LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

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: BP013134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	22	26	37	rVB	176584	237825	0.39%	0.096%
2	3.776	97	100	113	rBV	371311	565151	0.93%	0.227%
3	3.876	113	117	125	rVB	74778	109533	0.18%	0.044%
4	3.999	133	138	144	rVB	91695	138755	0.23%	0.056%
5	5.040	309	315	324	rVB	638739	913088	1.51%	0.367%
6	7.111	659	667	680	rBV	2701727	4379521	7.22%	1.761%
7	7.281	690	696	707	rBV	2449920	3744375	6.18%	1.506%
8	7.481	723	730	741	rBV	2829321	4487345	7.40%	1.804%
9	7.958	803	811	818	rBV	2044487	3186218	5.26%	1.281%
10	8.663	924	931	943	rBV	2693284	4286881	7.07%	1.724%
11	8.787	946	952	959	rVB	121800	198825	0.33%	0.080%
12	9.122	1002	1009	1022	rBV	2818058	4568080	7.53%	1.837%
13	9.528	1073	1078	1086	rBV	86058	138544	0.23%	0.056%
14	9.846	1122	1132	1150	rBV	2250240	3862903	6.37%	1.553%
15	9.987	1152	1156	1164	rVV2	33435	72087	0.12%	0.029%
16	10.387	1217	1224	1241	rBV	3503457	5815131	9.59%	2.338%
17	10.769	1280	1289	1296	rBV	2746231	4688691	7.73%	1.885%
18	10.910	1304	1313	1331	rBV	1329044	2539484	4.19%	1.021%
19	11.552	1412	1422	1428	rBV9	23244	68987	0.11%	0.028%
20	12.175	1524	1528	1535	rVB	73646	106835	0.18%	0.043%
21	12.293	1538	1548	1552	rBV2	43883	88430	0.15%	0.036%
22	12.352	1553	1558	1563	rVB2	62939	99002	0.16%	0.040%
23	13.410	1728	1738	1745	rVV	132496	223326	0.37%	0.090%
24	13.516	1747	1756	1762	rVV3	27525	83655	0.14%	0.034%
25	14.004	1832	1839	1848	rBV	6182934	8559524	14.12%	3.442%
26	14.122	1854	1859	1865	rVB6	42922	67714	0.11%	0.027%
27	14.187	1865	1870	1874	rBV	81749	110244	0.18%	0.044%
28	14.293	1881	1888	1898	rBV	7062889	10250462	16.91%	4.122%
29	14.481	1916	1920	1925	rVB	87696	117923	0.19%	0.047%
30	14.598	1928	1940	1947	rBV	4325187	6295523	10.38%	2.532%
31	14.787	1964	1972	1992	rBV	2060484	3289260	5.43%	1.323%
32	14.946	1995	1999	2004	rVV3	82949	143715	0.24%	0.058%
33	15.010	2004	2010	2019	rVV8	69054	177877	0.29%	0.072%
34	15.593	2102	2109	2115	rBV	8939016	12889031	21.26%	5.183%
35	15.640	2115	2117	2122	rVV2	43398	61296	0.10%	0.025%
36	15.704	2122	2128	2144	rVV	2619507	3728312	6.15%	1.499%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

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	15.828	2145	2149	2156	rVB2	46078	80745	0.13%	0.032%
38	15.957	2165	2171	2183	rVB	5485961	7202251	11.88%	2.896%
39	16.522	2262	2267	2273	rVB	269550	376145	0.62%	0.151%
40	17.351	2402	2408	2413	rVV	4884594	6904151	11.39%	2.776%
41	17.392	2413	2415	2419	rVV	155995	211334	0.35%	0.085%
42	17.451	2419	2425	2434	rVV	8738959	12282873	20.26%	4.939%
43	17.539	2438	2440	2448	rVB7	51260	79732	0.13%	0.032%
44	18.110	2532	2537	2541	rBV5	59628	106626	0.18%	0.043%
45	18.163	2542	2546	2552	rBV	357954	519871	0.86%	0.209%
46	18.228	2552	2557	2582	rVV	2874541	4386252	7.23%	1.764%
47	18.698	2635	2637	2641	rVB5	64280	79639	0.13%	0.032%
48	19.110	2702	2707	2715	rBV6	100135	228101	0.38%	0.092%
49	19.210	2720	2724	2727	rBV2	90647	130094	0.21%	0.052%
50	19.257	2729	2732	2738	rVB2	138675	198956	0.33%	0.080%
51	19.345	2738	2747	2762	rBV3	3496265	6884458	11.36%	2.768%
52	19.457	2762	2766	2781	rVB	966595	1638317	2.70%	0.659%
53	19.681	2799	2804	2816	rVB	9555388	13294317	21.93%	5.346%
54	20.192	2889	2891	2896	rVB2	149121	165403	0.27%	0.067%
55	21.133	3046	3051	3062	rBV	1474796	2744325	4.53%	1.104%
56	21.439	3097	3103	3107	rBV	4086011	5747739	9.48%	2.311%
57	23.133	3387	3391	3398	rBV2	1038019	1910220	3.15%	0.768%
58	23.757	3490	3497	3514	rVB2	5366259	11572133	19.09%	4.653%
59	23.922	3518	3525	3538	rVB2	2842682	5893164	9.72%	2.370%
60	24.539	3625	3630	3640	rVB	1384695	2922656	4.82%	1.175%
61	26.463	3950	3957	3976	rVB3	1374125	4859850	8.02%	1.954%
62	27.480	4121	4130	4151	rVB3	1827688	7336933	12.10%	2.950%
63	28.533	4293	4309	4331	rVB2	13895596	60627822	100.00%	24.380%

Sum of corrected areas: 248677660

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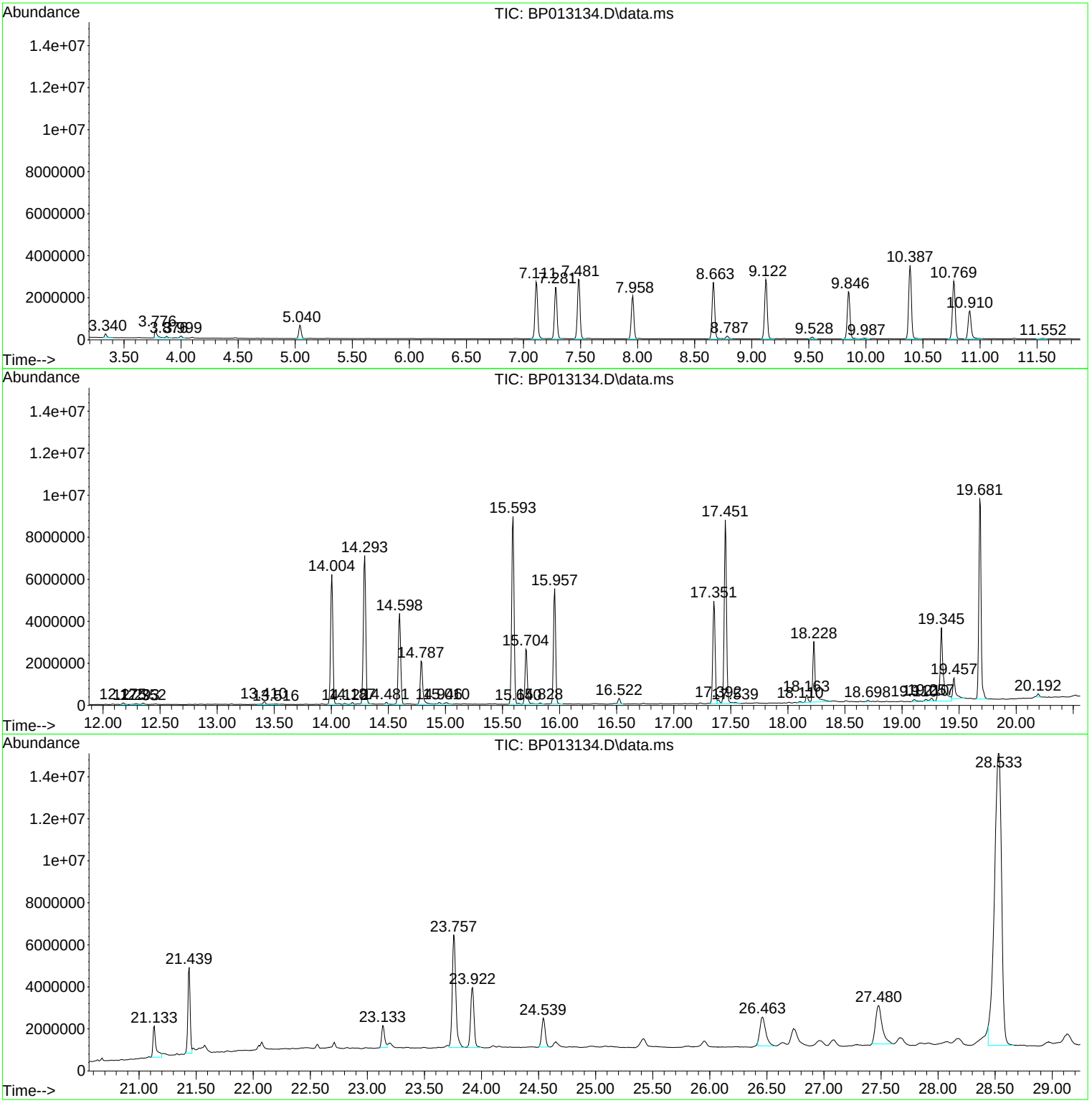
BNA_P
ClientSampleId :
DBXZ6

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\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
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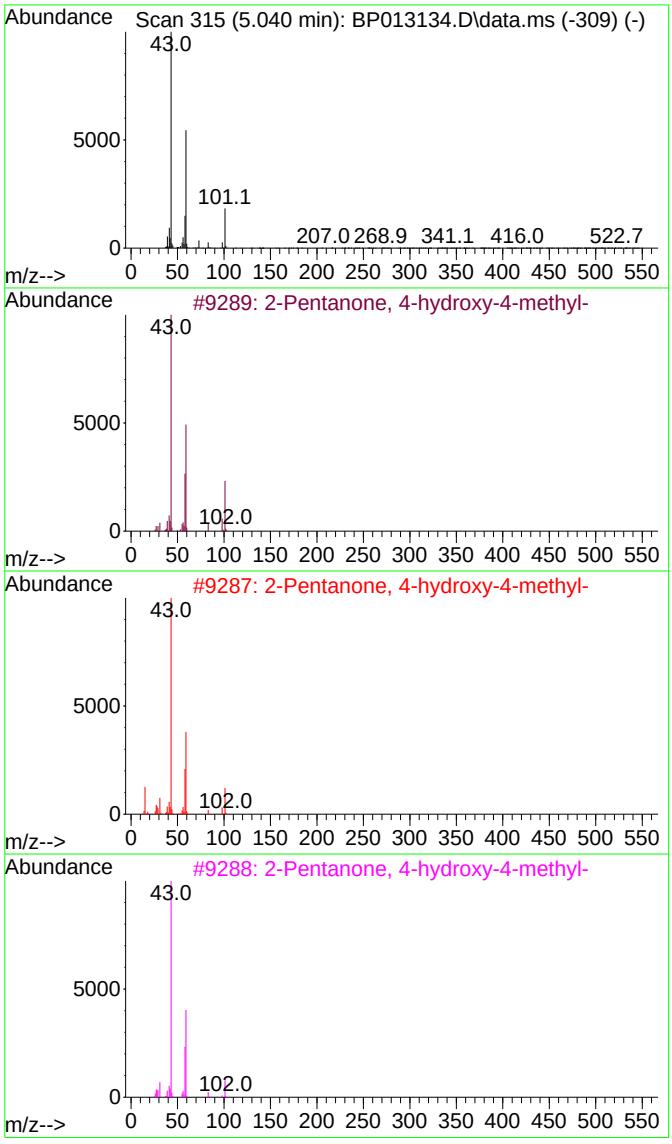
Quant Title : SVOA CALIBRATION

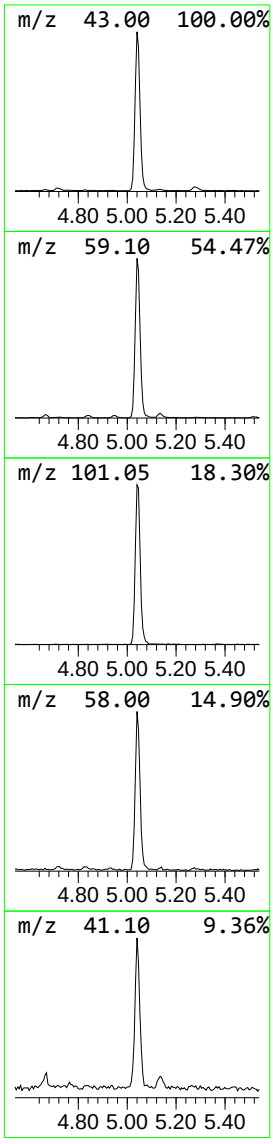
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	5.73 ng/ul	913088	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

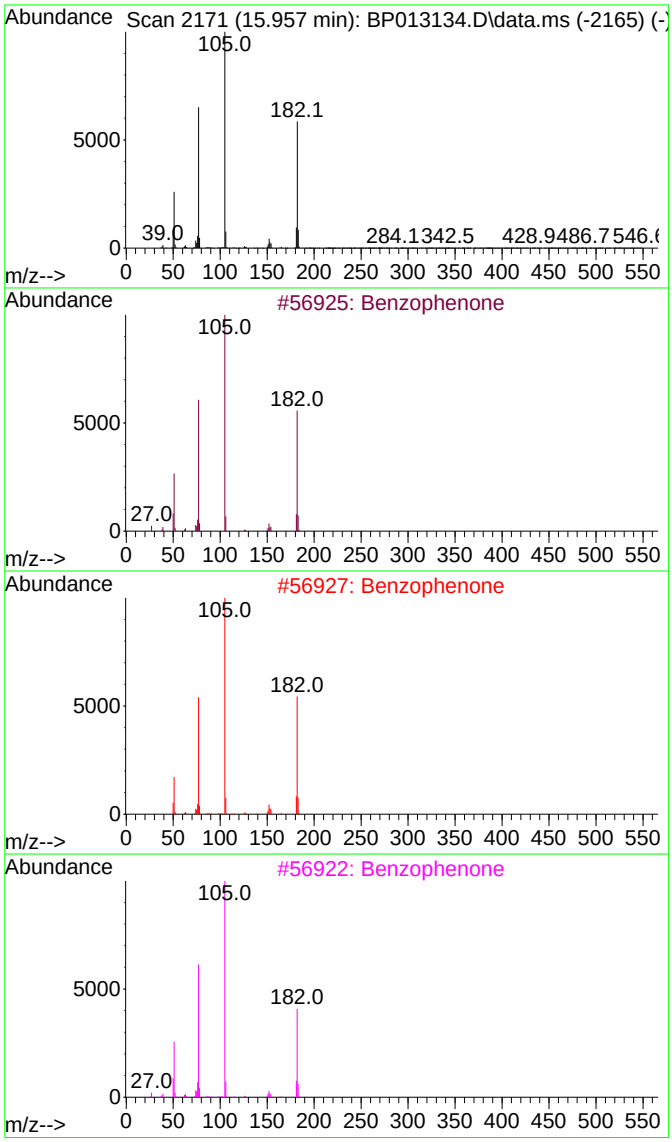
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

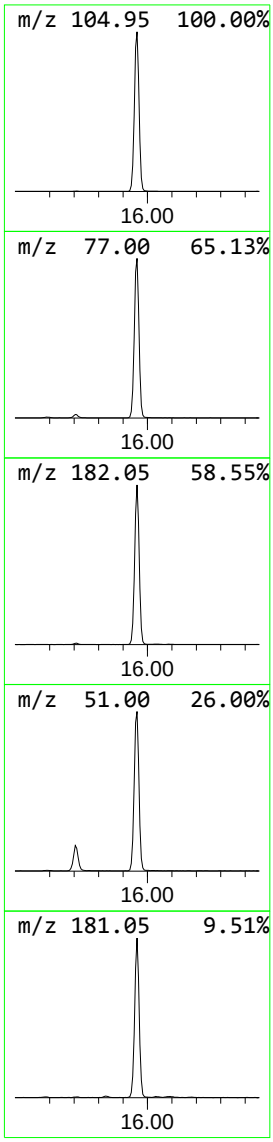
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	22.88 ng/ul	7202250	Acenaphthene-d10	14.599

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	93
5	Benzophenone	182	C13H10O	000119-61-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

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

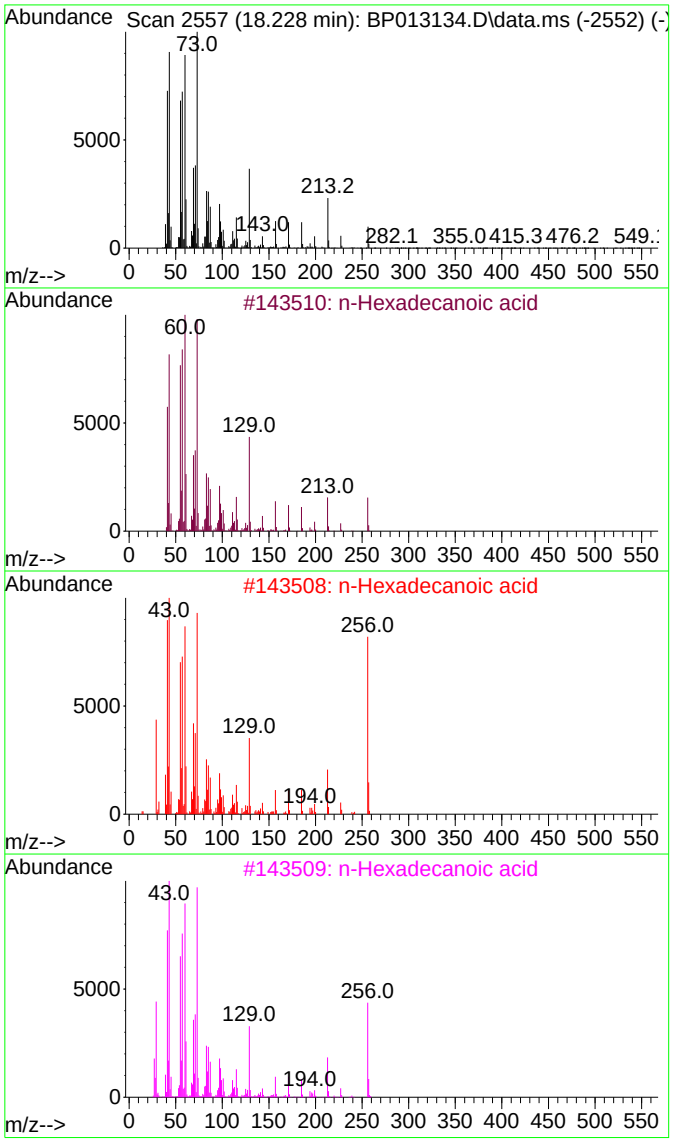
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

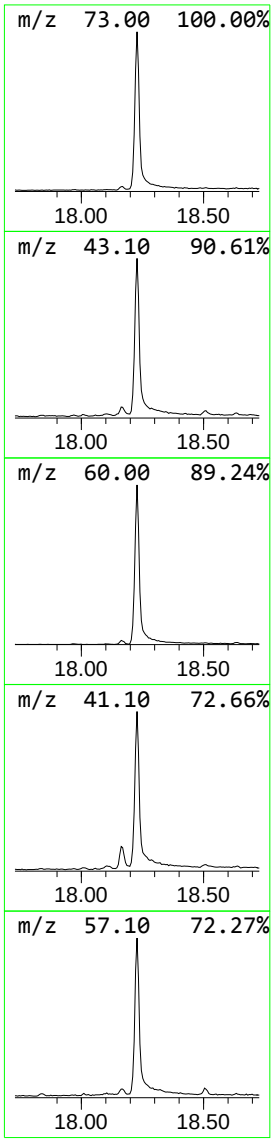
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.228	12.71 ng/ul	4386250	Phenanthrene-d10	17.351

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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

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

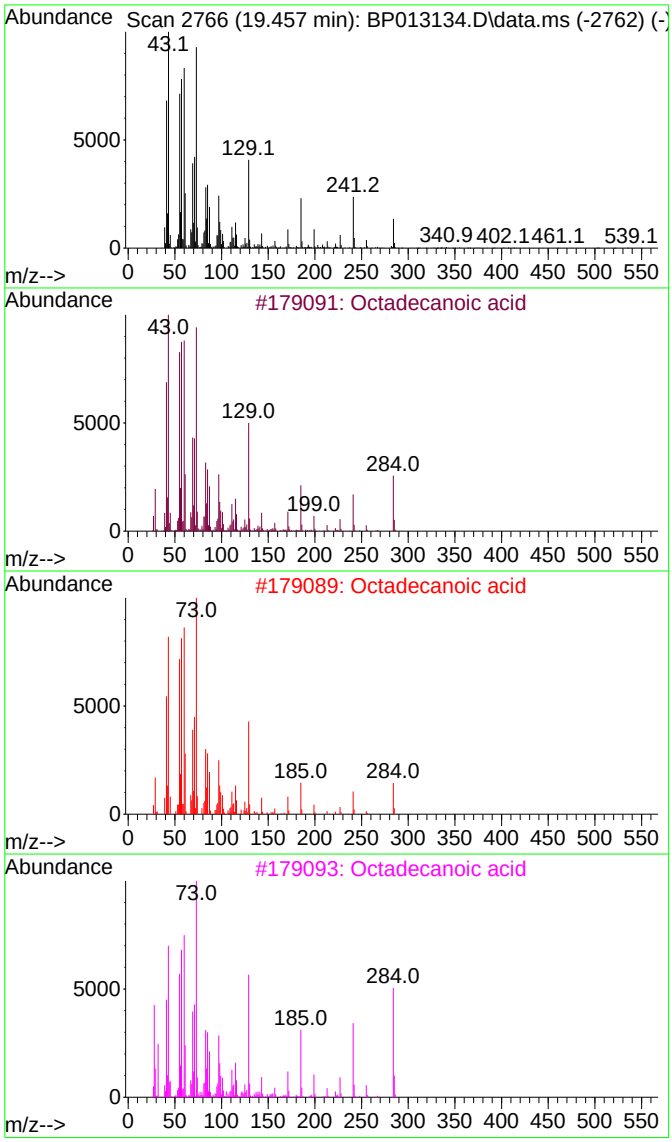
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

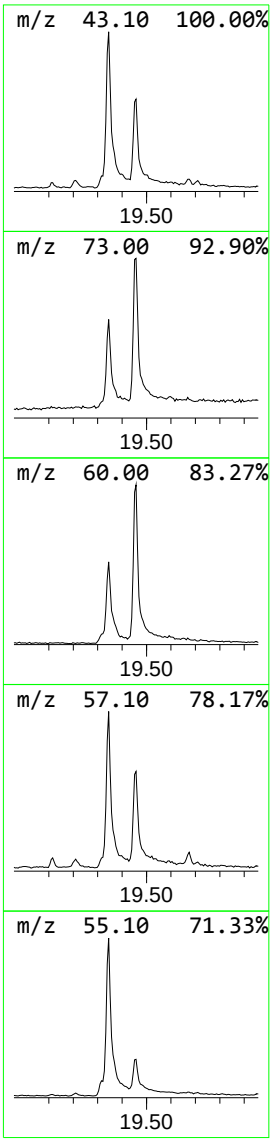
****

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	5.70 ng/ul	1638320	Chrysene-d12	21.439

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	97
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

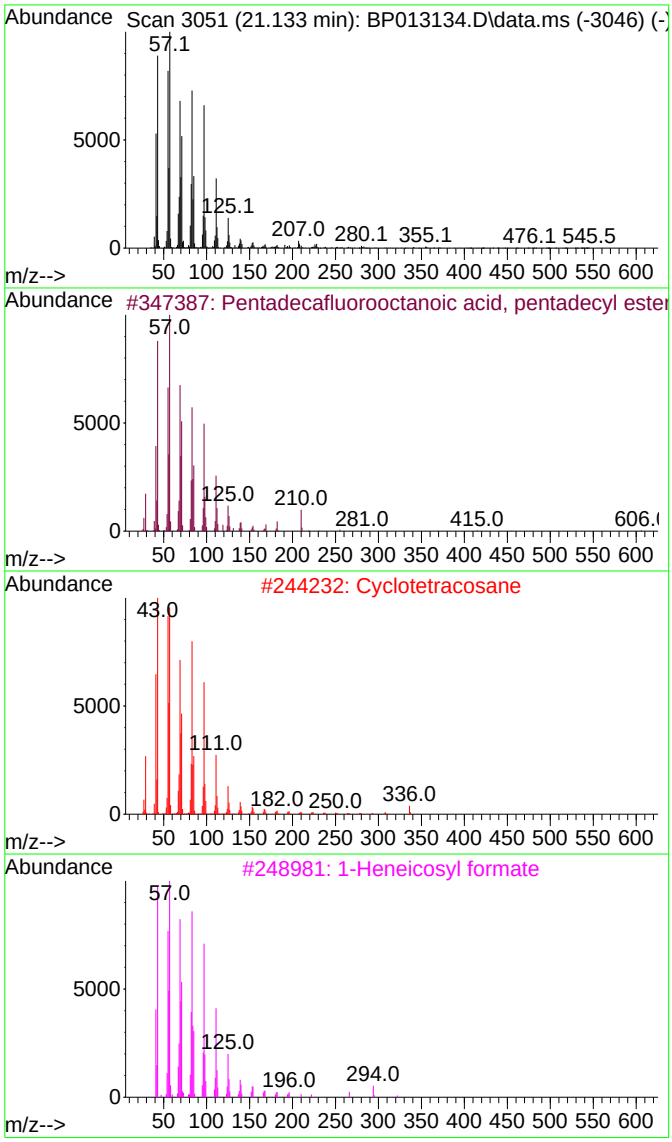
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

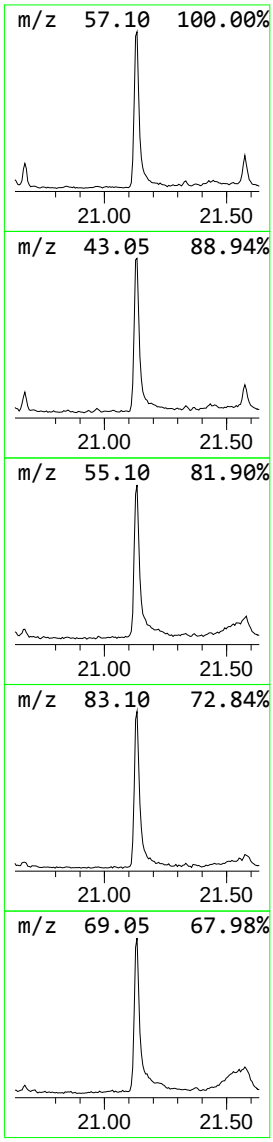
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	9.55 ng/ul	2744330	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





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Acq On : 19 Dec 2022 19:30
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Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
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DBXZ6

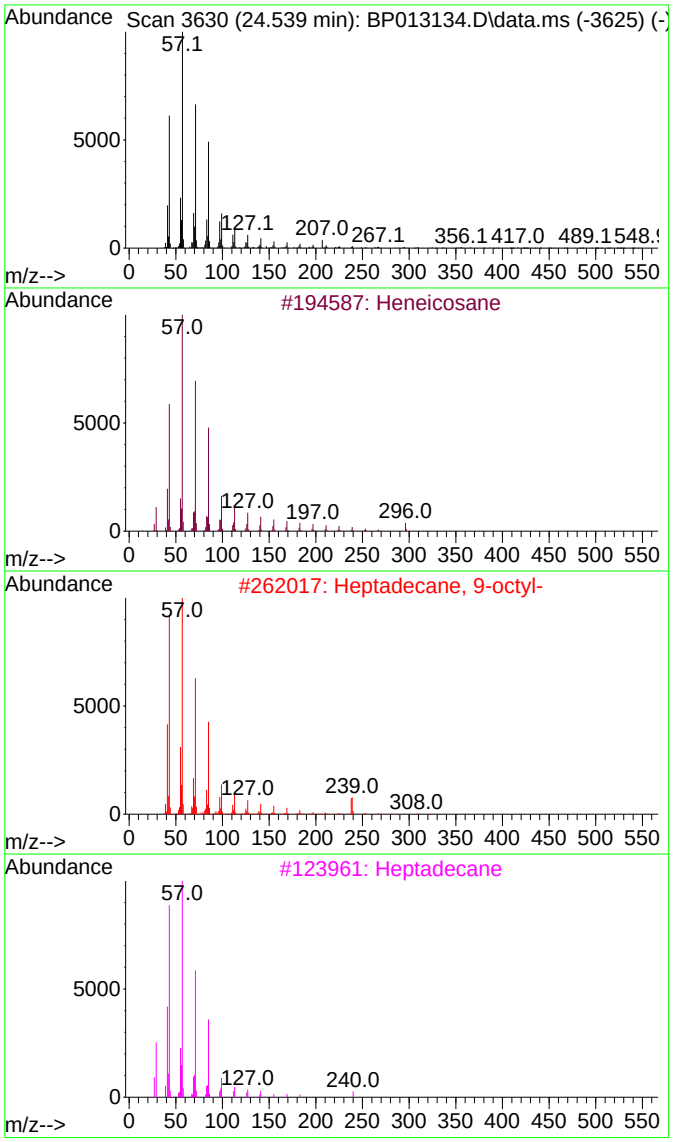
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

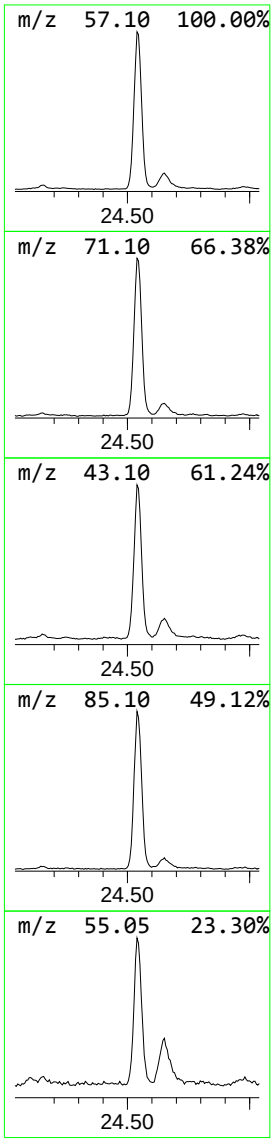
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	9.92 ng/ul	2922660	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3	Heptadecane	240	C17H36	000629-78-7	94
4	2-Methyltetracosane	352	C25H52	001560-78-7	94
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

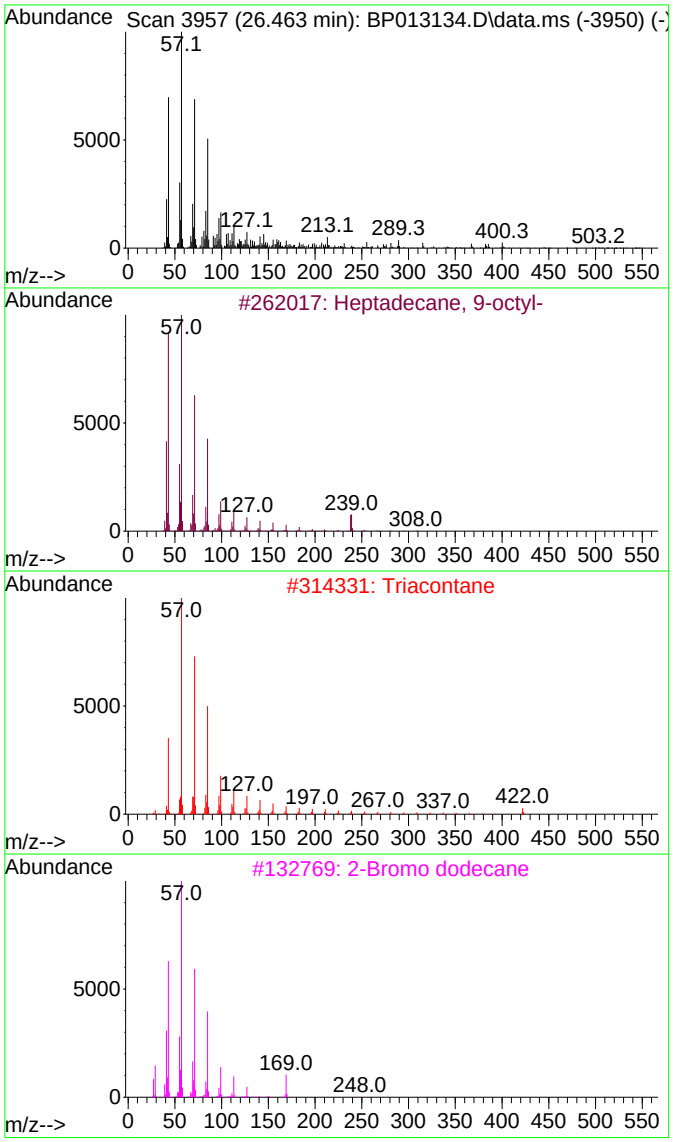
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

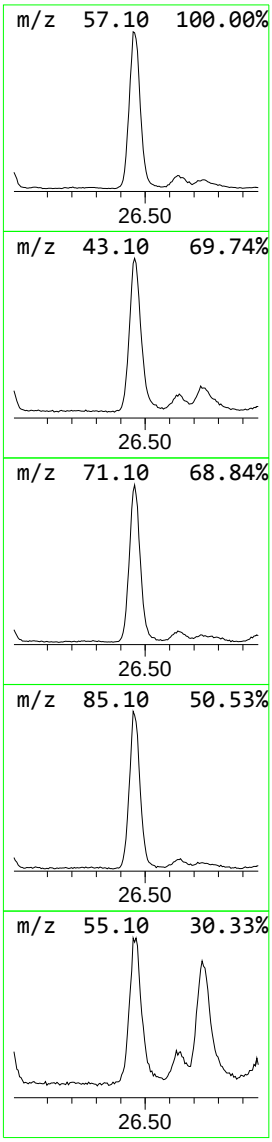
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.463	16.49 ng/ul	4859850	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2	Triacontane	422	C30H62	000638-68-6	92
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
4	2-Methylhexacosane	380	C27H56	001561-02-0	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

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

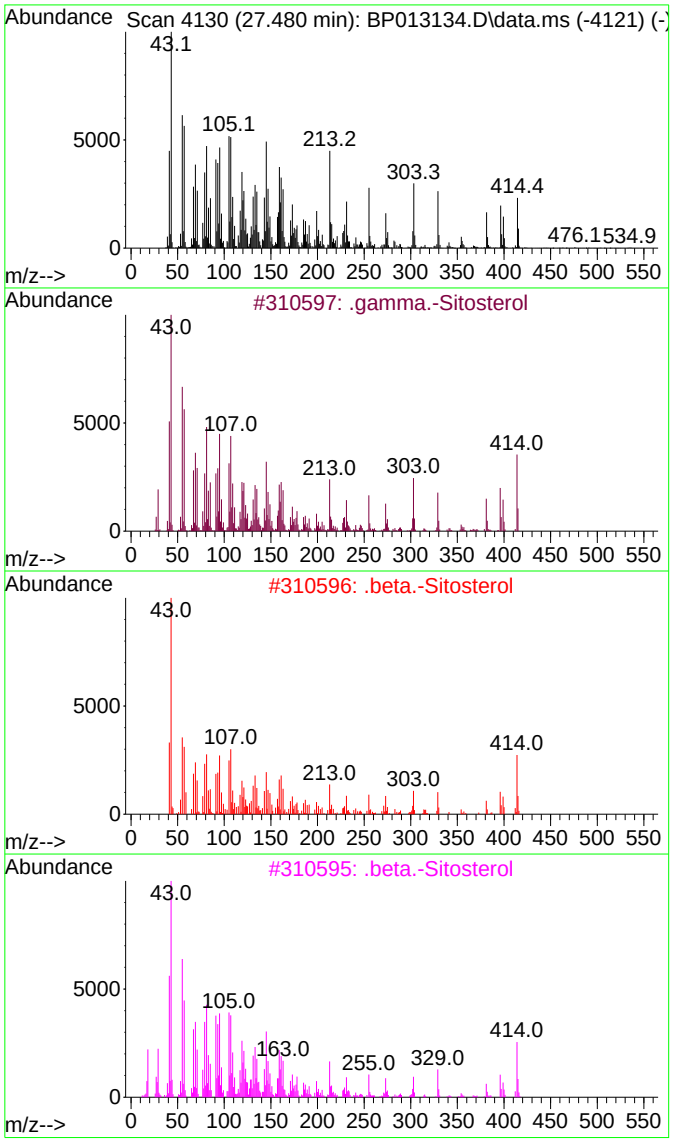
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

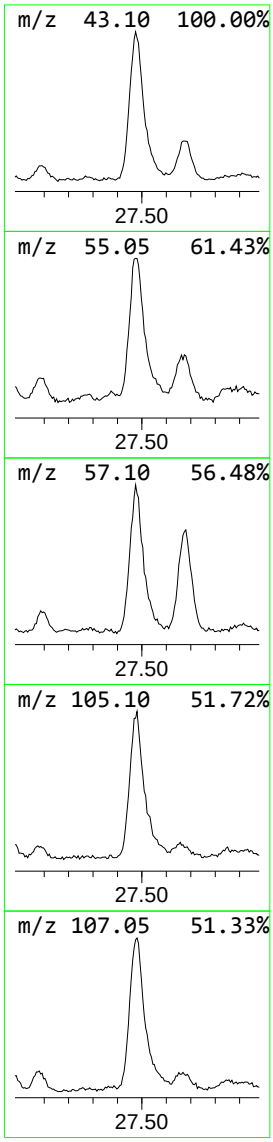
****

Peak Number 8 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.480	24.90 ng/ul	7336930	Perylene-d12	23.922

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	93
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
4	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	64
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

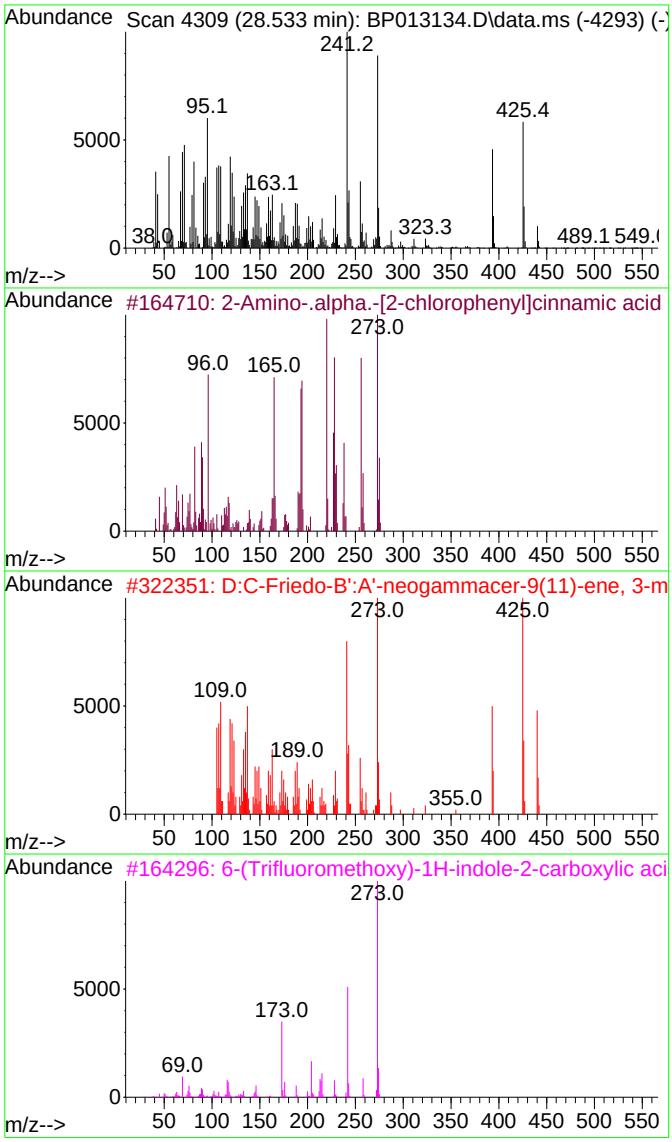
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

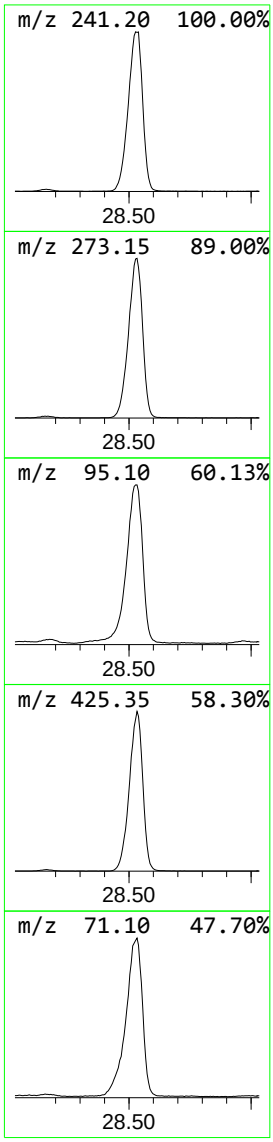
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.533	205.76 ng/ul	60627800	Perylene-d12	23.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	38
3	6-(Trifluoromethoxy)-1H-indole-2...	273	C12H10F3NO3	1000499-75-7	25
4	2-{[(4-Methyl-2-pyridinyl)amino]...	256	C13H16N4Si	1010494-07-4	15
5	Cobaltocene, 1,1'-diacetyl-	273	C14H14CoO2	073249-54-4	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013134.D
Acq On : 19 Dec 2022 19:30
Operator : CG/JU
Sample : N6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ6

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
2-Pentanone, 4-...	5.040	5.7	ng/ul	913088	1	7.958	3186220	20.0
Benzophenone	15.957	22.9	ng/ul	7202250	3	14.599	6295520	20.0
n-Hexadecanoic ...	18.228	12.7	ng/ul	4386250	4	17.351	6904150	20.0
Octadecanoic acid	19.457	5.7	ng/ul	1638320	5	21.439	5747740	20.0
Pentadecafluoro...	21.133	9.6	ng/ul	2744330	5	21.439	5747740	20.0
(DEL) Alkane: S...	24.539	9.9	ng/ul	2922660	6	23.922	5893160	20.0
(DEL) Alkane: S...	26.463	16.5	ng/ul	4859850	6	23.922	5893160	20.0
.gamma.-Sitosterol	27.480	24.9	ng/ul	7336930	6	23.922	5893160	20.0
2-Amino-.alpha....	28.533	205.8	ng/ul	60627800	6	23.922	5893160	20.0