LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

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: BP013260.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	30	rVB	131614	152525	0.39%	0.091%
2	3.764	95	98	114	rBV	1572981	2358320	5.97%	1.414%
3	4.087	150	153	161	rVB	55531	79371	0.20%	0.048%
4	5.040	309	315	320	rVB2	30061	53842	0.14%	0.032%
5	5.275	350	355	364	rVB3	21514	50290	0.13%	0.030%
6	7.105	660	666	677	rVB	2043945	3290823	8.33%	1.973%
7	7.275	688	695	703	rBV	1661640	2595916	6.57%	1.556%
8	7.475	722	729	737	rBV	2170644	3365644	8.52%	2.017%
9	7.946	801	809	816	rBV	2169512	3311843	8.39%	1.985%
10	8.658	922	930	940	rBV	2378522	3724572	9.43%	2.233%
11	9.116	1000	1008	1016	rBV	1926324	3148958	7.97%	1.888%
12	9.269	1030	1034	1043	rVB9	26723	46469	0.12%	0.028%
13	9.516	1070	1076	1080	rBV	45769	72017	0.18%	0.043%
14	9.840	1123	1131	1147	rBV	1607665	2681460	6.79%	1.607%
15	10.381	1215	1223	1235	rBV	2338532	4002916	10.14%	2.399%
16	10.758	1279	1287	1295	rBV	2714511	4452986	11.28%	2.669%
17	10.899	1303	1311	1332	rBV	1857555	3291825	8.34%	1.973%
18	12.340	1552	1556	1561	rBV	39068	61991	0.16%	0.037%
19	13.399	1727	1736	1742	rBV2	58112	110617	0.28%	0.066%
20	13.993	1828	1837	1846	rVV	3579041	4858535	12.30%	2.912%
21	14.110	1853	1857	1862	rVV8	28548	45213	0.11%	0.027%
22	14.175	1864	1868	1873	rVB	35781	43315	0.11%	0.026%
23	14.281	1879	1886	1902	rVB2	4125706	6034832	15.28%	3.617%
24	14.469	1916	1918	1924	rVB2	31698	41506	0.11%	0.025%
25	14.587	1927	1938	1947	rBV	3426141	4965208	12.57%	2.976%
26	14.787	1966	1972	1991	rBV	1088601	1892037	4.79%	1.134%
27	14.940	1995	1998	2002	rVV6	24679	40631	0.10%	0.024%
28	14.993	2003	2007	2013	rVB5	43612	66316	0.17%	0.040%
29	15.581	2100	2107	2120	rBV	4861966	7018100	17.77%	4.207%
30	15.698	2122	2127	2135	rBV	1023307	1422798	3.60%	0.853%
31	15.822	2145	2148	2154	rVB6	24738	41614	0.11%	0.025%
32	15.945	2159	2169	2181	rBV	2789286	3786223	9.59%	2.270%
33	16.516	2261	2266	2274	rVB	131380	193371	0.49%	0.116%
34	16.728	2299	2302	2311	rBV8	47334	84670	0.21%	0.051%
35	17.228	2383	2387	2392	rBV4	42475	59299	0.15%	0.036%
36	17.345	2401	2407	2417	rVV	3800308	5257947	13.31%	3.152%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

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	17.445	2417	2424	2432	rVV	4764729	6584282	16.67%	3.947%
38	17.698	2464	2467	2469	rBV3	32472	39801	0.10%	0.024%
39	18.157	2541	2545	2550	rBV3	99994	146897	0.37%	0.088%
40	18.216	2550	2555	2569	rBV	1150896	1707637	4.32%	1.024%
41	18.551	2608	2612	2618	rVB2	80913	122867	0.31%	0.074%
42	19.257	2729	2732	2737	rVB2	69636	85812	0.22%	0.051%
43	19.351	2737	2748	2753	rBV3	293001	847711	2.15%	0.508%
44	19.445	2761	2764	2772	rBV	219642	305091	0.77%	0.183%
45	19.675	2798	2803	2816	rBV	6404604	8836215	22.38%	5.297%
46	21.128	3046	3050	3061	rBV	1490837	2293704	5.81%	1.375%
47	21.433	3097	3102	3107	rBV	4907231	6299922	15.95%	3.776%
48	23.751	3490	3496	3512	rVB2	5090108	10999620	27.85%	6.593%
49	23.916	3517	3524	3531	rVB2	3280898	6828617	17.29%	4.093%
50	24.533	3624	3629	3637	rVB	859935	1815927	4.60%	1.088%
51	27.457	4119	4126	4148	rVB4	2068602	7721021	19.55%	4.628%
52	28.504	4292	4304	4319	rVB2	10050106	39491323	100.00%	23.672%

Sum of corrected areas: 166830447

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
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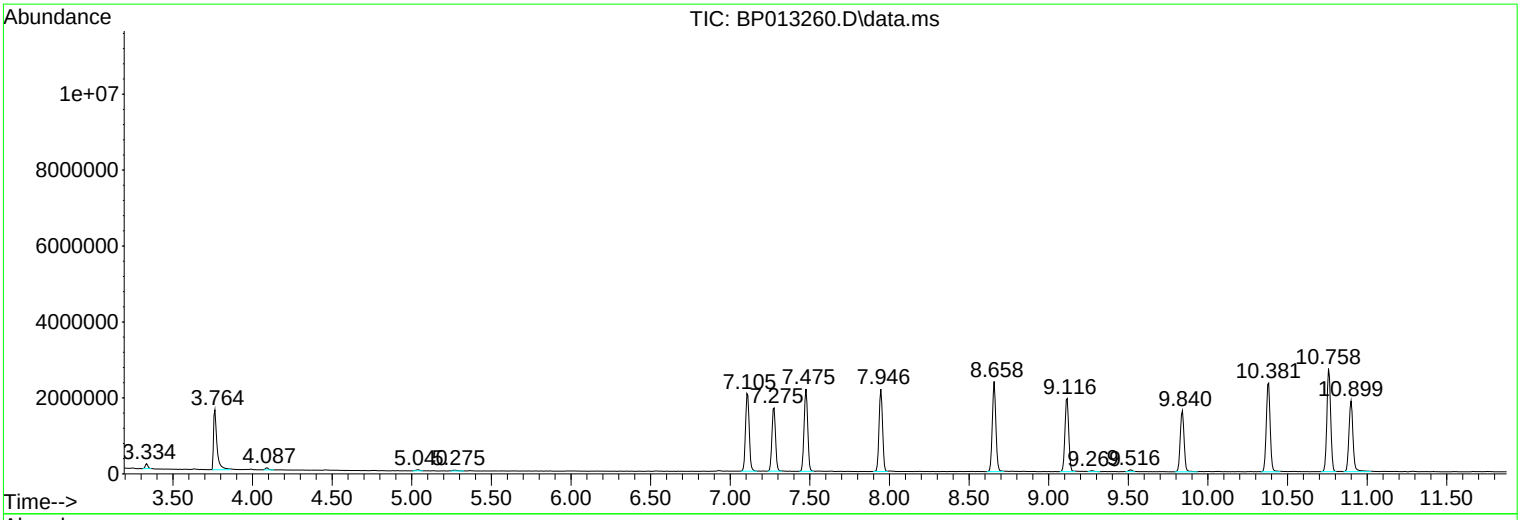
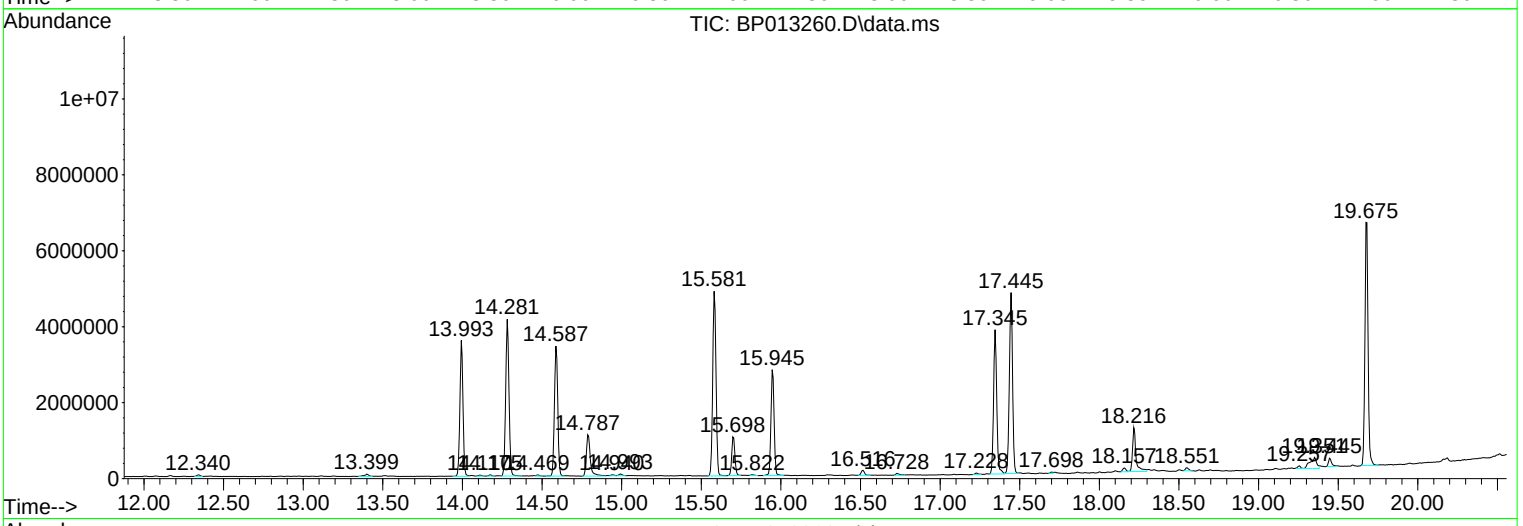
Misc :
ALS Vial : 27 Sample Multiplier: 1

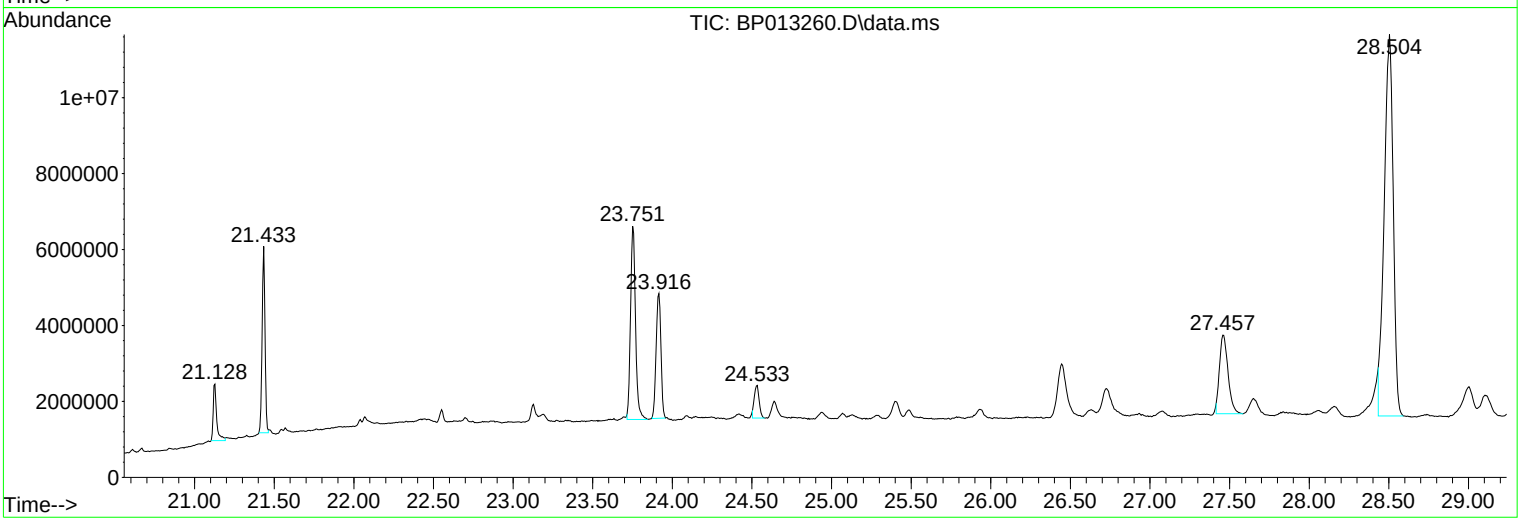
Instrument :
BNA_P
ClientSampleId :
DBXW5

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 : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

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

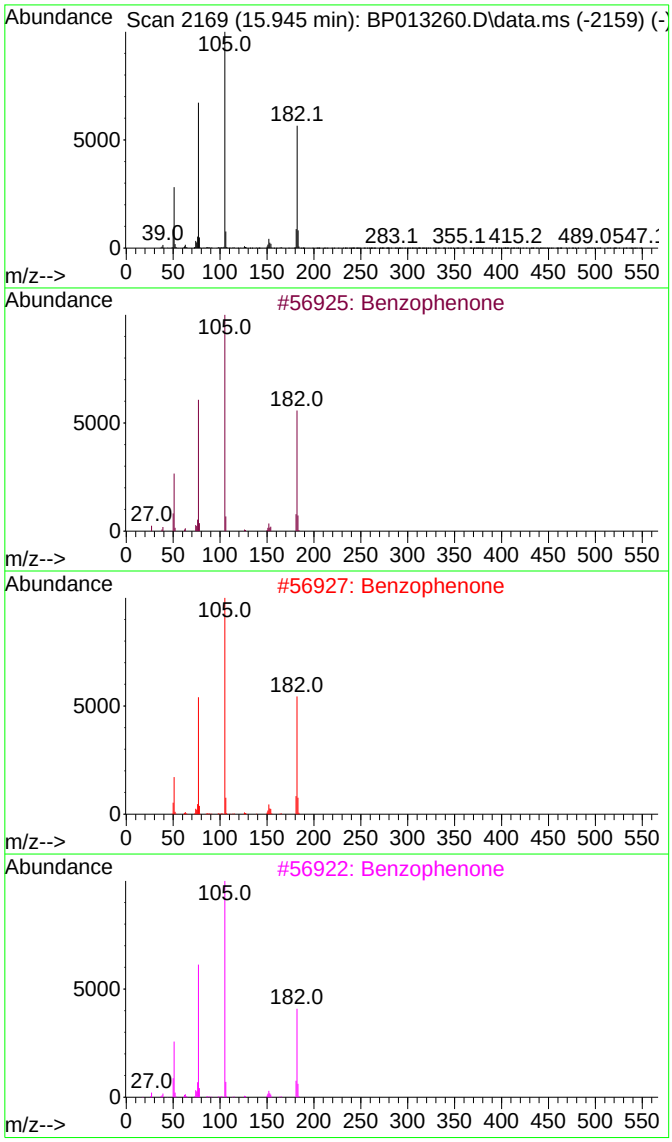
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

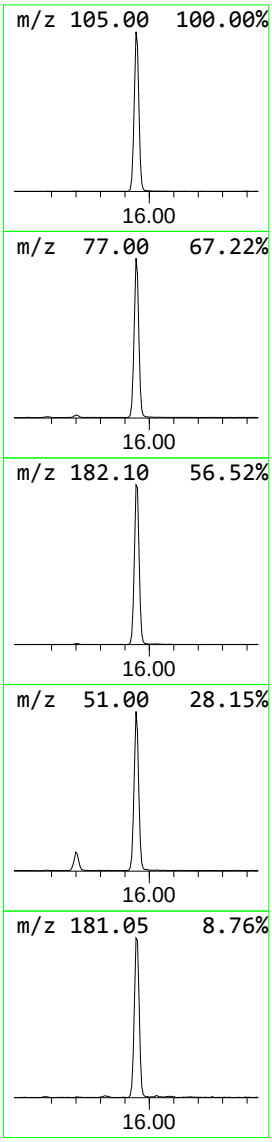
****

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	15.25 ng/ul	3786220	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 : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

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

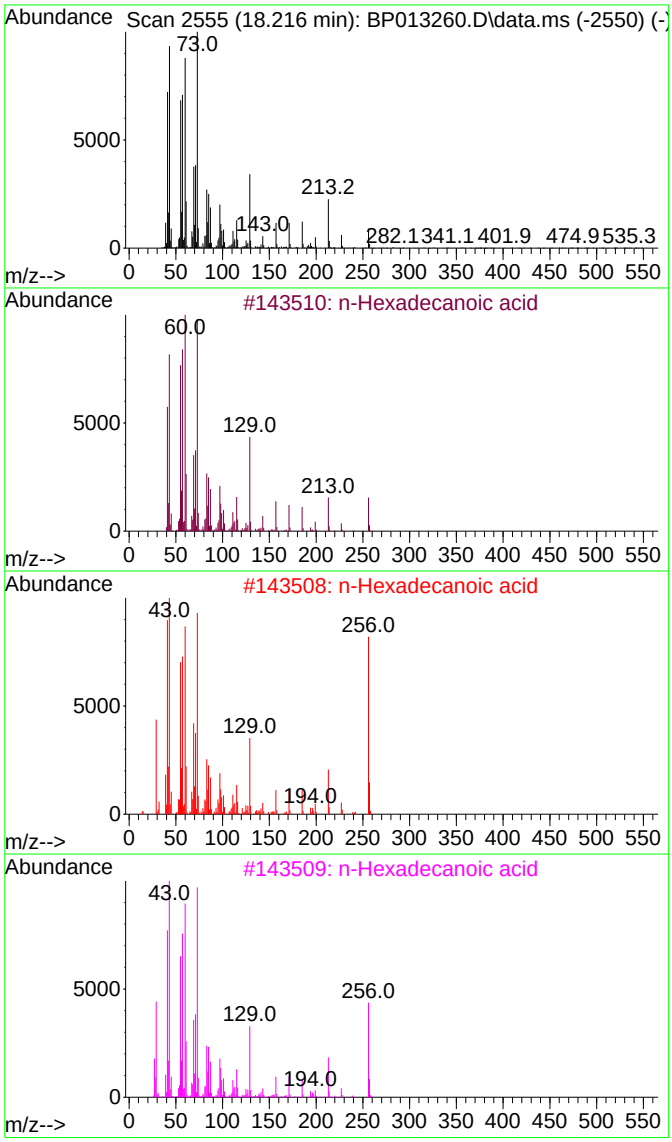
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

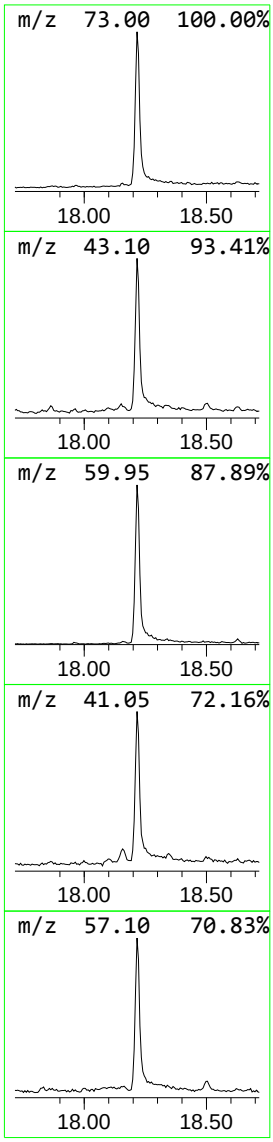
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	6.50 ng/ul	1707640	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	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

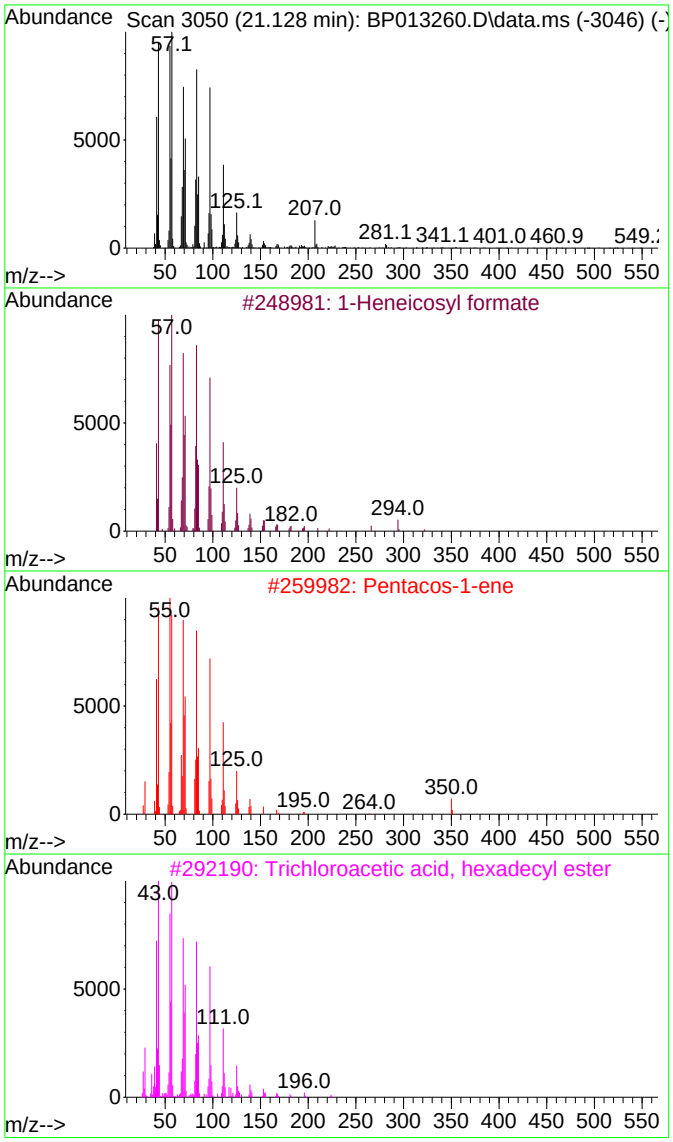
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

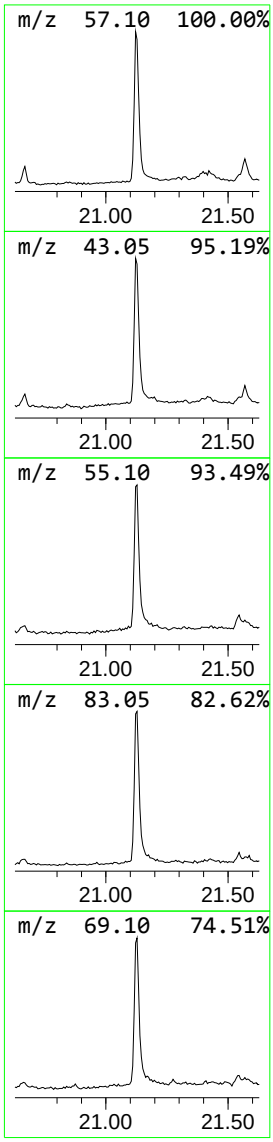
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	7.28 ng/ul	2293700	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

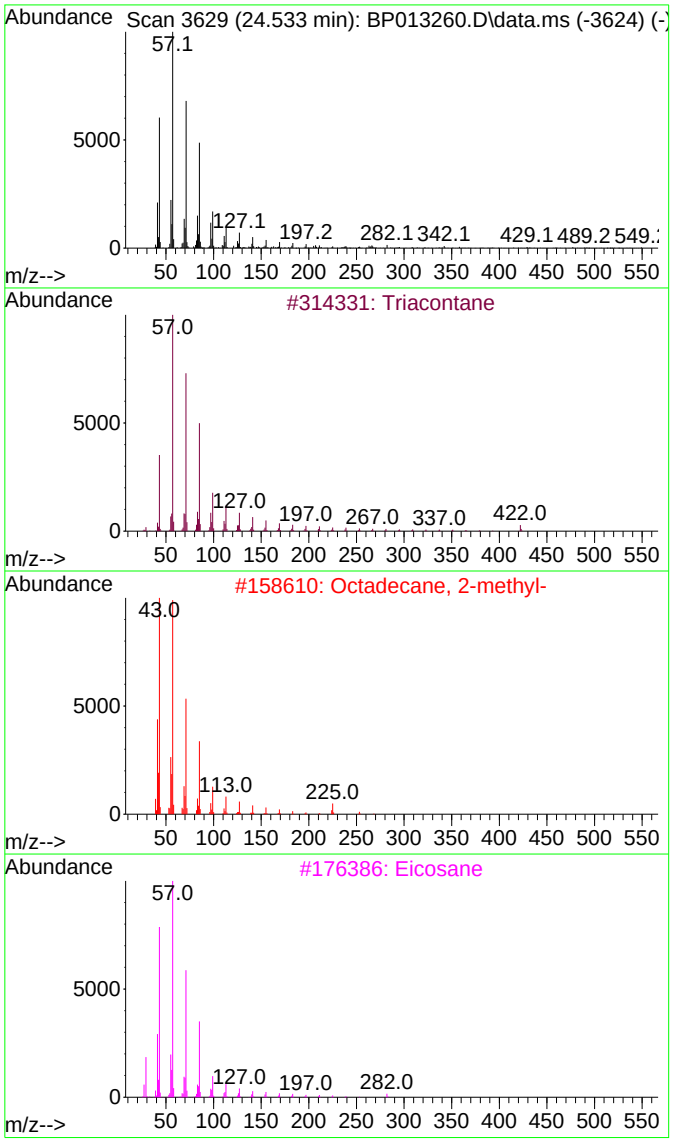
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

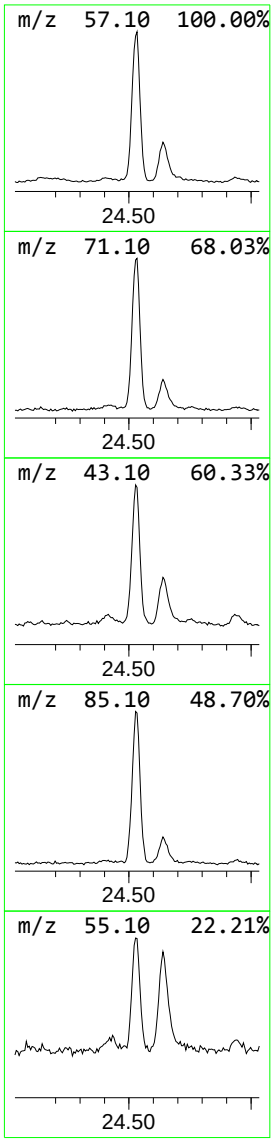
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	5.32 ng/ul	1815930	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	95
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Eicosane	282	C20H42	000112-95-8	92
4	Heneicosane	296	C21H44	000629-94-7	90
5	2-Methylheptacosane	394	C28H58	001561-00-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
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Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

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

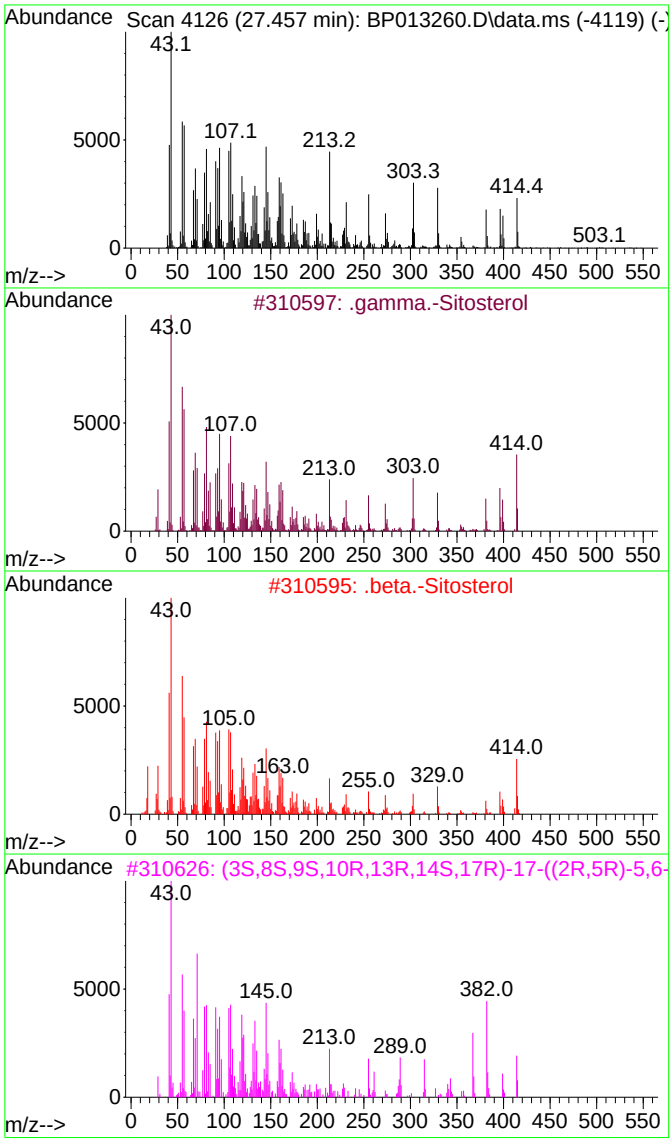
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

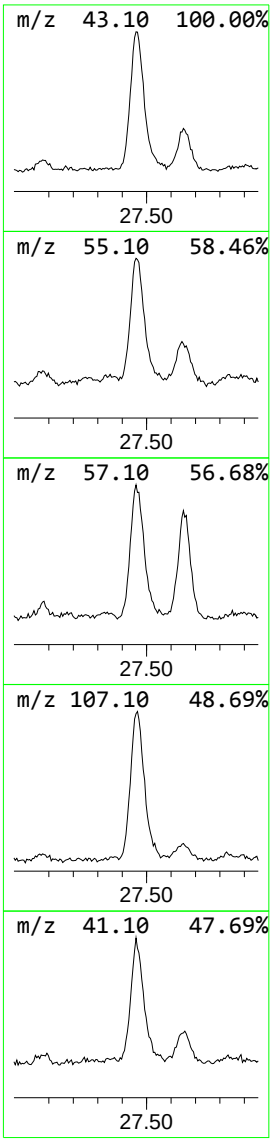
****

Peak Number 6 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.457	22.61 ng/ul	7721020	Perylene-d12	23.916

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	90
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	55
4	.beta.-Sitosterol	414	C29H50O	000083-46-5	55
5	Campesterol	400	C28H48O	000474-62-4	49





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Sample : N6015-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXW5

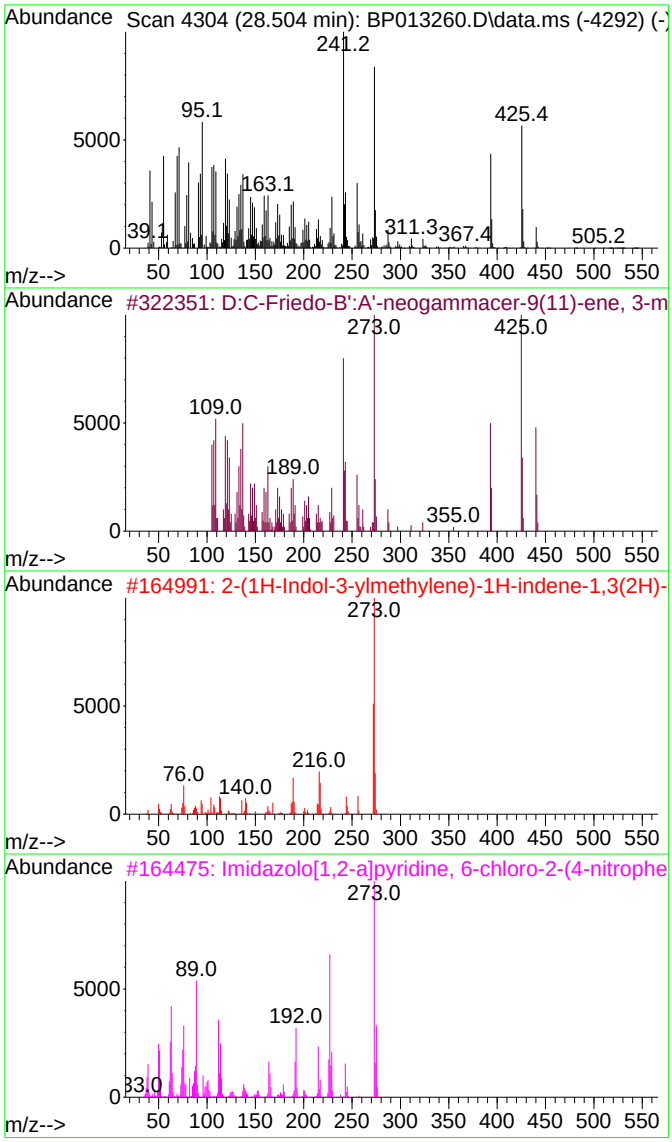
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

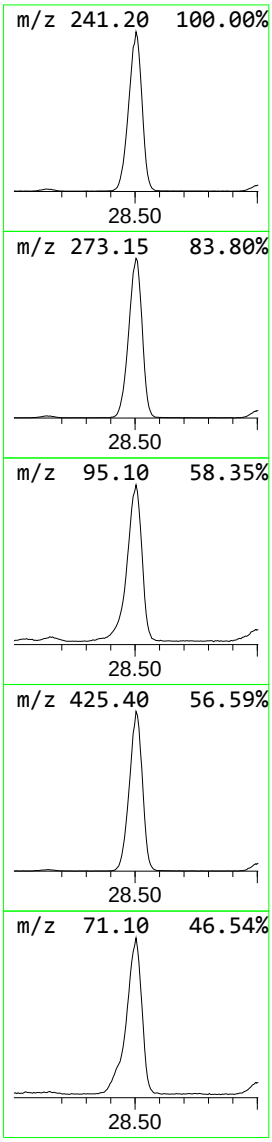
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.504	115.66 ng/ul	39491300	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	50
2	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25
3	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	15
4	Lupeol	426	C30H50O	000545-47-1	15
5	6-(Trifluoromethoxy)-1H-indole-2...	273	C12H10F3NO3	1000499-75-7	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013260.D
Acq On : 23 Dec 2022 00:09
Operator : CG/JU
Sample : N6015-15
Misc :
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Instrument :
BNA_P
ClientSampleId :
DBXW5

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	15.3	ng/ul	3786220	3	14.587	4965210	20.0
n-Hexadecanoic ...	18.216	6.5	ng/ul	1707640	4	17.345	5257950	20.0
1-Heneicosyl fo...	21.128	7.3	ng/ul	2293700	5	21.433	6299920	20.0
(DEL) Alkane: S...	24.533	5.3	ng/ul	1815930	6	23.916	6828620	20.0
.gamma.-Sitosterol	27.457	22.6	ng/ul	7721020	6	23.916	6828620	20.0
D:C-Friedo-B':A...	28.504	115.7	ng/ul	39491300	6	23.916	6828620	20.0