LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

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-BP100423.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP017551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.293	31	35	43	rVB	27605	39528	0.17%	0.059%
2	3.728	106	109	121	rBV	199159	309883	1.34%	0.464%
3	3.917	136	141	150	rVB7	9308	23298	0.10%	0.035%
4	4.558	245	250	255	rBV2	16668	24870	0.11%	0.037%
5	7.099	677	682	694	rVB	133089	216249	0.93%	0.324%
6	7.281	707	713	722	rBV	548303	860297	3.71%	1.289%
7	7.458	737	743	755	rBV	513584	843322	3.64%	1.264%
8	7.940	818	825	834	rBV	477418	737010	3.18%	1.105%
9	8.663	941	948	963	rBV	402825	668695	2.88%	1.002%
10	9.146	1023	1030	1044	rBV	669824	1095567	4.73%	1.642%
11	9.863	1143	1152	1163	rBV	569360	919353	3.97%	1.378%
12	10.393	1235	1242	1252	rBV	786267	1321805	5.70%	1.981%
13	10.775	1299	1307	1314	rBV	625400	1027633	4.43%	1.540%
14	10.946	1326	1336	1351	rBV	713074	1255406	5.42%	1.881%
15	11.222	1376	1383	1387	rBV	17905	29858	0.13%	0.045%
16	11.269	1387	1391	1397	rVB3	21919	33274	0.14%	0.050%
17	11.804	1475	1482	1495	rBV3	47473	126329	0.54%	0.189%
18	12.122	1525	1536	1546	rBV	96783	188165	0.81%	0.282%
19	12.369	1572	1578	1586	rBV4	13198	25689	0.11%	0.038%
20	12.569	1603	1612	1617	rBV	44471	70188	0.30%	0.105%
21	13.469	1756	1765	1771	rBV	25416	45351	0.20%	0.068%
22	13.945	1841	1846	1857	rVB	99251	158456	0.68%	0.237%
23	14.051	1857	1864	1869	rBV	1734032	2358638	10.18%	3.535%
24	14.110	1869	1874	1878	rVB	260996	352794	1.52%	0.529%
25	14.334	1904	1912	1920	rBV	1740601	2569477	11.08%	3.851%
26	14.422	1923	1927	1932	rVB	18597	31457	0.14%	0.047%
27	14.634	1954	1963	1972	rBV	997428	1426537	6.15%	2.138%
28	14.798	1986	1991	1998	rVB	32300	47082	0.20%	0.071%
29	14.881	1998	2005	2023	rBV	91948	206922	0.89%	0.310%
30	15.022	2025	2029	2036	rBV6	15521	27816	0.12%	0.042%
31	15.122	2041	2046	2054	rBV	185274	272631	1.18%	0.409%
32	15.634	2126	2133	2142	rBV	2360277	3366312	14.52%	5.045%
33	15.775	2151	2157	2162	rBV	741146	1020779	4.40%	1.530%
34	15.834	2162	2167	2173	rVV	471422	631099	2.72%	0.946%
35	16.298	2231	2246	2265	rBV	9303627	23180204	100.00%	34.740%
36	16.469	2273	2275	2288	rVB2	37977	71173	0.31%	0.107%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

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-BP100423.MA.M
Title : SVOA CALIBRATION

37	16.563	2288	2291	2296	rVB5	16967	26659	0.12%	0.040%
38	16.981	2358	2362	2369	rVB	108303	144065	0.62%	0.216%
39	17.316	2413	2419	2431	rBV	194803	396577	1.71%	0.594%
40	17.422	2431	2437	2445	rVV	1286383	1757783	7.58%	2.634%
41	17.522	2448	2454	2466	rVB	2799100	3867605	16.68%	5.796%
42	18.269	2576	2581	2595	rBV	352023	517395	2.23%	0.775%
43	18.422	2603	2607	2610	rBV2	23433	27666	0.12%	0.041%
44	19.204	2737	2740	2745	rBV	37909	51486	0.22%	0.077%
45	19.345	2761	2764	2767	rBV2	36353	39188	0.17%	0.059%
46	19.386	2767	2771	2772	rBV	52902	66972	0.29%	0.100%
47	19.516	2788	2793	2799	rBV3	149210	224974	0.97%	0.337%
48	19.775	2832	2837	2843	rBV	3755219	4827670	20.83%	7.235%
49	21.210	3078	3081	3088	rBV4	117740	169658	0.73%	0.254%
50	21.557	3135	3140	3146	rBV	1579072	1976787	8.53%	2.963%
51	23.968	3542	3550	3560	rVB2	2510402	5032290	21.71%	7.542%
52	24.139	3572	3579	3587	rVB	994768	2015840	8.70%	3.021%

Sum of corrected areas: 66725762

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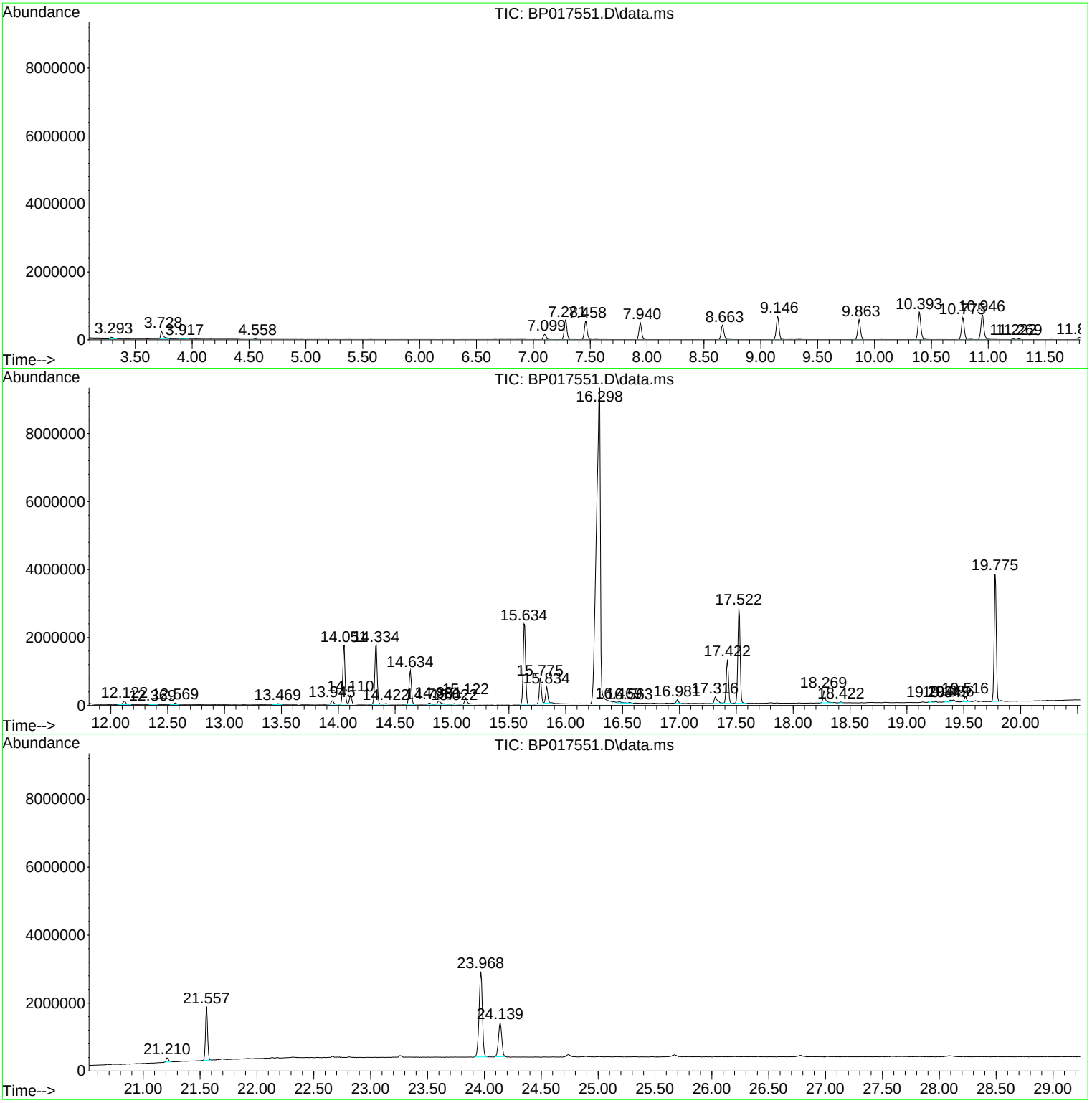
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.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\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

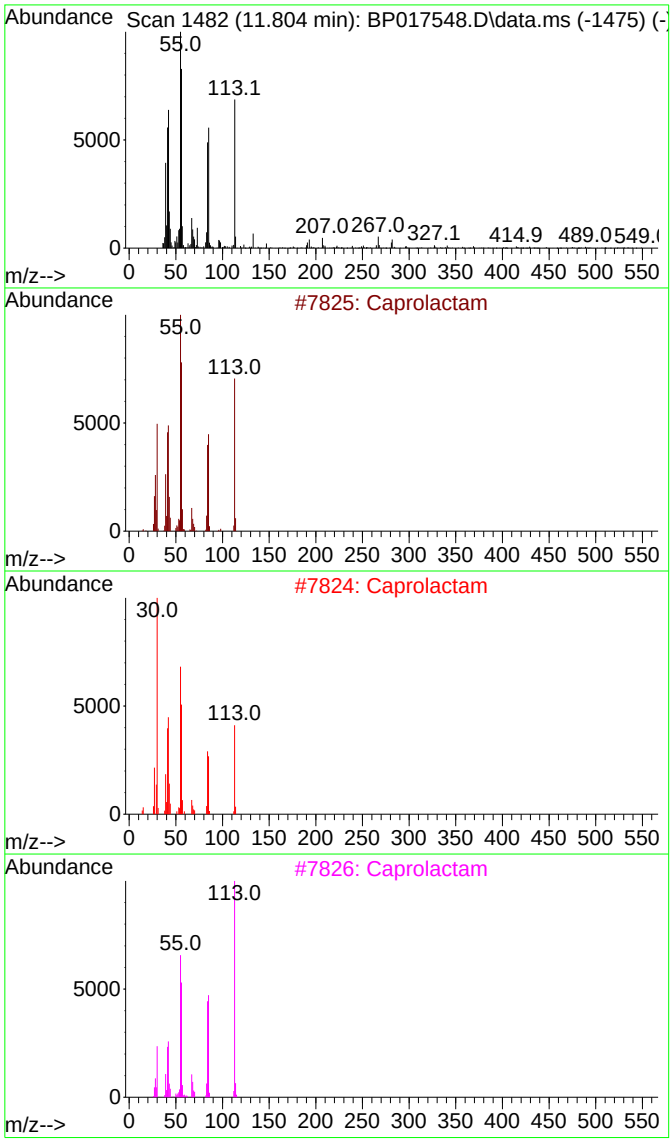
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

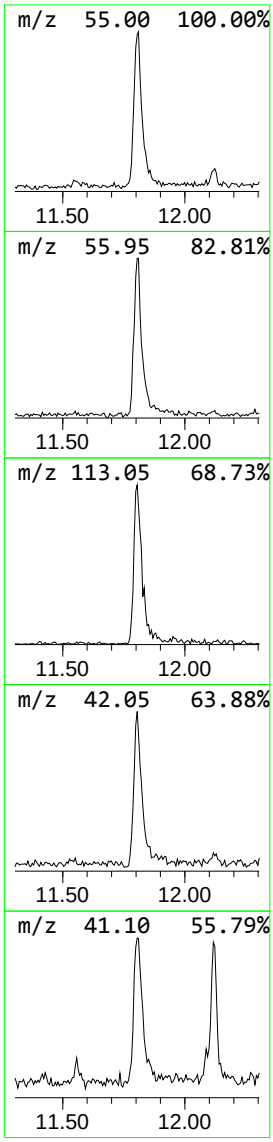
****

Peak Number 1 Capro lactam Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.46 ng/ul	126329	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caprolactam	113	C6H11NO	000105-60-2	95
2	Caprolactam	113	C6H11NO	000105-60-2	94
3	Caprolactam	113	C6H11NO	000105-60-2	87
4	Caprolactam	113	C6H11NO	000105-60-2	81
5	Caprolactam	113	C6H11NO	000105-60-2	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

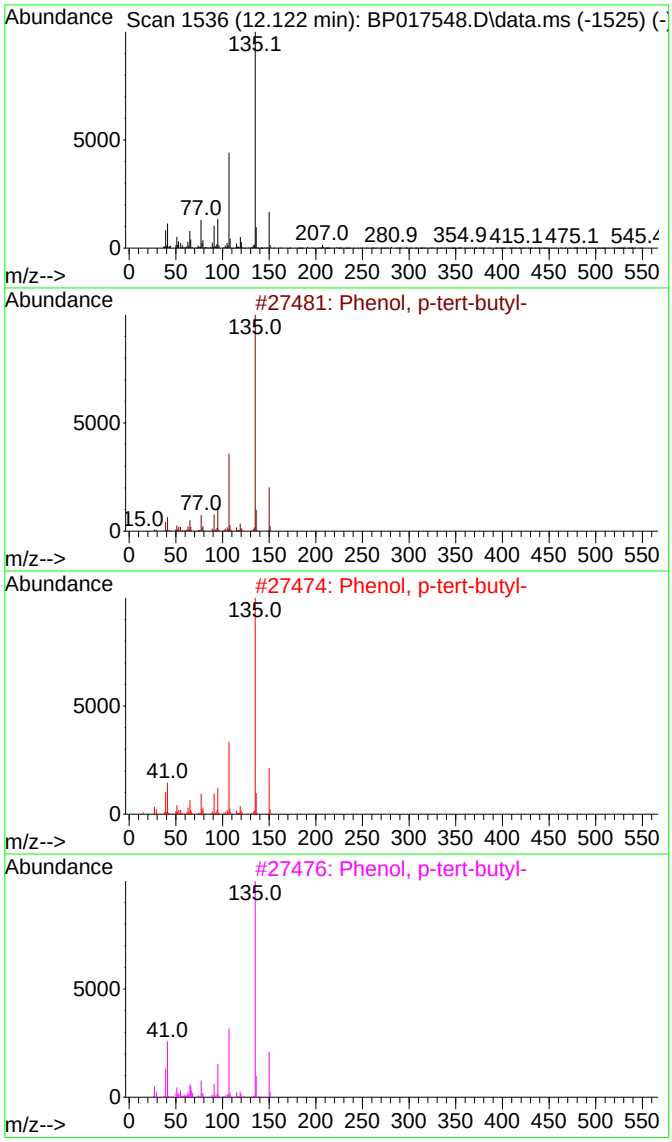
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

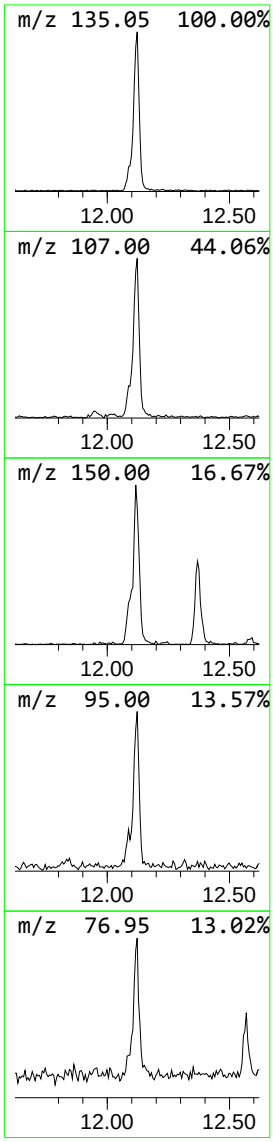
****

Peak Number 2 Phenol, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.122	3.66 ng/ul	188165	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	87
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	81
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

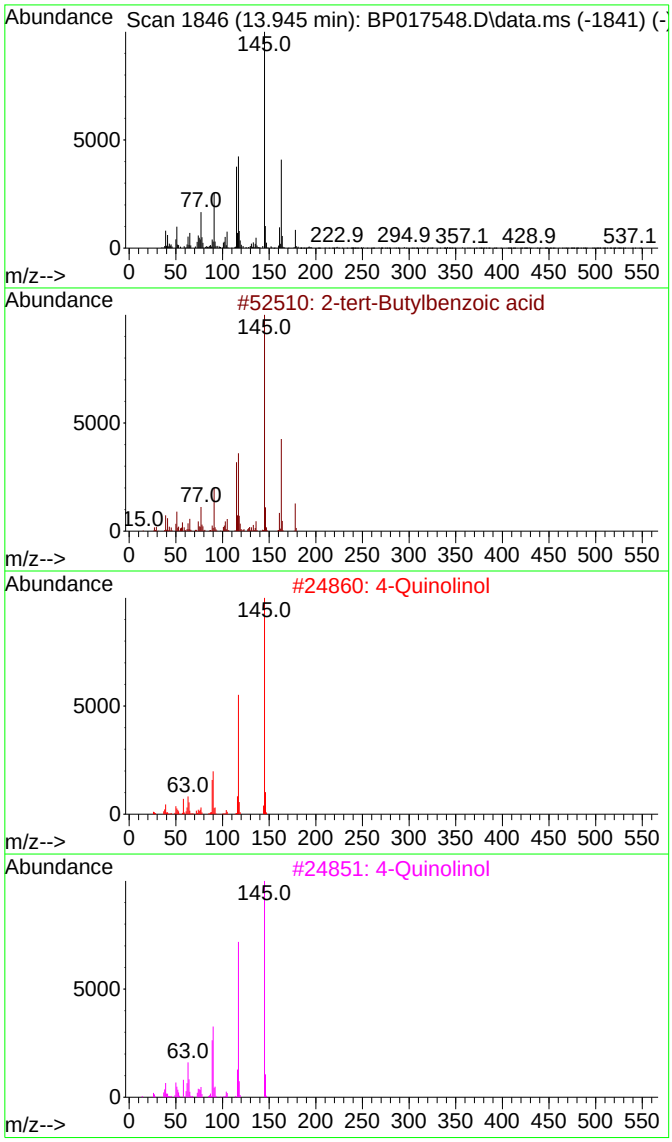
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

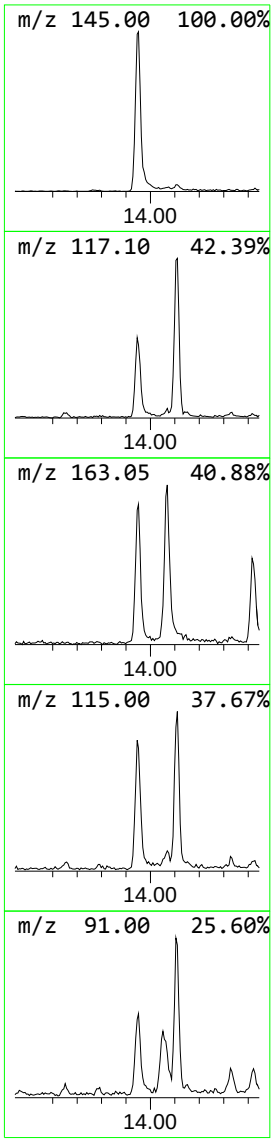
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-tert-Butylbenzoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.22 ng/ul	158456	Acenaphthene-d10	14.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-tert-Butylbenzoic acid	178	C11H14O2	001077-58-3	96
2	4-Quinolinol	145	C9H7NO	000611-36-9	49
3	4-Quinolinol	145	C9H7NO	000611-36-9	47
4	Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	47
5	Cyclopropanecarboxylic acid, tra...	272	C16H13ClO2	1000406-84-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

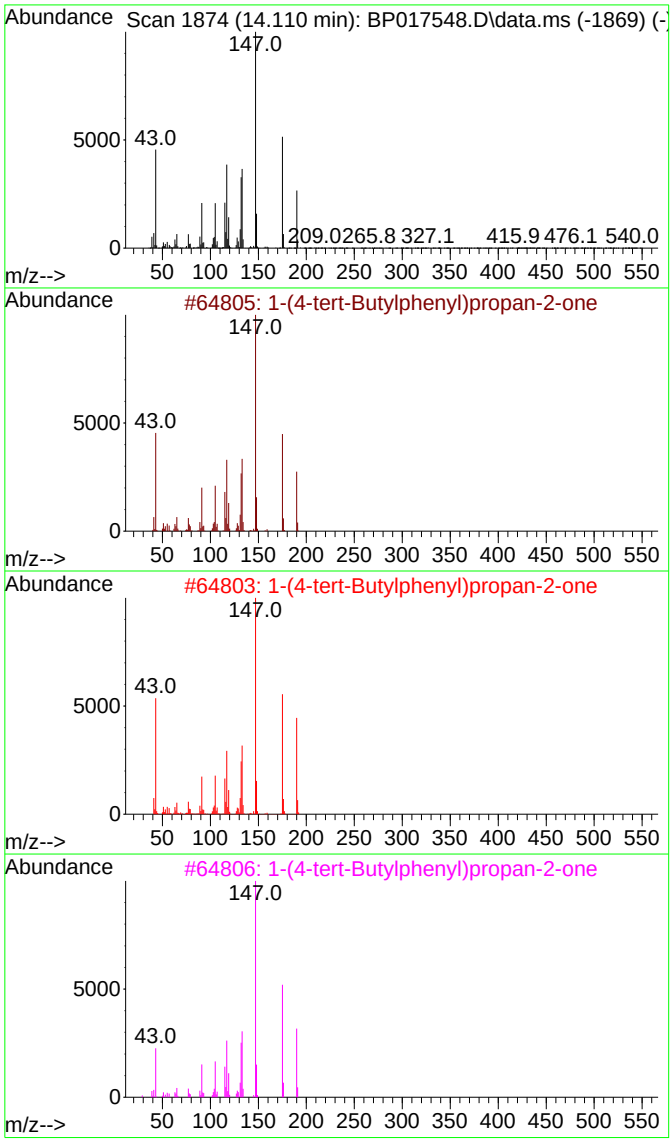
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

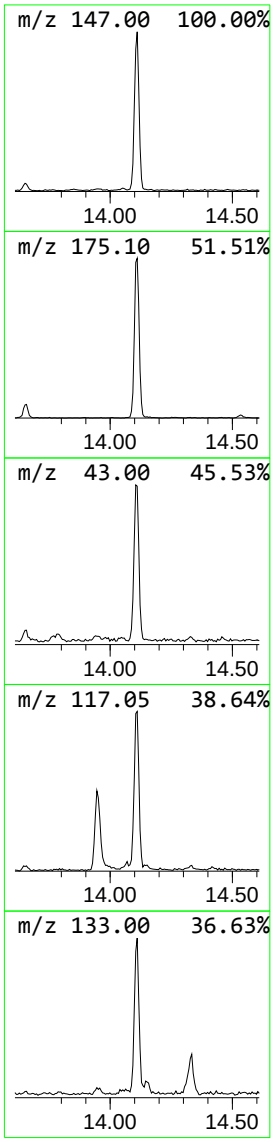
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-(4-tert-Butylphenyl)propa... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	4.95 ng/ul	352794	Acenaphthene-d10	14.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	99
2	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	98
3	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	97
4	4,5-Dimethylindoline-2,3-dione	175	C10H9NO2	1010443-10-6	46
5	1-Methyl-1H-benzimidazol-5-amine	147	C8H9N3	010394-38-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

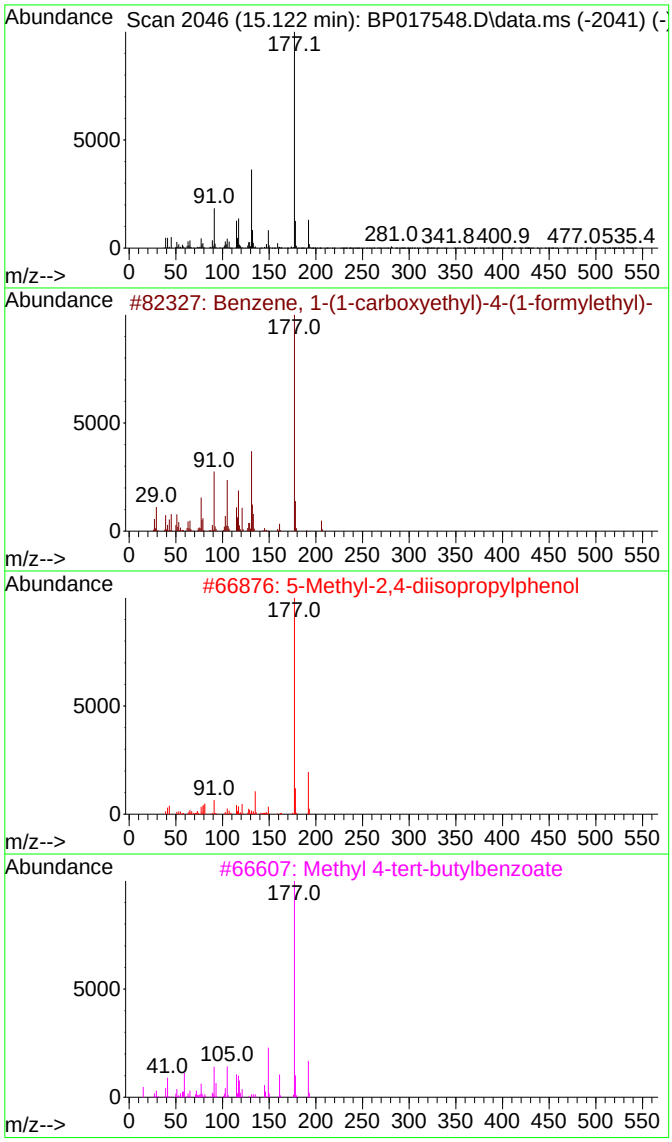
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

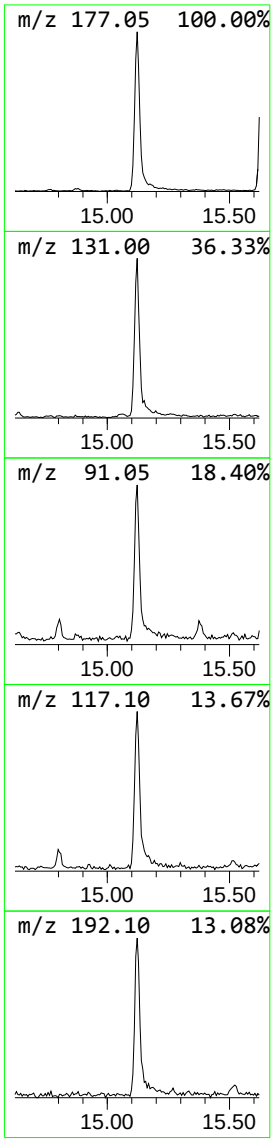
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-(1-carboxyethyl)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.122	3.82 ng/ul	272631	Acenaphthene-d10	14.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1-carboxyethyl)-4-(1...	206	C12H14O3	1000161-22-9	72
2	5-Methyl-2,4-diisopropylphenol	192	C13H20O	040625-96-5	64
3	Methyl 4-tert-butylbenzoate	192	C12H16O2	026537-19-9	64
4	Benzene, 1,4-bis(1-carboxyethyl)-	222	C12H14O4	150552-26-4	64
5	3-tert-Butylbenzoic acid, methyl...	192	C12H16O2	027330-57-0	59





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Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

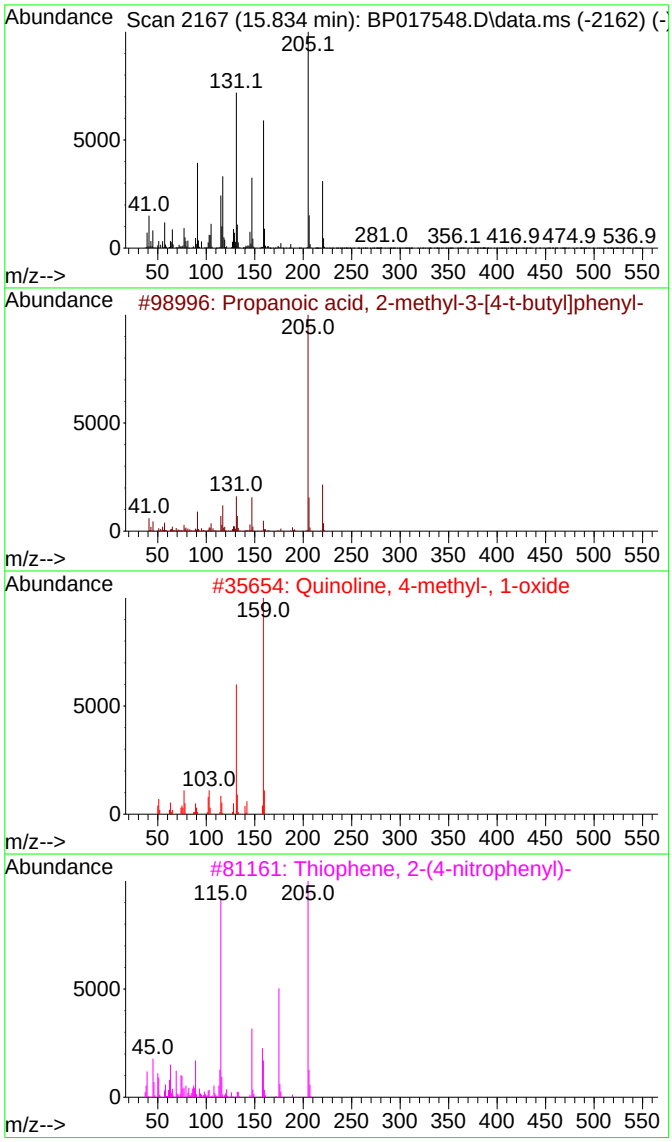
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

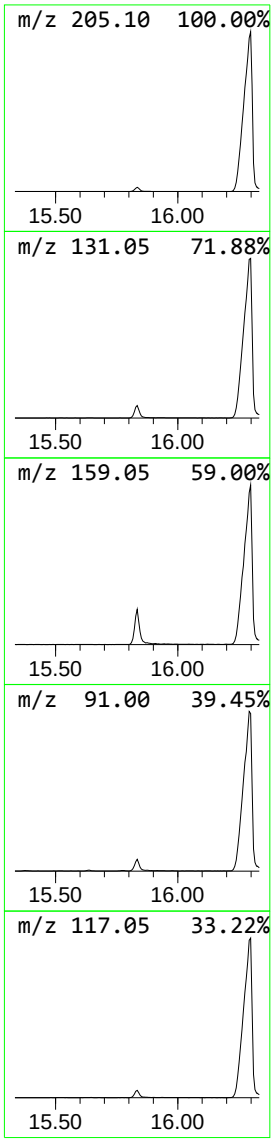
****

Peak Number 6 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	8.85 ng/ul	631099	Acenaphthene-d10	14.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	49
2	Quinoline, 4-methyl-, 1-oxide	159	C10H9NO	004053-40-1	38
3	Thiophene, 2-(4-nitrophenyl)-	205	C10H7NO2S	059156-21-7	35
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	30
5	Ethyl 4-acetyl-3,5-dimethylbenzoate	220	C13H16O3	1000431-98-6	30





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Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

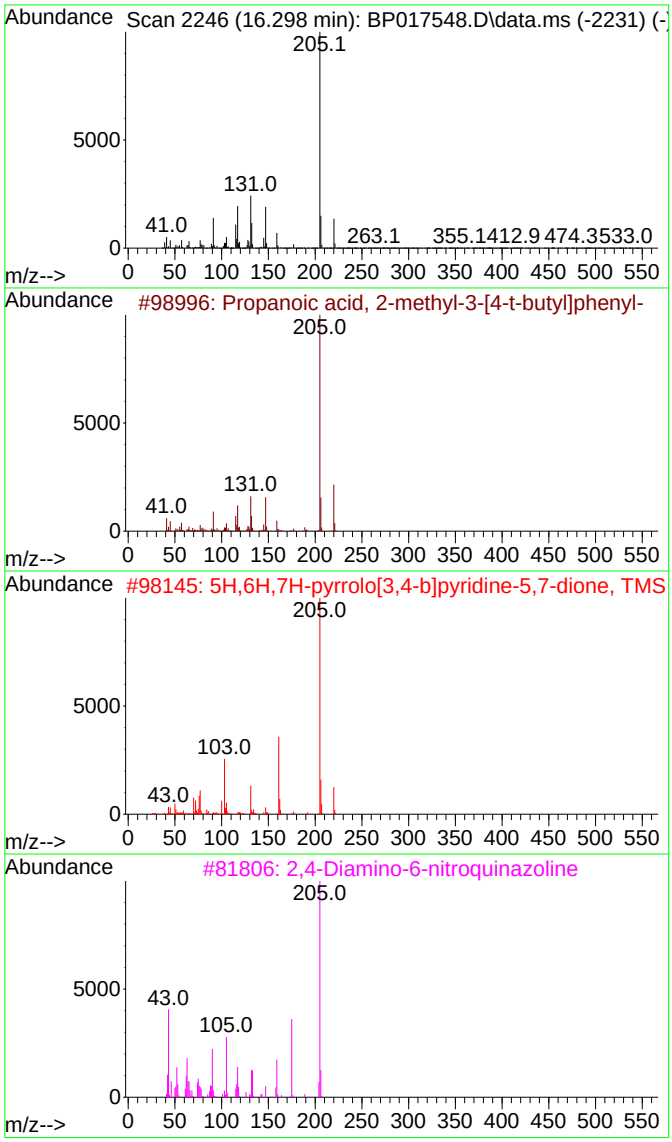
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

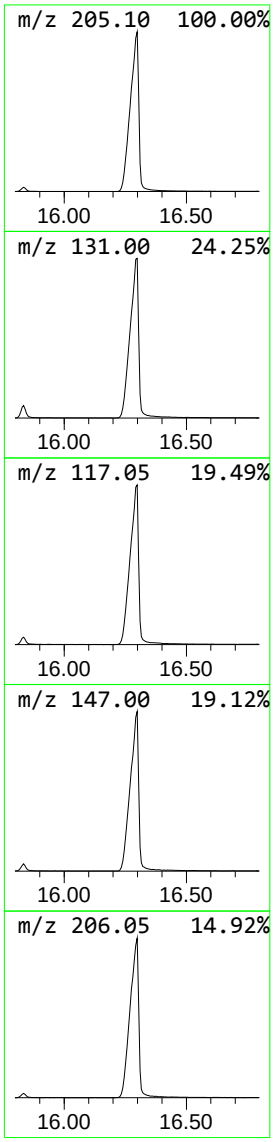
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, 2-methyl-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.298	263.74 ng/ul	23180200	Phenanthrene-d10	17.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	97
2	5H,6H,7H-pyrrolo[3,4-b]pyridine-...	220	C10H12N2O2Si	1000485-20-1	47
3	2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	46
4	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	43
5	(4S)-Perhydro-3-benzyl-4-methyl-...	205	C12H15NO2	1000434-17-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

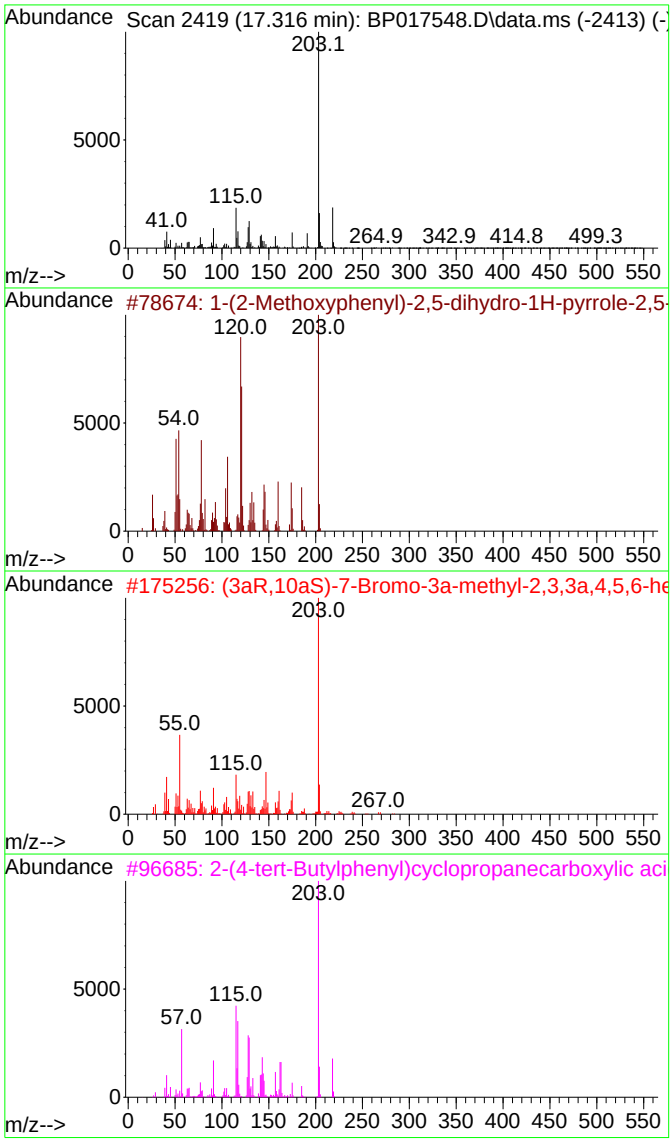
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

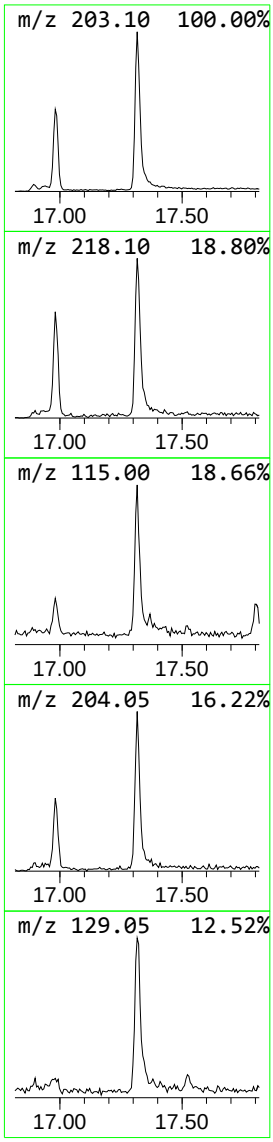
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-(2-Methoxyphenyl)-2,5-dih... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.316	4.51 ng/ul	396577	Phenanthrene-d10	17.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Methoxyphenyl)-2,5-dihydro-...	203	C11H9NO3	017392-68-6	91
2	(3aR,10aS)-7-Bromo-3a-methyl-2,3...	282	C13H15BrO2	1010482-61-0	80
3	2-(4-tert-Butylphenyl)cyclopropa...	218	C14H18O2	1000474-95-9	64
4	Eupatoriochromene	218	C13H14O3	019013-03-7	64
5	Benzoic acid, 4-(3-hydroxy-3-met...	218	C13H14O3	033577-98-9	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

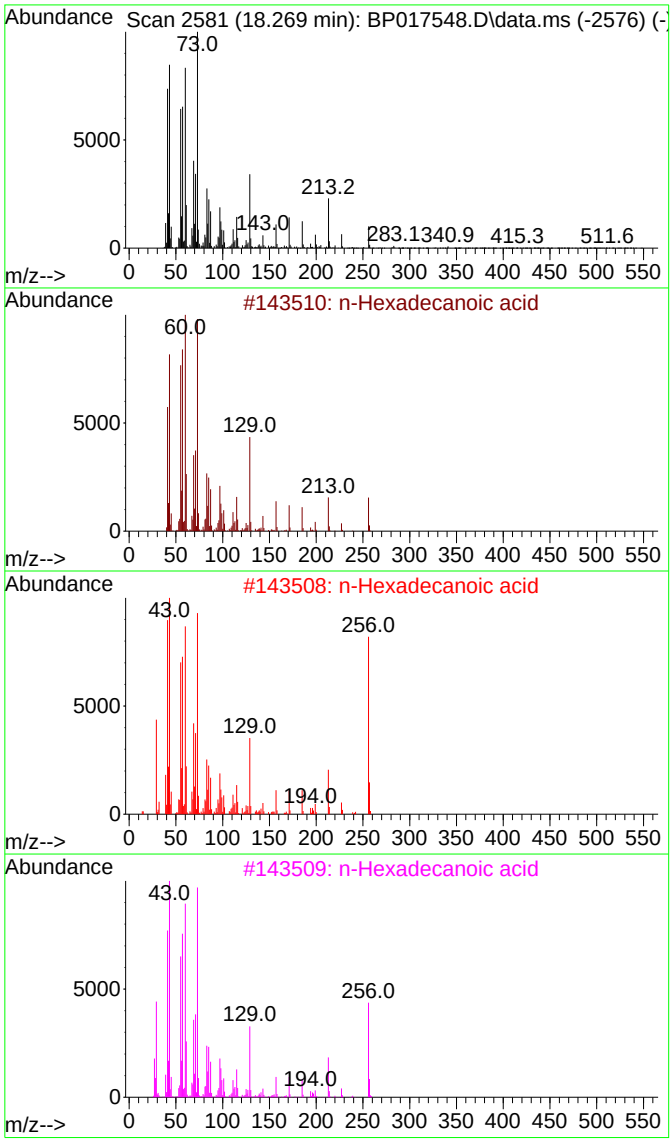
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

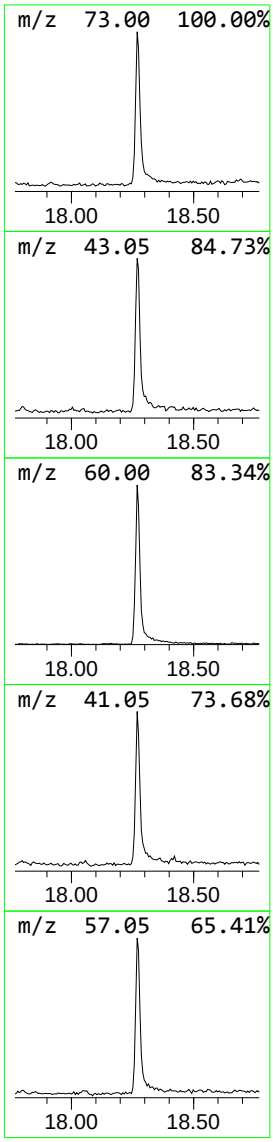
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.269	5.89 ng/ul	517395	Phenanthrene-d10	17.422

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	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

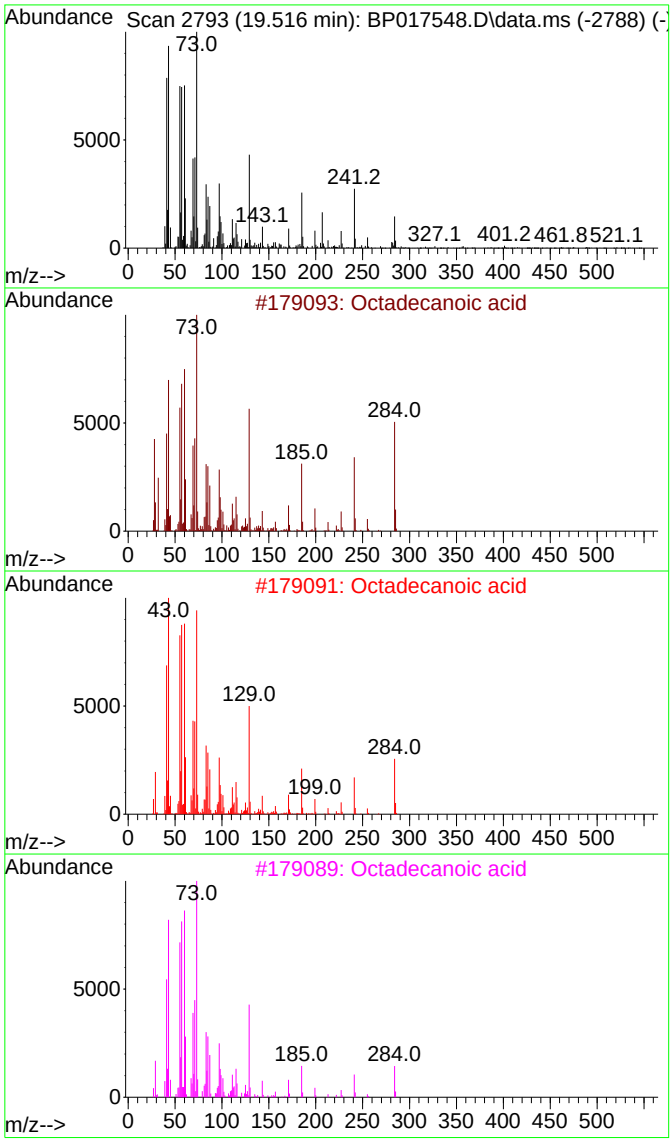
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

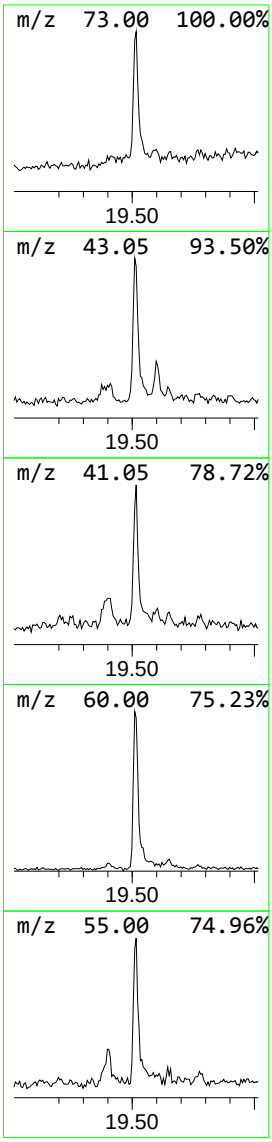
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	2.28 ng/ul	224974	Chrysene-d12	21.557

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	95
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017548.D
Acq On : 05 Oct 2023 01:40
Operator : MA/JU
Sample : 04679-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PMW-1(20230926)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.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
Capro lactam	11.804	2.5	ng/ul	126329	2	10.775	1027630	20.0
Phenol, p-tert-...	12.122	3.7	ng/ul	188165	2	10.775	1027630	20.0
2-tert-Butylben...	13.945	2.2	ng/ul	158456	3	14.634	1426540	20.0
1-(4-tert-Butyl...	14.110	5.0	ng/ul	352794	3	14.634	1426540	20.0
Benzene, 1-(1-c...	15.122	3.8	ng/ul	272631	3	14.634	1426540	20.0
unknown-01	15.834	8.8	ng/ul	631099	3	14.634	1426540	20.0
Propanoic acid,...	16.298	263.7	ng/ul	23180200	4	17.422	1757780	20.0
1-(2-Methoxyphe...	17.316	4.5	ng/ul	396577	4	17.422	1757780	20.0
n-Hexadecanoic ...	18.269	5.9	ng/ul	517395	4	17.422	1757780	20.0
Octadecanoic acid	19.516	2.3	ng/ul	224974	5	21.557	1976790	20.0