LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXQ3

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: BP013162.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	22	25	32	rVB	133354	172252	0.41%	0.097%
2	3.622	71	74	79	rBV	50763	73714	0.17%	0.041%
3	3.769	95	99	112	rBV	894492	1342207	3.18%	0.752%
4	3.869	114	116	121	rVB	39641	49848	0.12%	0.028%
5	3.999	134	138	143	rVB	57164	84840	0.20%	0.048%
6	4.099	151	155	158	rBV	33025	43313	0.10%	0.024%
7	5.040	309	315	322	rBV2	197201	305770	0.72%	0.171%
8	7.110	660	667	683	rVB	1985761	3077229	7.29%	1.724%
9	7.281	689	696	704	rBV	1695730	2526620	5.98%	1.416%
10	7.481	723	730	738	rBV	2078167	3201579	7.58%	1.794%
11	7.952	803	810	818	rBV	1712269	2753380	6.52%	1.543%
12	8.663	920	931	943	rBV	2139249	3397603	8.05%	1.904%
13	8.781	947	951	957	rVB	37288	62147	0.15%	0.035%
14	9.122	1002	1009	1021	rBV	1907469	3026569	7.17%	1.696%
15	9.528	1069	1078	1084	rBV2	39663	69324	0.16%	0.039%
16	9.846	1122	1132	1147	rBV	1615362	2596318	6.15%	1.455%
17	10.063	1164	1169	1175	rVB3	28350	47889	0.11%	0.027%
18	10.387	1216	1224	1240	rBV	2342233	3870248	9.16%	2.169%
19	10.546	1245	1251	1260	rVB2	71992	123240	0.29%	0.069%
20	10.769	1281	1289	1298	rBV	2311292	3768469	8.92%	2.112%
21	10.904	1305	1312	1327	rBV	1749237	3122744	7.39%	1.750%
22	12.345	1553	1557	1565	rVB	37630	62294	0.15%	0.035%
23	13.410	1728	1738	1744	rBV	54782	89072	0.21%	0.050%
24	13.587	1760	1768	1772	rVB	55155	90588	0.21%	0.051%
25	13.998	1832	1838	1854	rBV	3561760	5044783	11.95%	2.827%
26	14.122	1854	1859	1864	rVB7	28110	45433	0.11%	0.025%
27	14.181	1864	1869	1873	rBV	44276	63776	0.15%	0.036%
28	14.287	1881	1887	1904	rVB2	4052241	6301382	14.92%	3.531%
29	14.598	1933	1940	1947	rBV	3014355	4513867	10.69%	2.529%
30	14.792	1966	1973	1988	rBV	1138907	1895143	4.49%	1.062%
31	15.010	2004	2010	2015	rVB7	44339	81594	0.19%	0.046%
32	15.586	2102	2108	2122	rBV	5203530	7600138	18.00%	4.259%
33	15.704	2122	2128	2140	rBV	1369238	1931088	4.57%	1.082%
34	15.828	2146	2149	2157	rVB4	27956	46134	0.11%	0.026%
35	15.951	2161	2170	2182	rVV	2453059	3461834	8.20%	1.940%
36	16.522	2262	2267	2275	rVB	174556	240197	0.57%	0.135%

LSC Area Percent Report

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Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

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	17.351	2402	2408	2414	rBV	3338353	4829096	11.43%	2.706%
38	17.451	2419	2425	2433	rVV	5211384	7247493	17.16%	4.061%
39	17.539	2437	2440	2448	rVB7	45763	75593	0.18%	0.042%
40	17.728	2469	2472	2477	rVB4	48442	65544	0.16%	0.037%
41	18.010	2516	2520	2524	rBV6	29370	47063	0.11%	0.026%
42	18.163	2542	2546	2550	rBV	162226	209333	0.50%	0.117%
43	18.222	2551	2556	2566	rBV	998782	1376397	3.26%	0.771%
44	18.633	2622	2626	2632	rBV	499560	594153	1.41%	0.333%
45	19.051	2694	2697	2702	rVB5	70417	90677	0.21%	0.051%
46	19.263	2729	2733	2737	rVB4	84948	117264	0.28%	0.066%
47	19.333	2739	2745	2747	rBV3	142527	315073	0.75%	0.177%
48	19.451	2761	2765	2776	rBV	417640	633583	1.50%	0.355%
49	19.680	2799	2804	2817	rVB	6564541	9246107	21.89%	5.181%
50	20.192	2888	2891	2893	rBV2	187507	239530	0.57%	0.134%
51	20.674	2971	2973	2976	rVB	137211	126523	0.30%	0.071%
52	21.127	3046	3050	3055	rBV	1281322	1820361	4.31%	1.020%
53	21.439	3098	3103	3107	rBV	4654043	6135043	14.53%	3.438%
54	23.133	3386	3391	3398	rBV	3112236	5201183	12.32%	2.914%
55	23.762	3491	3498	3512	rVB2	5449966	11551736	27.35%	6.473%
56	23.921	3518	3525	3536	rVB2	3382183	7043655	16.68%	3.947%
57	24.545	3625	3631	3640	rVB	1644338	3495543	8.28%	1.959%
58	28.521	4294	4307	4325	rVB2	10501063	42232301	100.00%	23.665%
59	29.021	4382	4392	4406	rVB3	2799689	10586201	25.07%	5.932%

Sum of corrected areas: 178462078

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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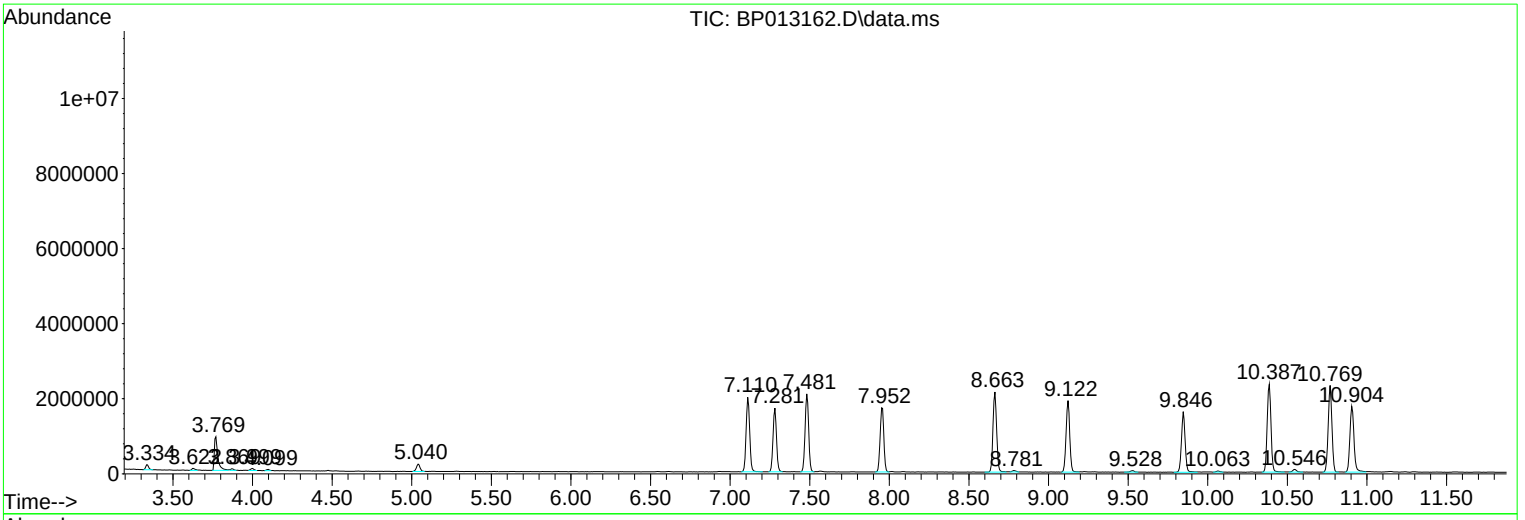
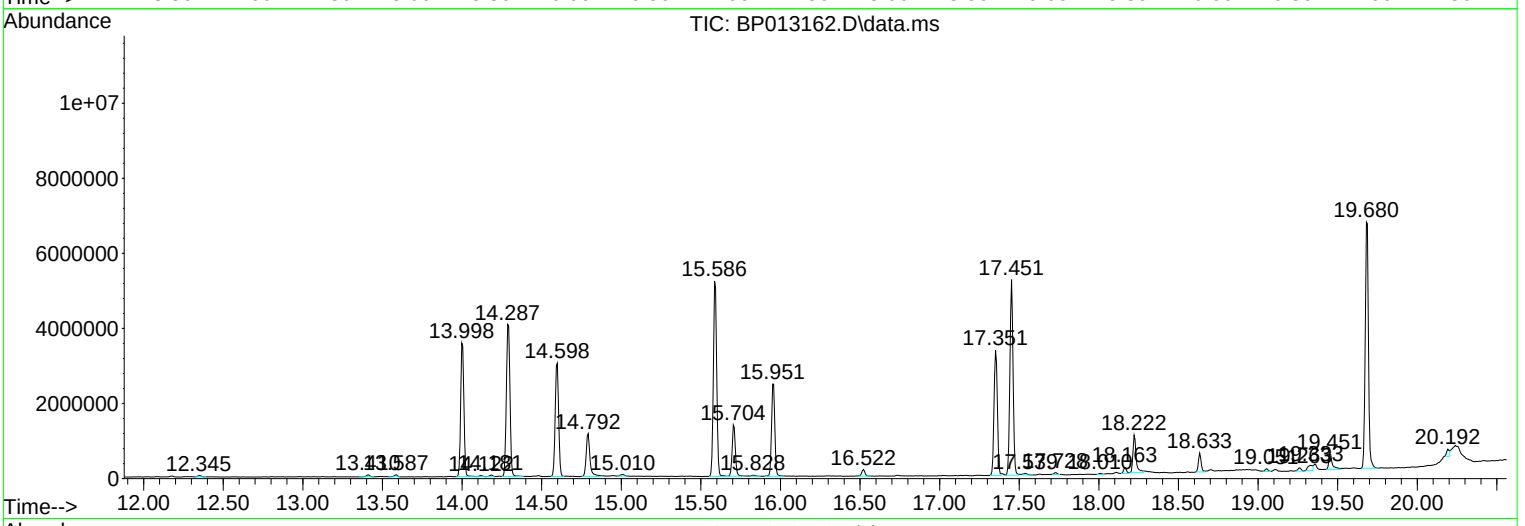
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

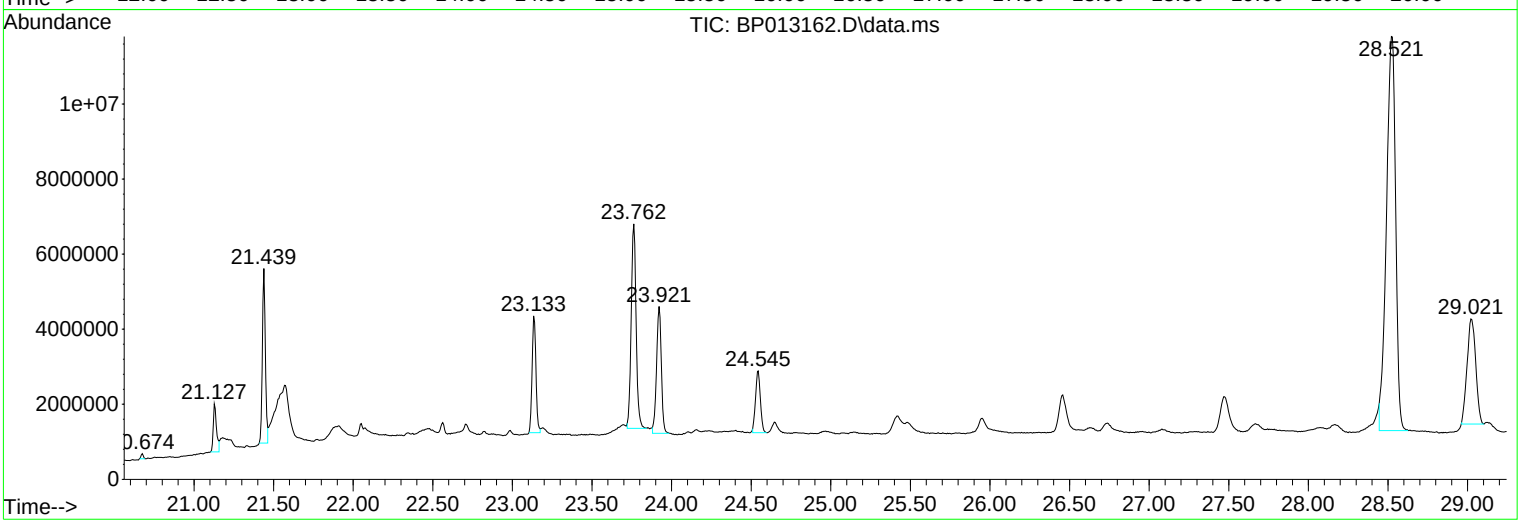
Instrument :
BNA_P
ClientSampleId :
DBXQ3

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 : BP013162.D
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Operator : CG/JU
Sample : N6003-12
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Instrument :
BNA_P
ClientSampleId :
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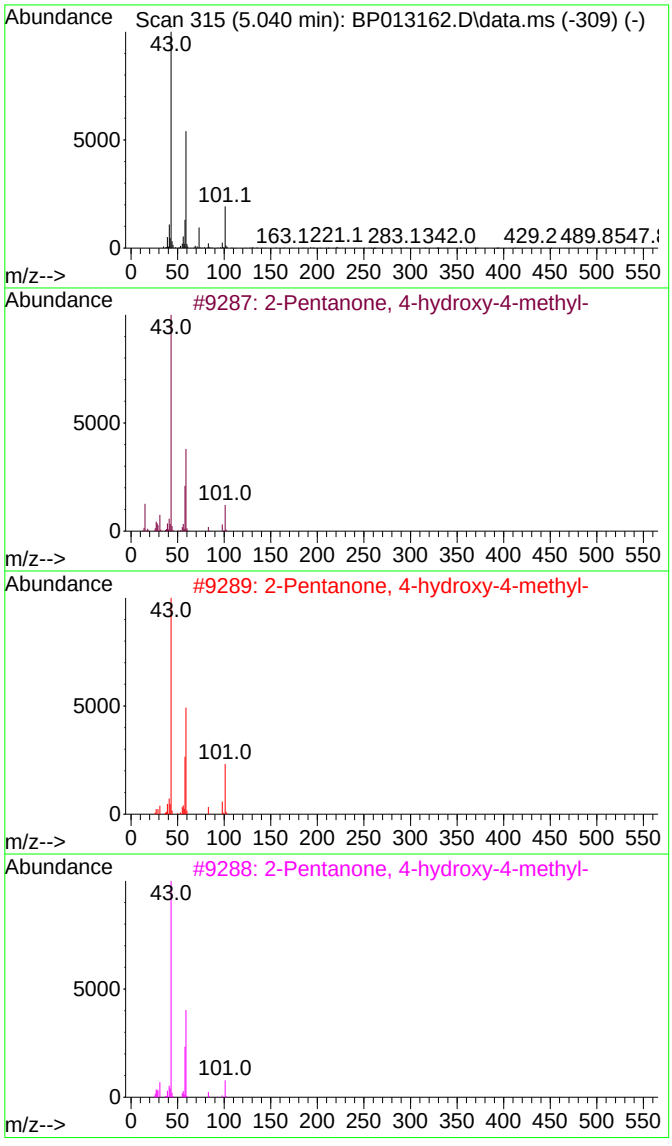
Quant Title : SVOA CALIBRATION

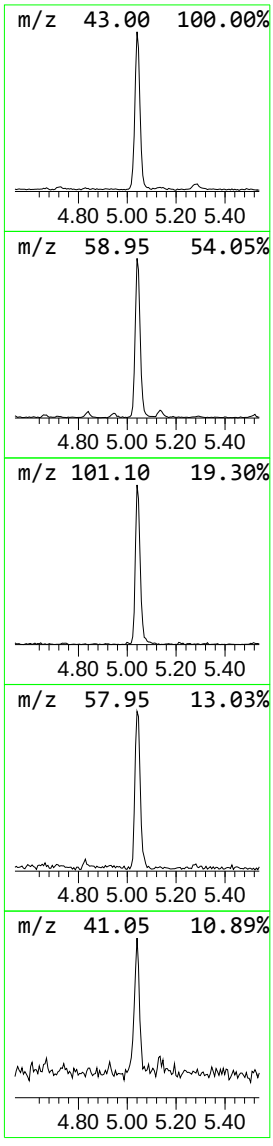
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.22 ng/ul	305770	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

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

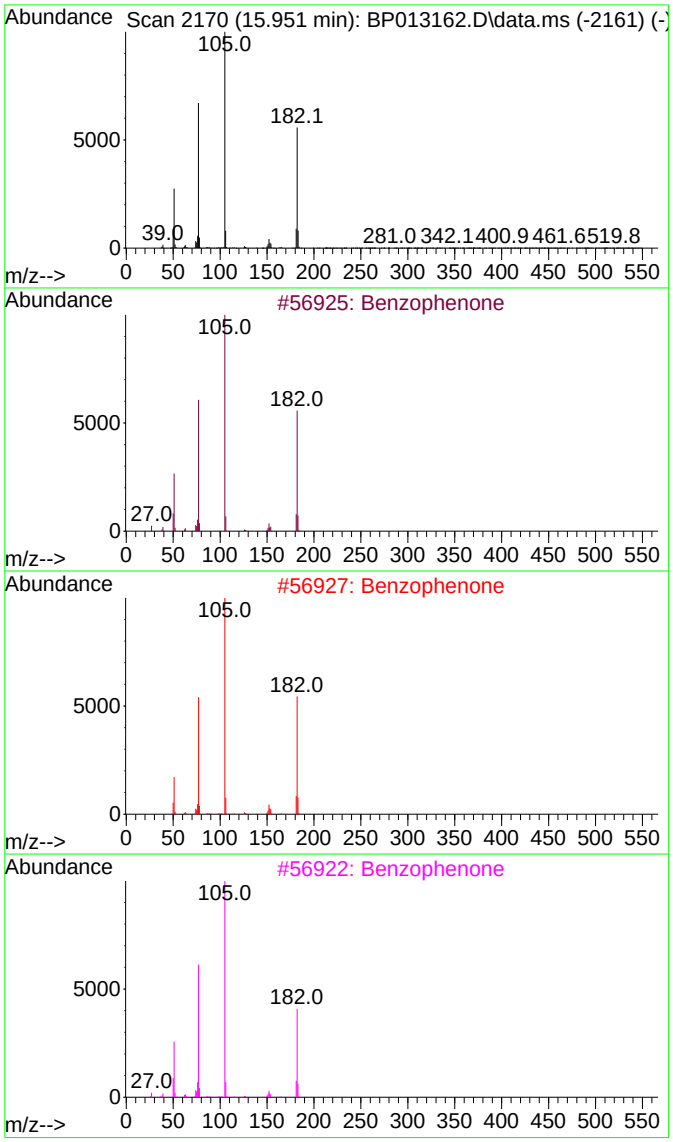
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

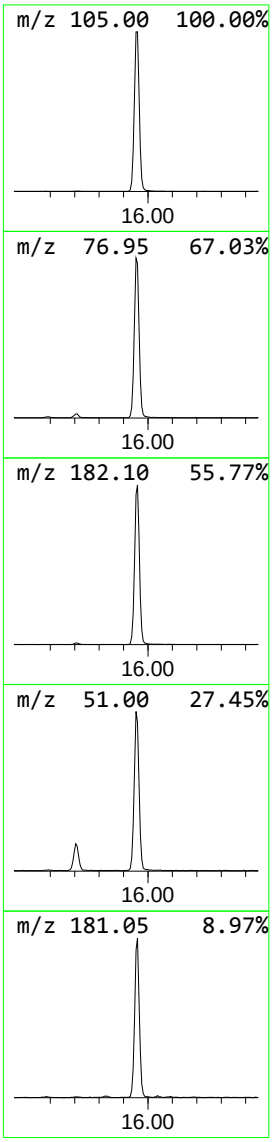
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	15.34 ng/ul	3461830	Acenaphthene-d10	14.598

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	90
5	Azobenzene	182	C12H10N2	000103-33-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

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

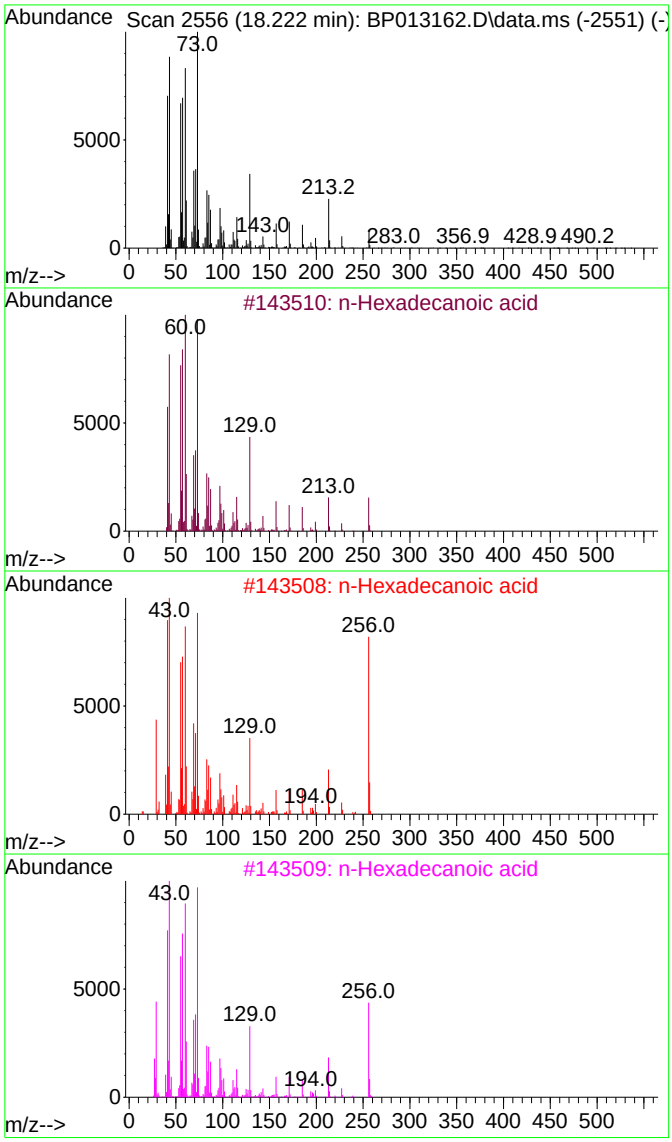
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

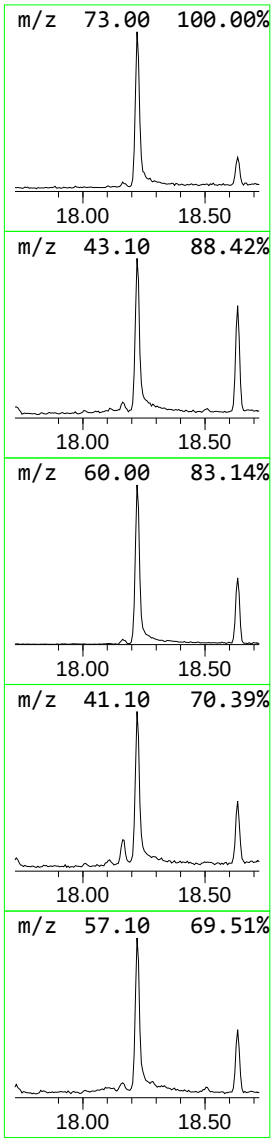
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	5.70 ng/ul	1376400	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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	Tridecanoic acid	214	C13H26O2	000638-53-9	95
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

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

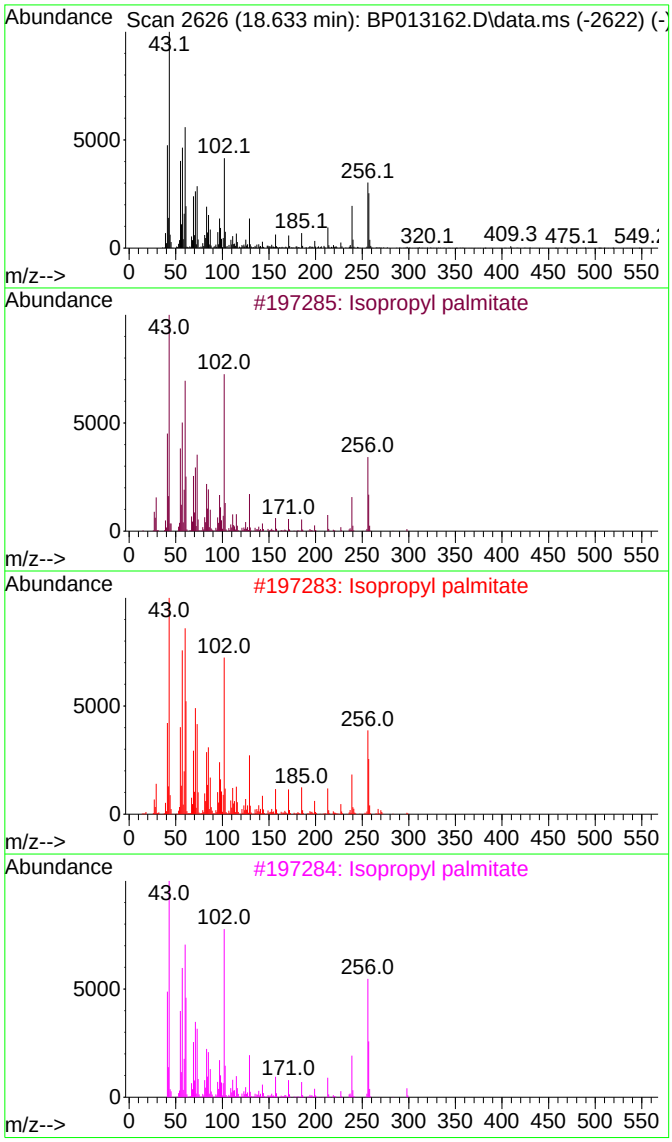
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

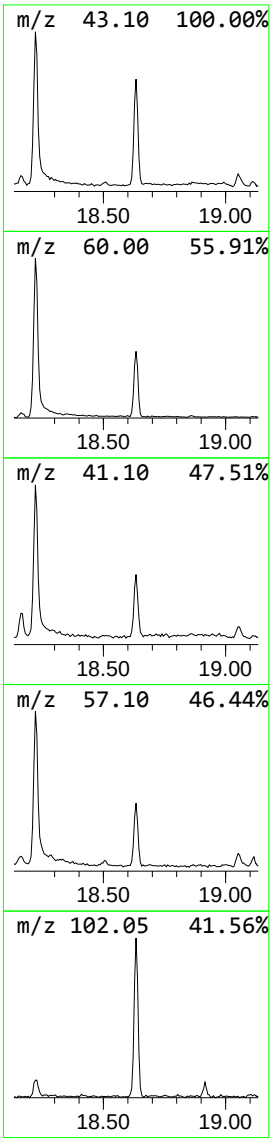
****

Peak Number 4 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.633	2.46 ng/ul	594153	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	96
2	Isopropyl palmitate	298	C19H38O2	000142-91-6	62
3	Isopropyl palmitate	298	C19H38O2	000142-91-6	52
4	8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	43
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
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Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

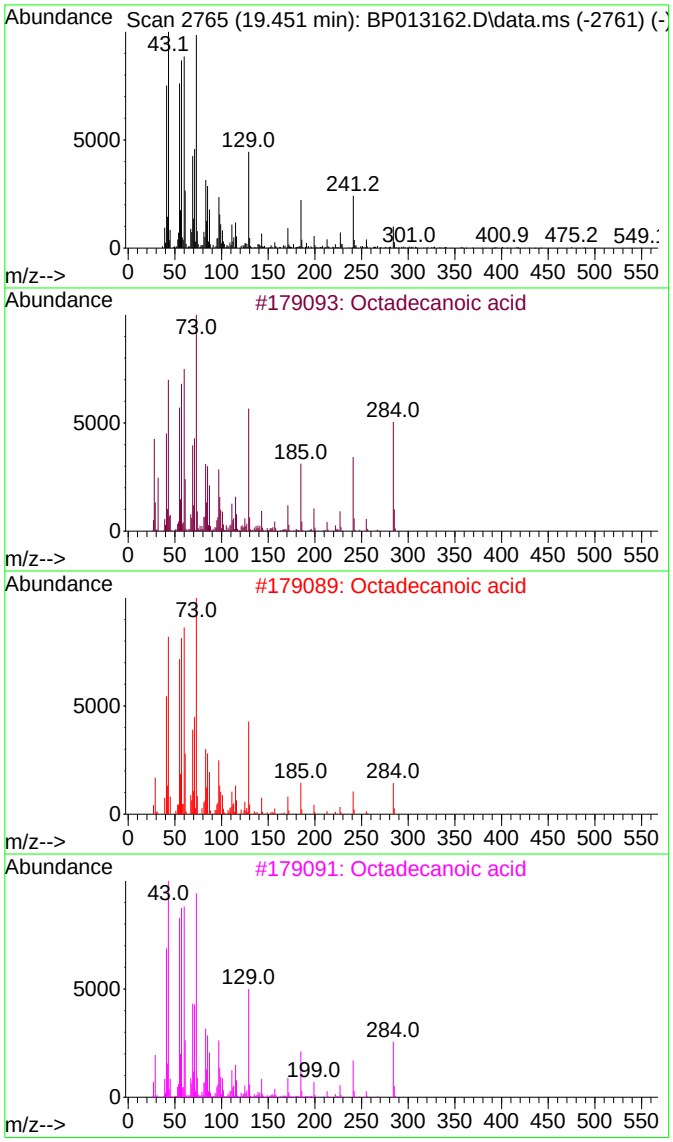
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

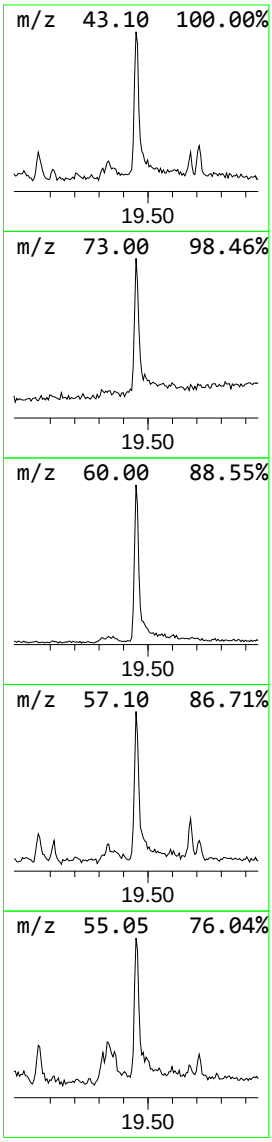
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.07 ng/ul	633583	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

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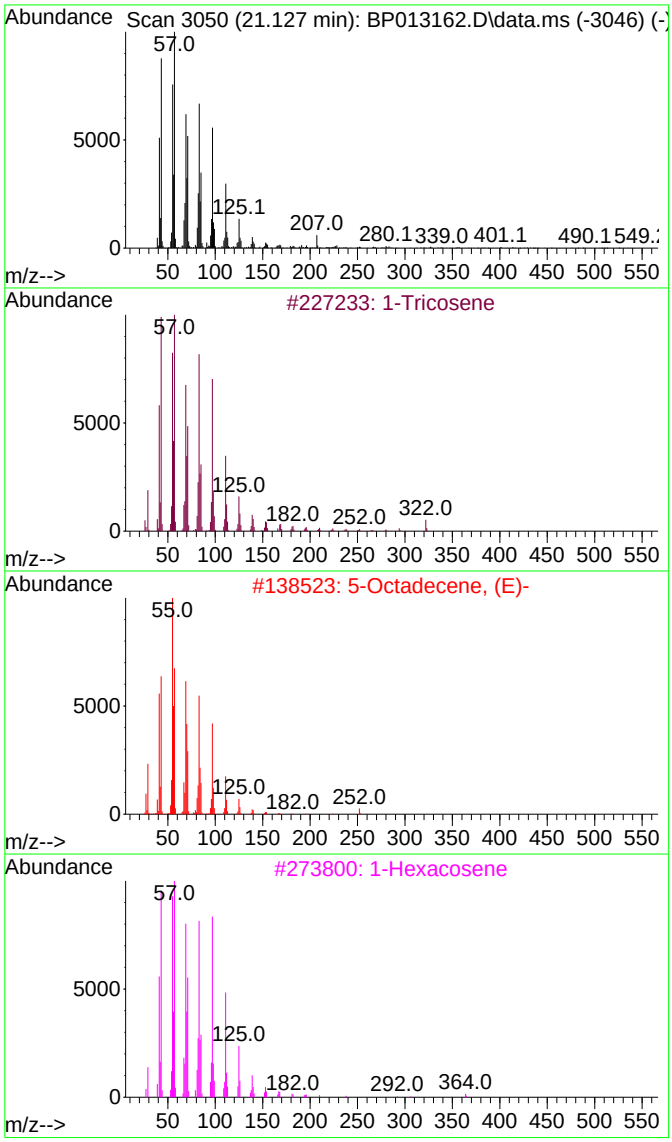
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

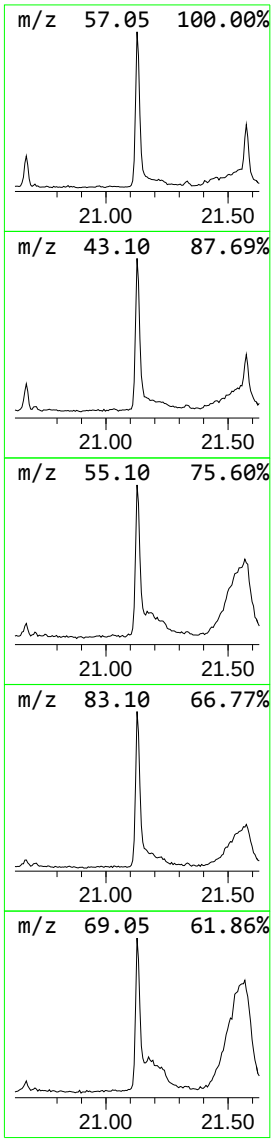
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	5.93 ng/ul	1820360	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	94
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

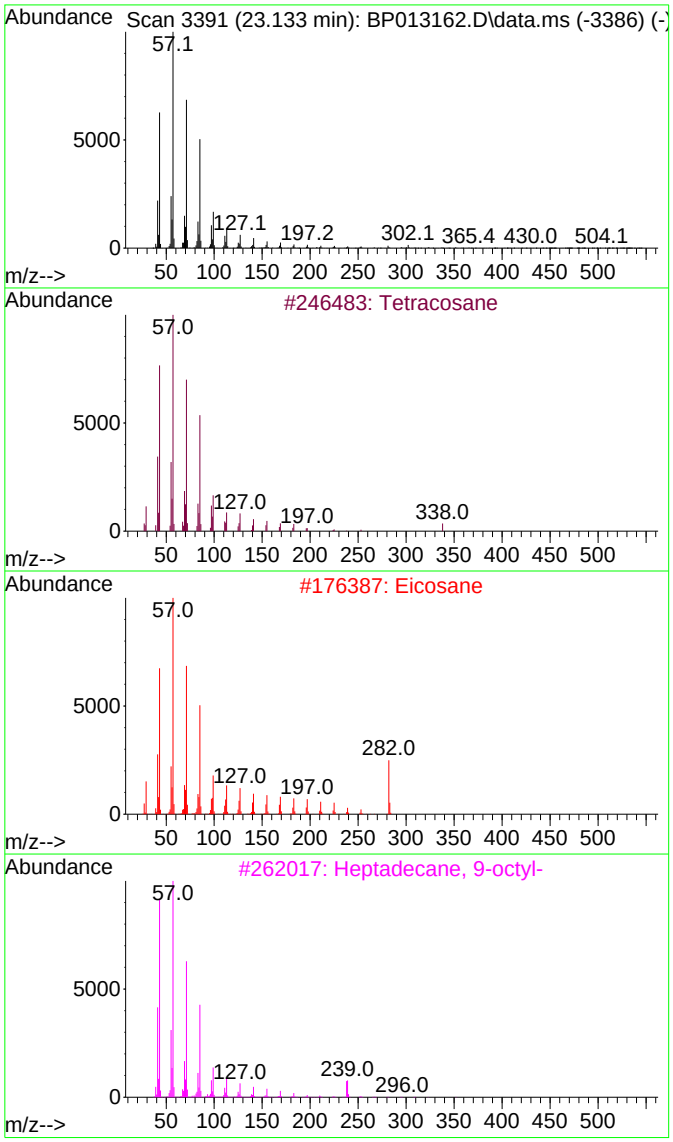
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

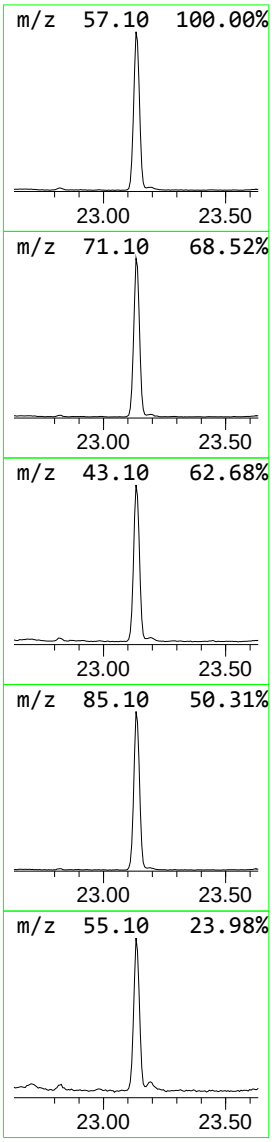
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.133	14.77 ng/ul	5201180	Perylene-d12	23.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Eicosane	282	C20H42	000112-95-8	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013162.D
Acq On : 20 Dec 2022 12:30
Operator : CG/JU
Sample : N6003-12
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

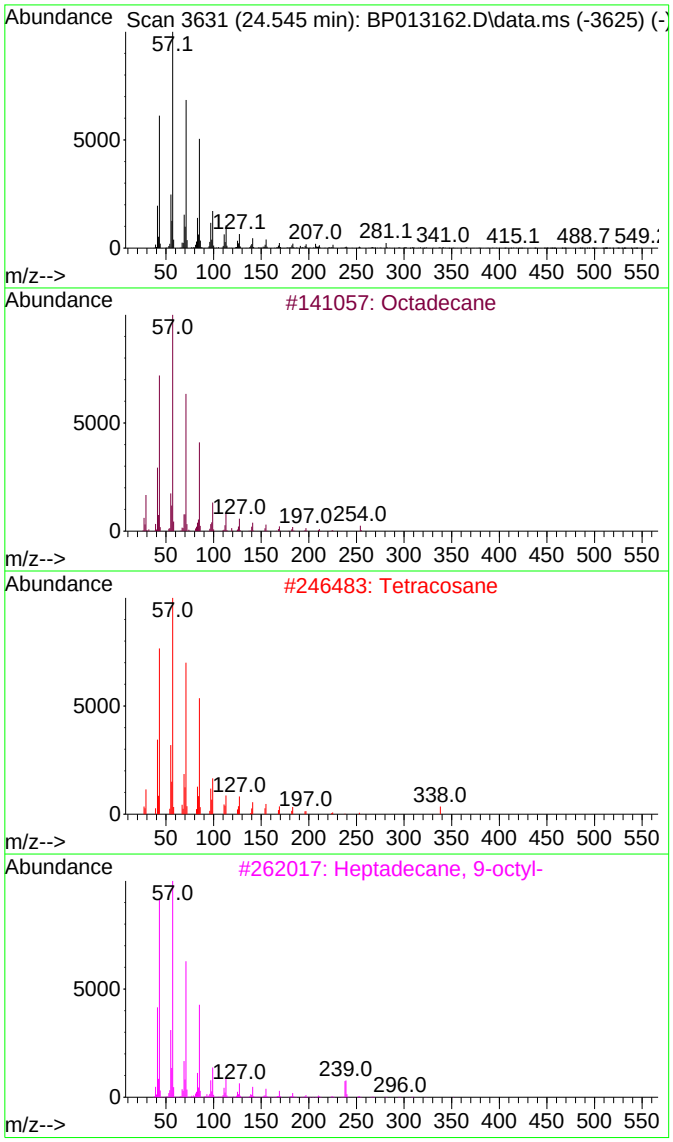
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

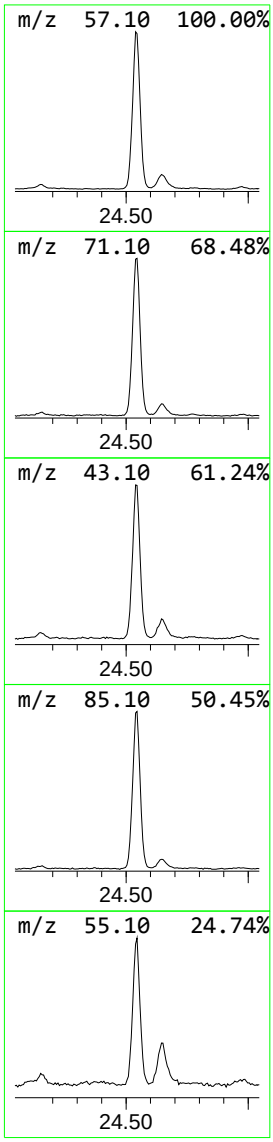
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.545	9.93 ng/ul	3495540	Perylene-d12	23.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Tetracosane	338	C24H50	000646-31-1	95
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
5	2-Methylpentacosane	366	C26H54	000629-87-8	93





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Data File : BP013162.D
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Instrument :
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ClientSampleId :
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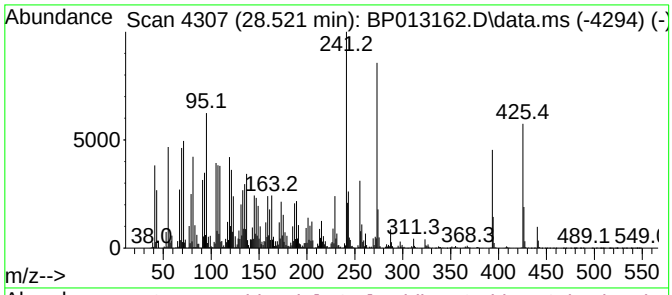
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

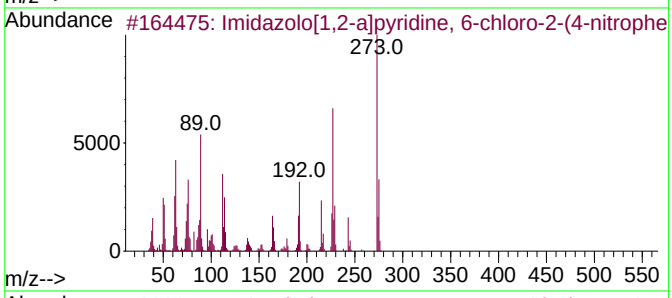
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

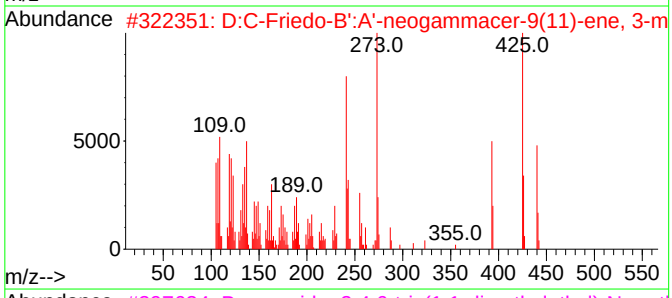
****
Peak Number 9 Imidazolo[1,2-a]pyridine, 6... Concentration Rank 1

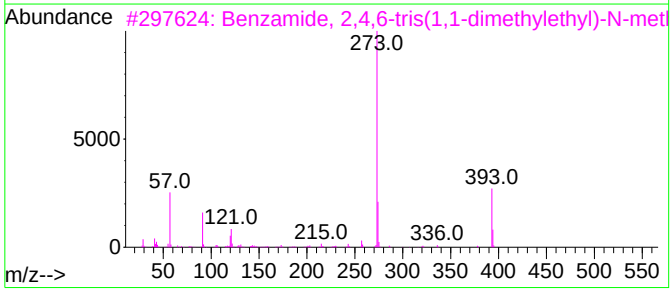
R.T.	EstConc	Area	Relative to ISTD	R.T.
28.521	119.92 ng/ul	42232300	Perylene-d12	23.921

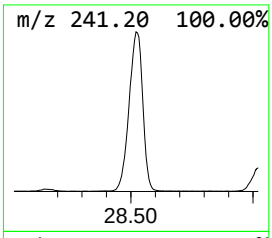
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	53
2	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	47
3	Benzamide, 2,4,6-tris(1,1-dimeth...	393	C27H39NO	016420-52-3	18
4	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	15
5	2-(Phenylmethyl)phenol, tert-but...	298	C19H26OSi	1417315-87-7	15

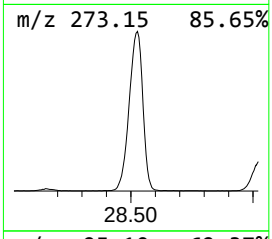


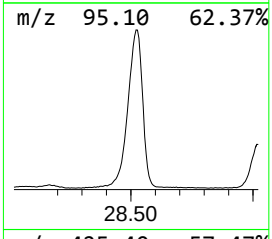


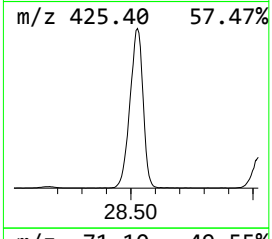


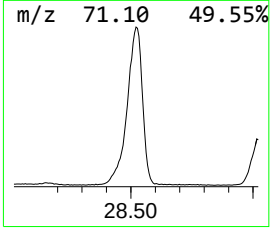












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ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXQ3

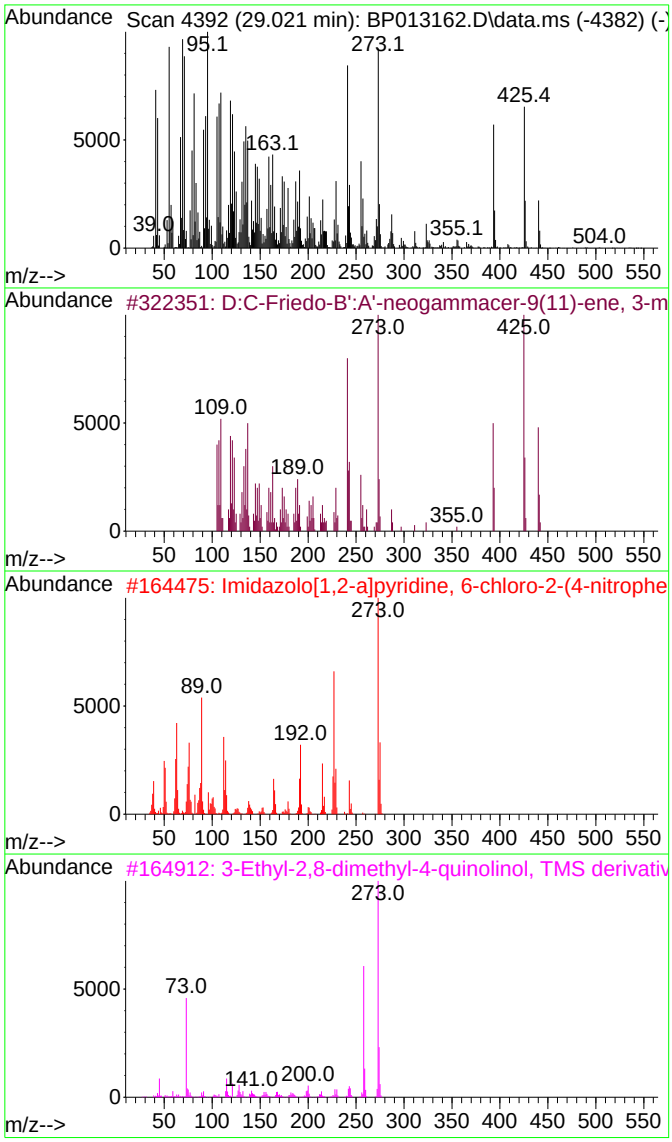
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

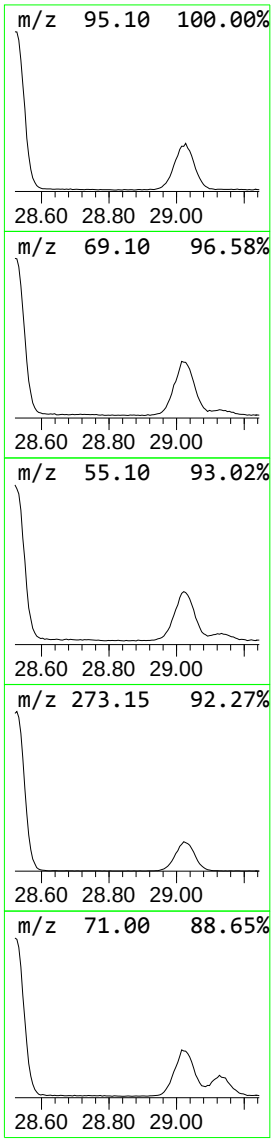
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 D:C-Friedo-B':A'-neogammace... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.021	30.06 ng/ul	10586200	Perylene-d12	23.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	96
2	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	56
3	3-Ethyl-2,8-dimethyl-4-quinolino...	273	C16H23NOSi	1000474-26-4	44
4	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	38
5	1-(4-Methyl-6-chloro-quinolin-2-...	273	C14H12ClN3O	111784-26-0	25





Tentatively Identified Compound (LSC) summary

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BNA_P
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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	2.2	ng/ul	305770	1	7.952	2753380	20.0
Benzophenone	15.951	15.3	ng/ul	3461830	3	14.598	4513870	20.0
n-Hexadecanoic ...	18.222	5.7	ng/ul	1376400	4	17.351	4829100	20.0
Isopropyl palmi...	18.633	2.5	ng/ul	594153	4	17.351	4829100	20.0
Octadecanoic acid	19.451	2.1	ng/ul	633583	5	21.439	6135040	20.0
(DEL) Alkane: S...	21.127	5.9	ng/ul	1820360	5	21.439	6135040	20.0
(DEL) Alkane: S...	23.133	14.8	ng/ul	5201180	6	23.921	7043660	20.0
(DEL) Alkane: S...	24.545	9.9	ng/ul	3495540	6	23.921	7043660	20.0
Imidazolo[1,2-a...	28.521	119.9	ng/ul	42232300	6	23.921	7043660	20.0
D:C-Friedo-B':A...	29.021	30.1	ng/ul	10586200	6	23.921	7043660	20.0