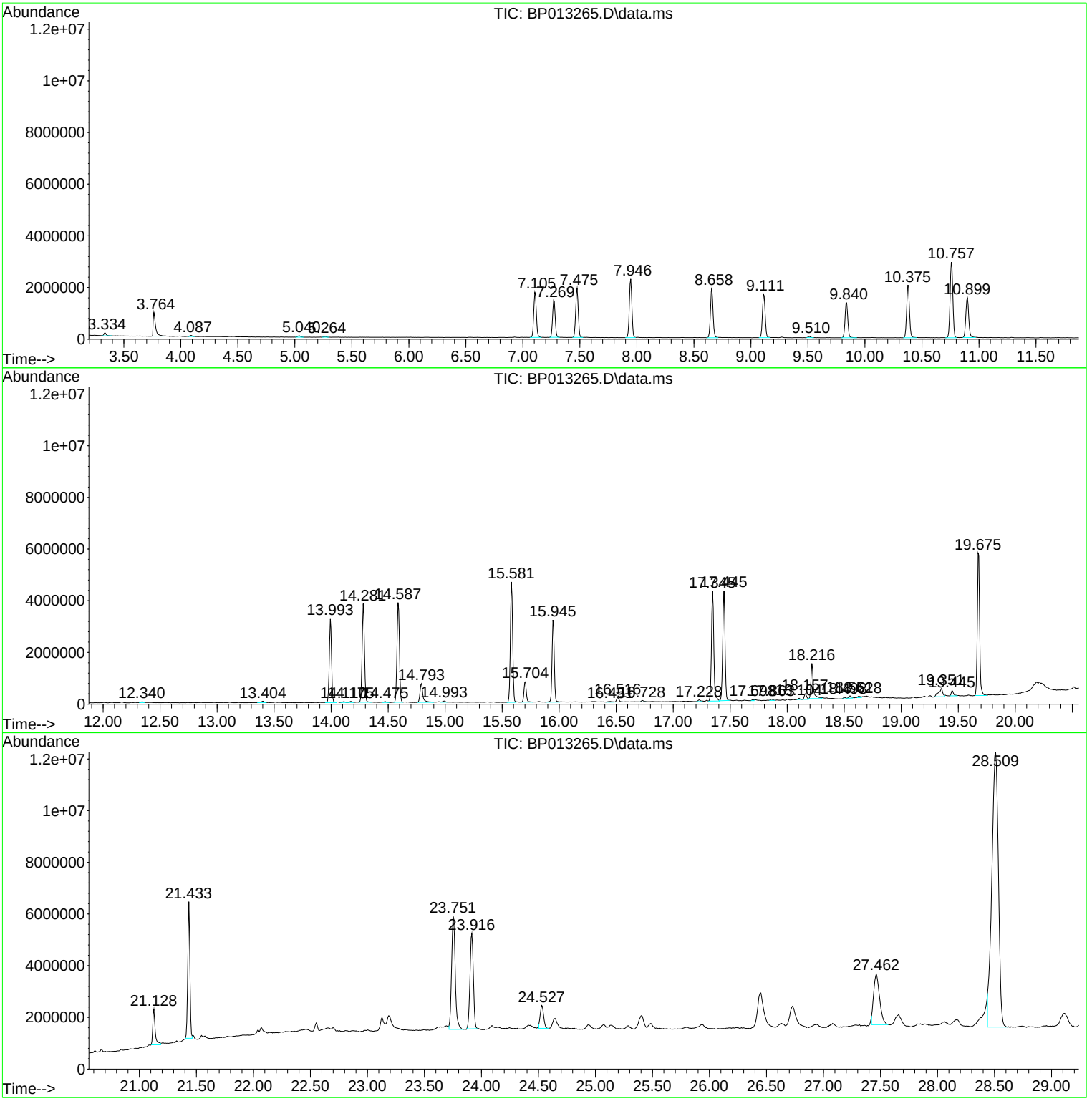
Sum of corrected areas: 163222750

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

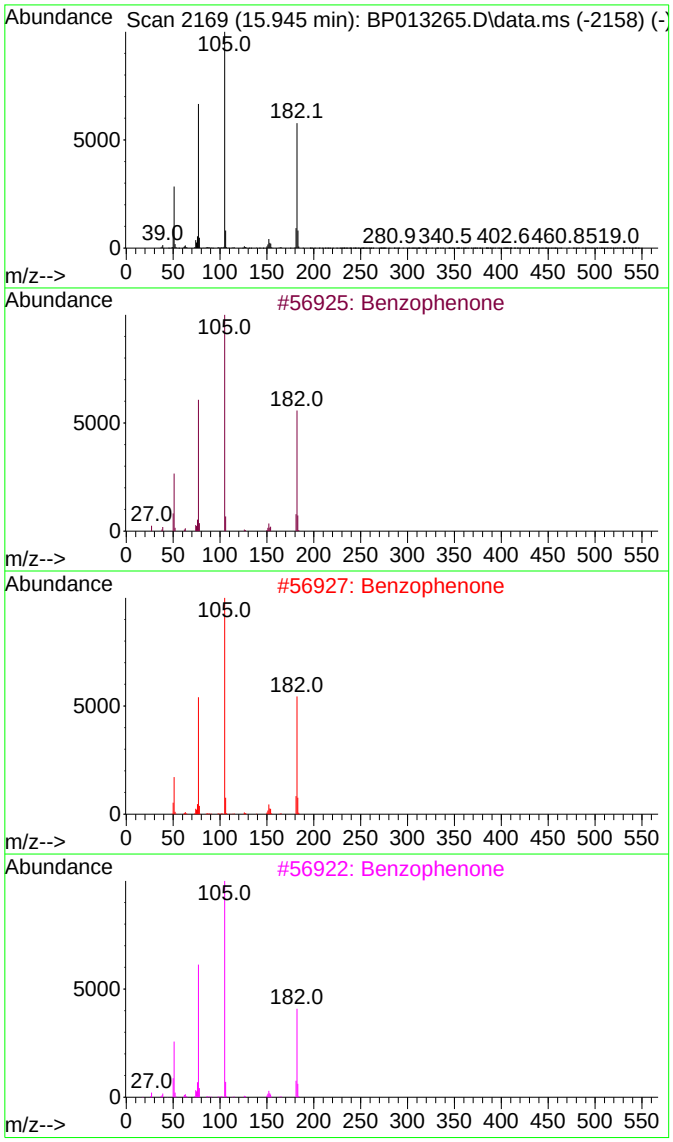
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

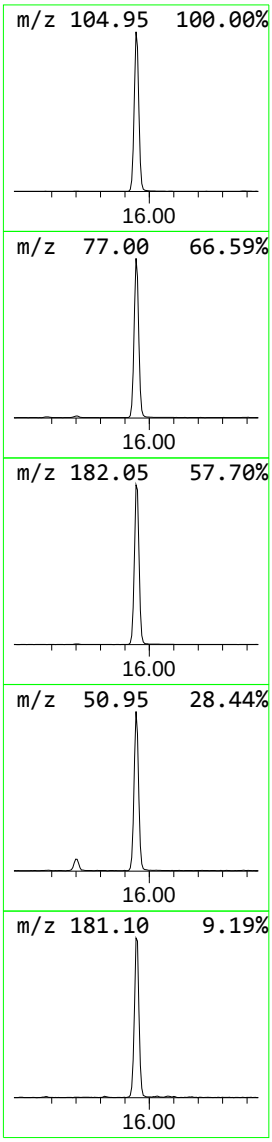
****

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	14.83 ng/ul	4225240	Acenaphthene-d10	14.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

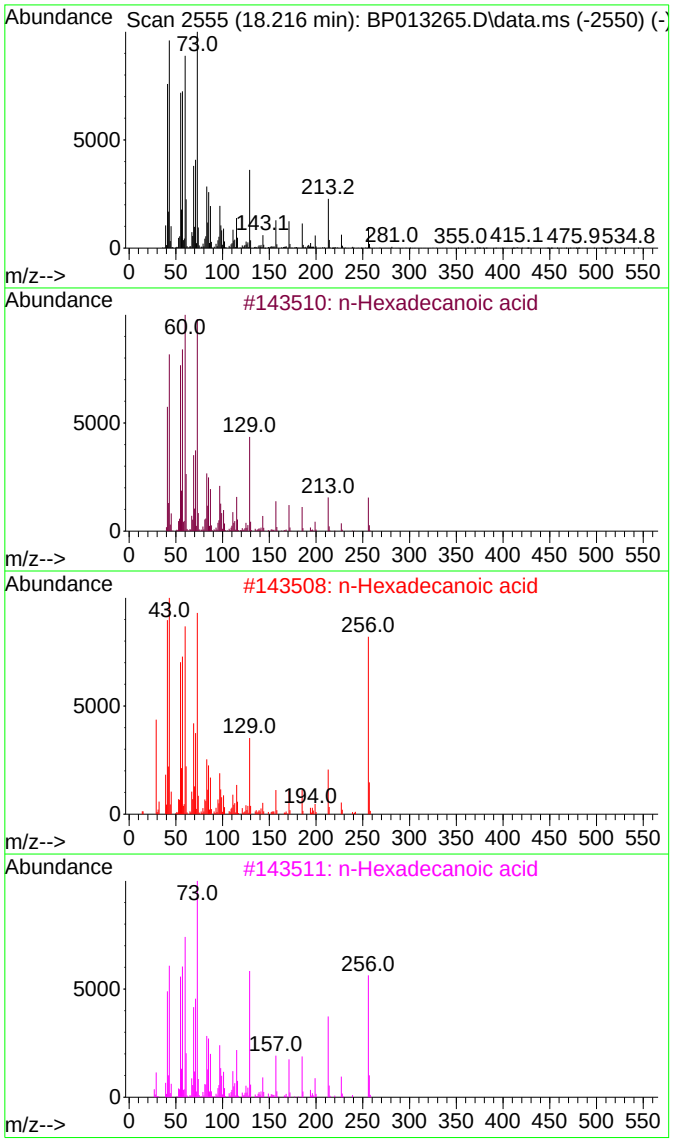
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

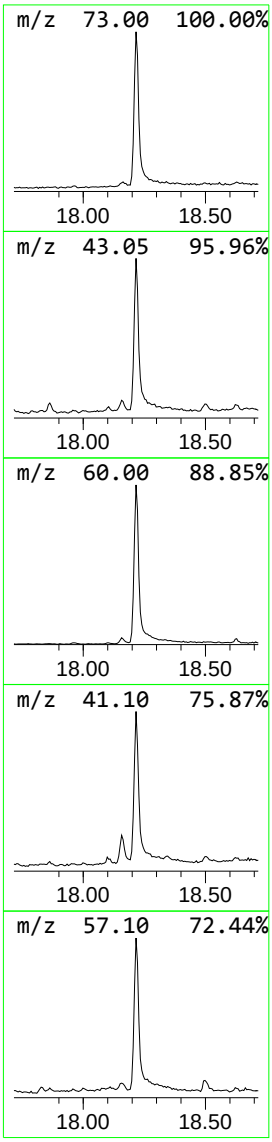
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	6.59 ng/ul	1995150	Phenanthrene-d10	17.345

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

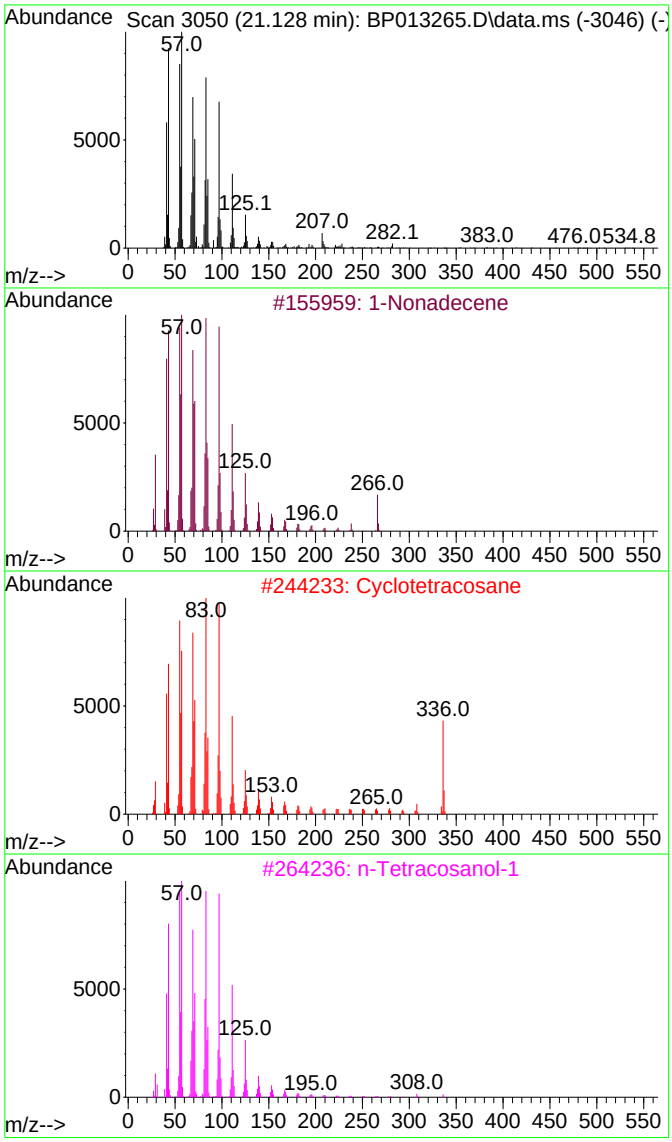
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

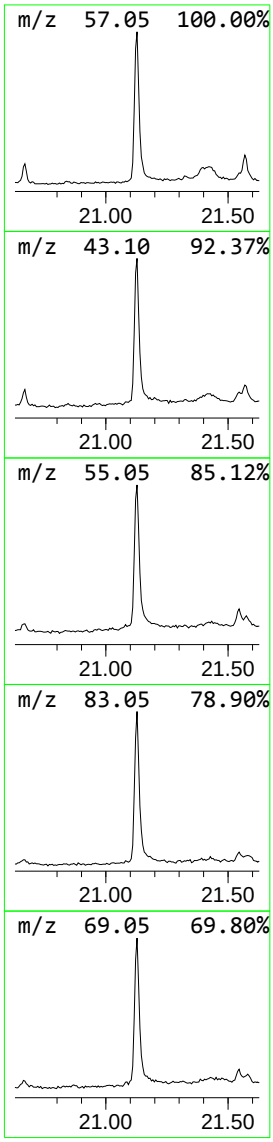
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	5.95 ng/ul	2038510	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Cyclotetracosane	336	C24H48	000297-03-0	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

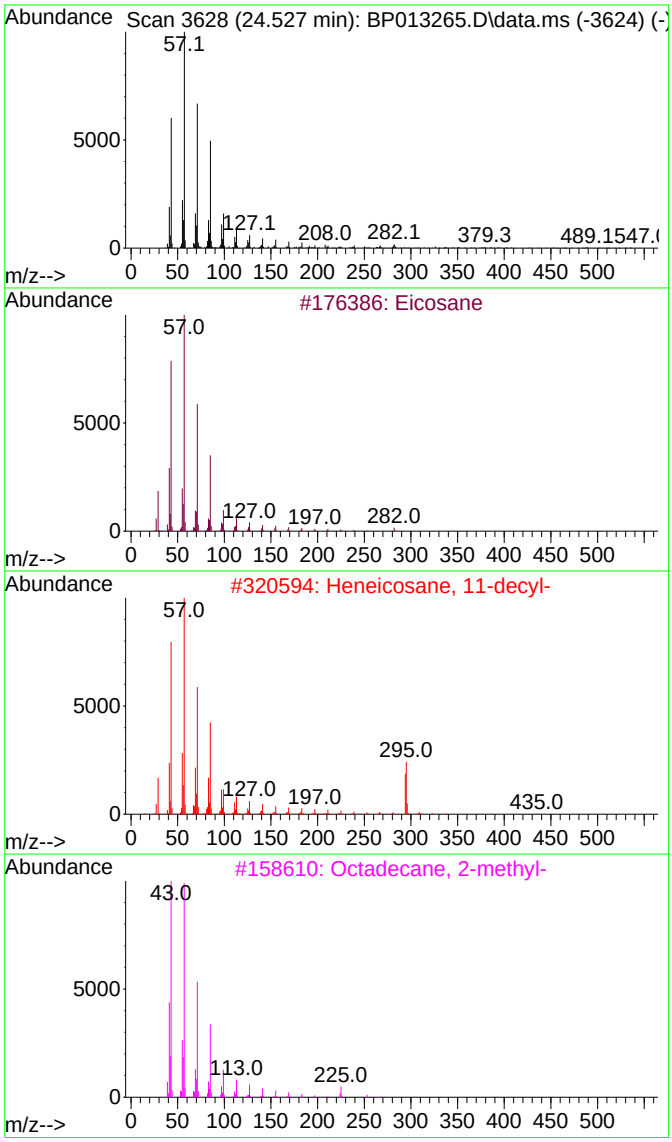
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

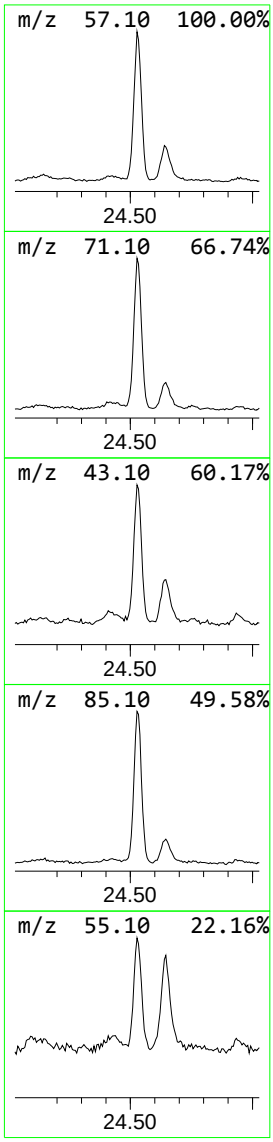
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.527	4.91 ng/ul	1833820	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4	2-Methylpentacosane	366	C26H54	000629-87-8	90
5	Tetracosane	338	C24H50	000646-31-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

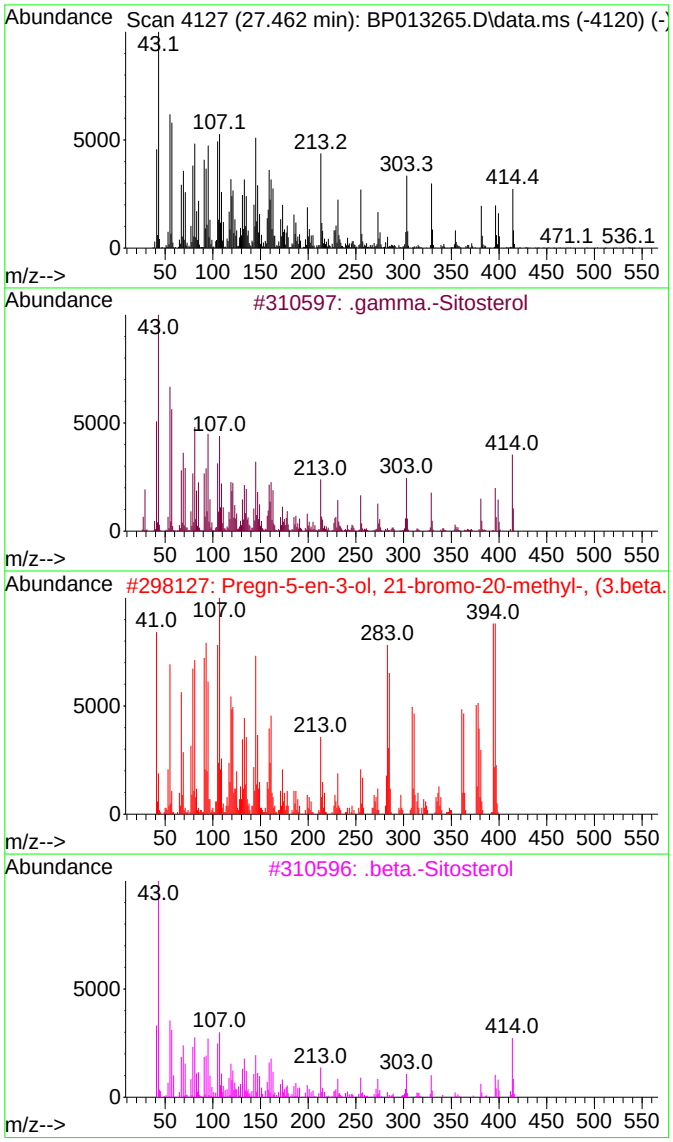
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

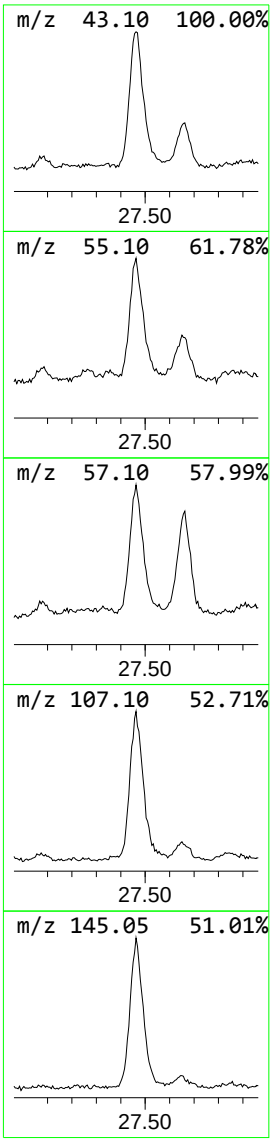
****

Peak Number 6 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.462	19.02 ng/ul	7098710	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	94
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	92
4	.beta.-Sitosterol	414	C29H50O	000083-46-5	70
5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

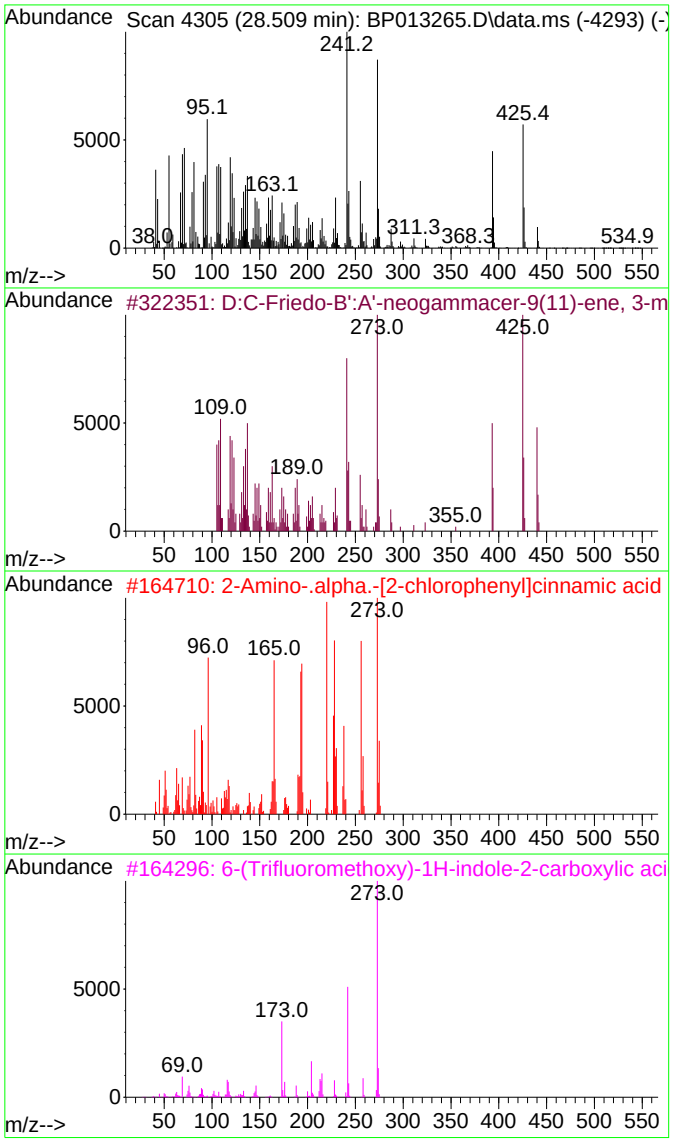
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

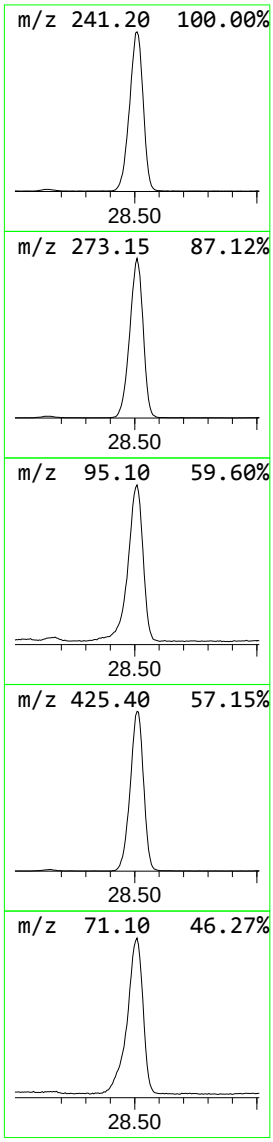
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	113.38 ng/ul	42316300	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	72
2	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
3	6-(Trifluoromethoxy)-1H-indole-2...	273	C12H10F3NO3	1000499-75-7	25
4	Phenol, 2,6-dimethyl-, phosphite...	394	C24H27O3P	052830-49-6	25
5	2-{[(4-Methyl-2-pyridinyl)amino]...	256	C13H16N4Si	1010494-07-4	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013265.D
Acq On : 23 Dec 2022 03:00
Operator : CG/JU
Sample : N6015-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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	15.945	14.8	ng/ul	4225240	3	14.587	5696930	20.0
n-Hexadecanoic ...	18.216	6.6	ng/ul	1995150	4	17.345	6059490	20.0
(DEL) Alkane: S...	21.128	6.0	ng/ul	2038510	5	21.433	6855070	20.0
(DEL) Alkane: S...	24.527	4.9	ng/ul	1833820	6	23.916	7464460	20.0
.gamma.-Sitosterol	27.462	19.0	ng/ul	7098710	6	23.916	7464460	20.0
D:C-Friedo-B':A...	28.509	113.4	ng/ul	42316300	6	23.916	7464460	20.0