LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

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-BP120123.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	27	30	38	rVB	81256	109097	0.89%	0.091%
2	3.552	76	79	89	rVB2	21098	33150	0.27%	0.028%
3	3.687	98	102	114	rBV	271287	381697	3.10%	0.319%
4	3.922	138	142	150	rVB3	22638	37629	0.31%	0.031%
5	4.016	155	158	163	rVB	26367	32349	0.26%	0.027%
6	4.393	218	222	226	rVB6	11188	17332	0.14%	0.015%
7	5.775	453	457	463	rBV3	11500	21163	0.17%	0.018%
8	6.846	635	639	643	rVB3	12443	19253	0.16%	0.016%
9	7.016	659	668	675	rBV	329731	532843	4.33%	0.446%
10	7.187	690	697	707	rVB	1500639	2282925	18.56%	1.911%
11	7.381	723	730	739	rBV	1293197	2034107	16.54%	1.702%
12	7.469	742	745	754	rVB3	12418	20631	0.17%	0.017%
13	7.852	803	810	817	rBV	1377965	2153787	17.51%	1.802%
14	7.922	817	822	826	rVB3	20123	35583	0.29%	0.030%
15	8.563	923	931	940	rBV	1039141	1683323	13.69%	1.409%
16	9.010	999	1007	1019	rBV	1766868	2824271	22.97%	2.364%
17	9.181	1032	1036	1042	rVB5	21370	31925	0.26%	0.027%
18	9.434	1073	1079	1084	rVB	30304	42499	0.35%	0.036%
19	9.734	1120	1130	1141	rBV	1311264	2160263	17.57%	1.808%
20	9.969	1165	1170	1178	rBV3	56684	92978	0.76%	0.078%
21	10.269	1214	1221	1239	rBV	1971621	3323481	27.03%	2.781%
22	10.645	1277	1285	1292	rBV	1886985	3193307	25.97%	2.672%
23	10.704	1292	1295	1300	rVB6	13474	22468	0.18%	0.019%
24	10.787	1300	1309	1321	rBV	1597334	2656379	21.60%	2.223%
25	11.440	1415	1420	1427	rBV5	16121	30246	0.25%	0.025%
26	11.928	1498	1503	1507	rBV2	16707	24996	0.20%	0.021%
27	12.234	1549	1555	1560	rBV3	41799	68046	0.55%	0.057%
28	12.763	1636	1645	1652	rBV5	19657	45764	0.37%	0.038%
29	13.104	1698	1703	1705	rBV5	7196	12573	0.10%	0.011%
30	13.387	1745	1751	1757	rBV2	80440	132206	1.08%	0.111%
31	13.898	1831	1838	1844	rVV	3931908	5536035	45.02%	4.633%
32	14.004	1855	1856	1864	rVB3	6407	12993	0.11%	0.011%
33	14.175	1875	1885	1899	rBV	4529714	6775090	55.09%	5.670%
34	14.481	1929	1937	1947	rBV	3013290	4462311	36.29%	3.734%
35	14.563	1947	1951	1957	rVB2	33555	46791	0.38%	0.039%
36	14.681	1965	1971	1982	rBV	239076	419221	3.41%	0.351%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : C0AK6

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-BP120123.MA.M
Title : SVOA CALIBRATION

37	14.898	2002	2008	2014	rVB7	24954	45450	0.37%	0.038%
38	15.157	2047	2052	2059	rVB3	27389	49729	0.40%	0.042%
39	15.286	2069	2074	2075	rBV2	28220	35993	0.29%	0.030%
40	15.475	2099	2106	2114	rBV	5627917	8143793	66.22%	6.816%
41	15.592	2118	2126	2135	rBV	1328100	1921235	15.62%	1.608%
42	15.710	2142	2146	2153	rVB3	27103	45805	0.37%	0.038%
43	15.839	2164	2168	2173	rBV3	18104	25963	0.21%	0.022%
44	16.257	2235	2239	2248	rVB9	8423	16982	0.14%	0.014%
45	16.828	2330	2336	2339	rBV	19823	29703	0.24%	0.025%
46	17.227	2393	2404	2411	rBV	3012722	4291850	34.90%	3.592%
47	17.327	2414	2421	2430	rBV2	6212791	8663123	70.45%	7.250%
48	17.516	2451	2453	2462	rVB3	11520	18059	0.15%	0.015%
49	17.845	2506	2509	2512	rBV4	10068	14213	0.12%	0.012%
50	17.898	2514	2518	2523	rVV	333373	420034	3.42%	0.352%
51	18.116	2551	2555	2561	rBV2	107629	154250	1.25%	0.129%
52	18.186	2565	2567	2572	rVB	19082	25917	0.21%	0.022%
53	19.139	2725	2729	2735	rVB	84556	104996	0.85%	0.088%
54	19.204	2736	2740	2749	rBV	79460	126074	1.03%	0.106%
55	19.351	2761	2765	2770	rBV2	109728	153224	1.25%	0.128%
56	19.563	2795	2801	2807	rBV	6843891	9139199	74.32%	7.649%
57	21.316	3094	3099	3108	rBV	3040215	3985646	32.41%	3.336%
58	21.510	3129	3132	3143	rBV	282678	488530	3.97%	0.409%
59	22.468	3291	3295	3305	rVB2	279562	523009	4.25%	0.438%
60	23.533	3469	3476	3483	rBV2	4787959	9440104	76.76%	7.900%
61	23.686	3496	3502	3512	rVB	2199416	4416263	35.91%	3.696%
62	24.598	3650	3657	3667	rVB	2814901	6286296	51.12%	5.261%
63	26.403	3953	3964	3982	rVB2	3786619	12297606	100.00%	10.292%
64	28.868	4372	4383	4402	rVB2	1713547	7317268	59.50%	6.124%

Sum of corrected areas: 119489026

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
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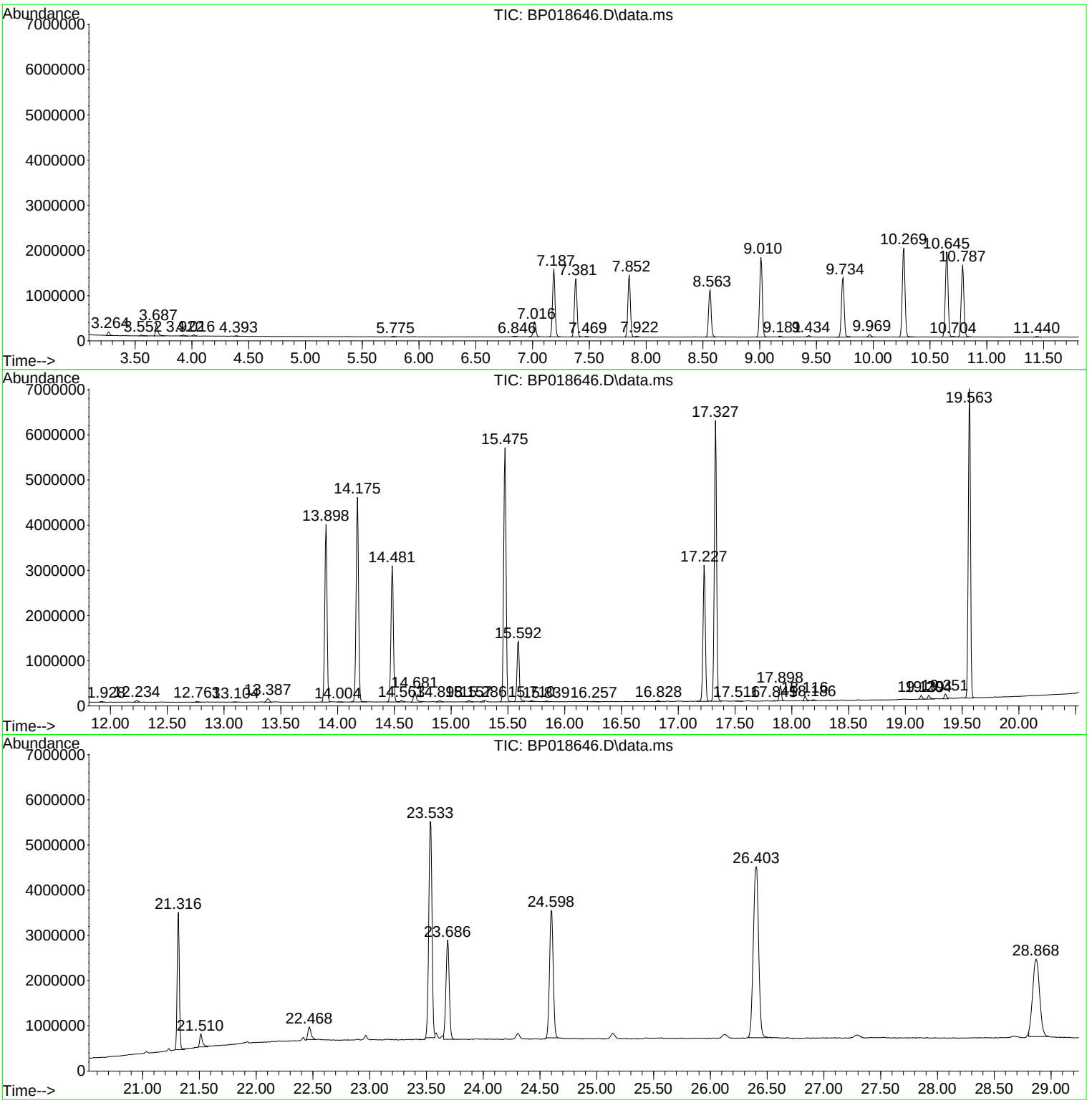
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

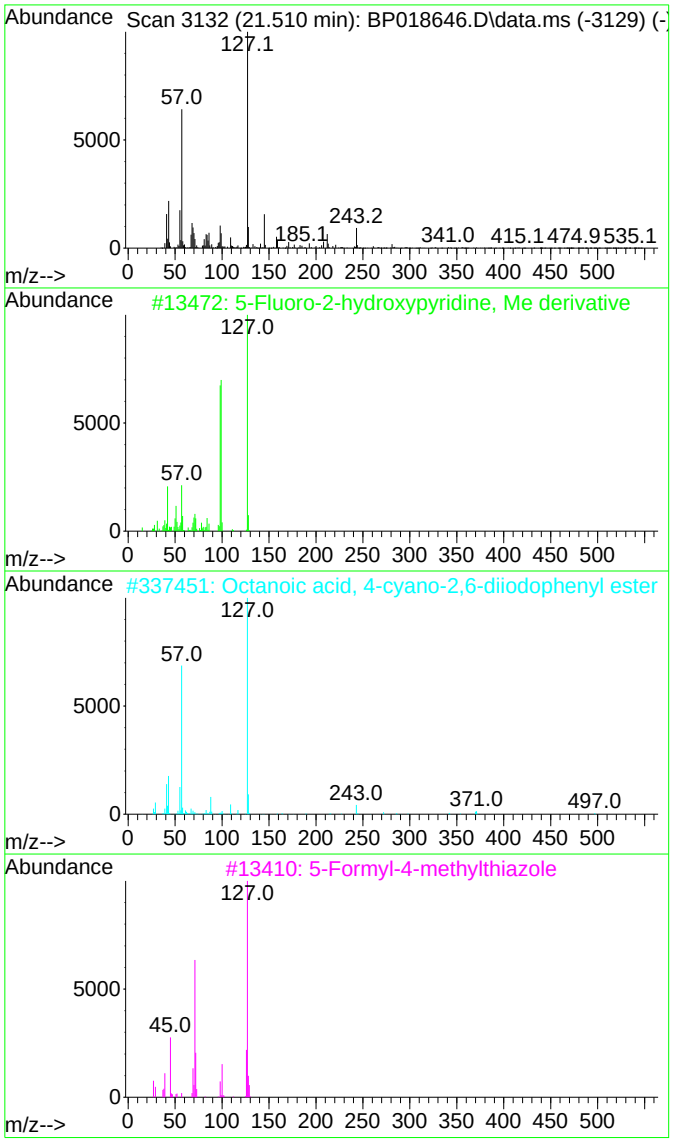
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

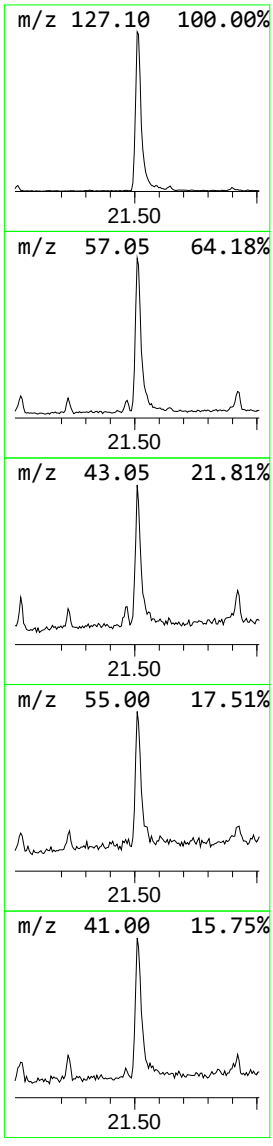
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 5-Fluoro-2-hydroxypyridine,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.510	2.45 ng/ul	488530	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-hydroxypyridine, Me d...	127	C6H6FNO	1000496-67-4	59
2	Octanoic acid, 4-cyano-2,6-diiod...	497	C15H17I2NO2	003861-47-0	59
3	5-Formyl-4-methylthiazole	127	C5H5NOS	082294-70-0	59
4	Oxalic acid, monoamide, monohydr...	213	C10H19N3O2	1000265-20-0	59
5	Caprylic anhydride	270	C16H30O3	000623-66-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

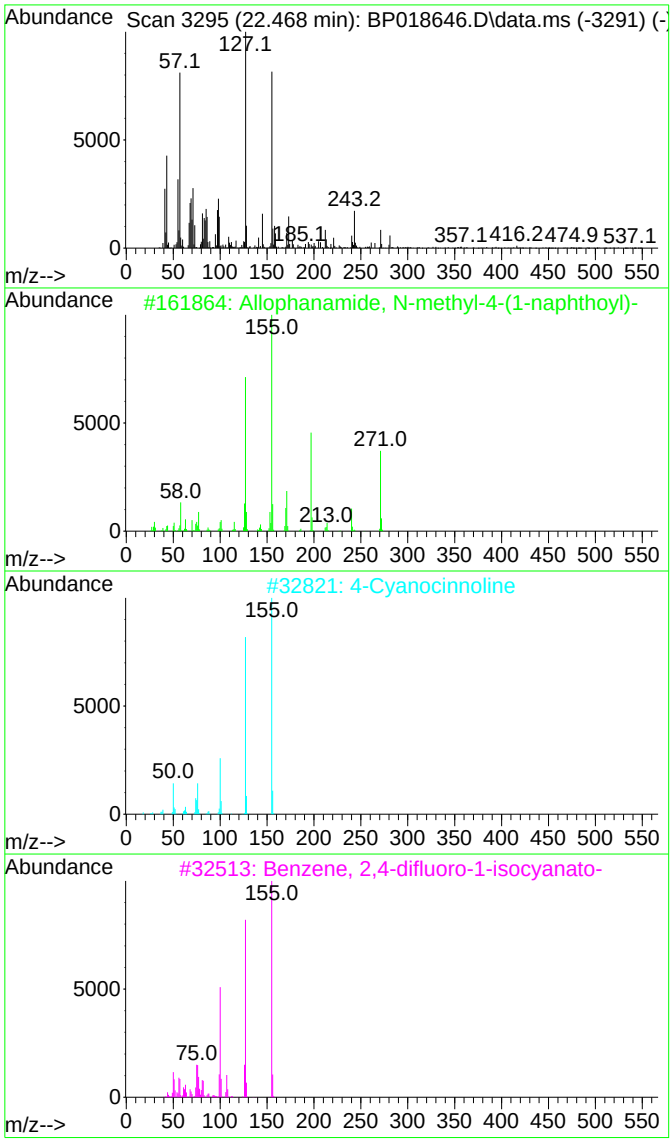
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

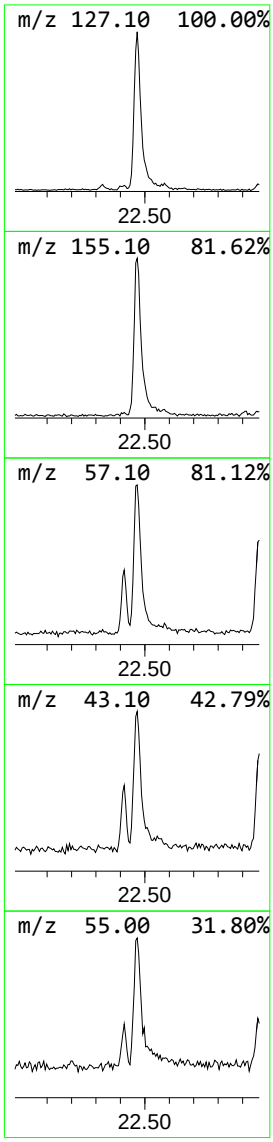
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Allophanamide, N-methyl-4-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.468	2.62 ng/ul	523009	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allophanamide, N-methyl-4-(1-nap...	271	C14H13N3O3	1000160-42-1	64
2	4-Cyanocinnoline	155	C9H5N3	016470-90-9	64
3	Benzene, 2,4-difluoro-1-isocyanato-	155	C7H3F2NO	059025-55-7	59
4	1-Naphthamide, N-butyl-N-isobutyl-	283	C19H25NO	1000415-71-5	59
5	.beta.-Naphthoylhydrazine	186	C11H10N2O	039627-84-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

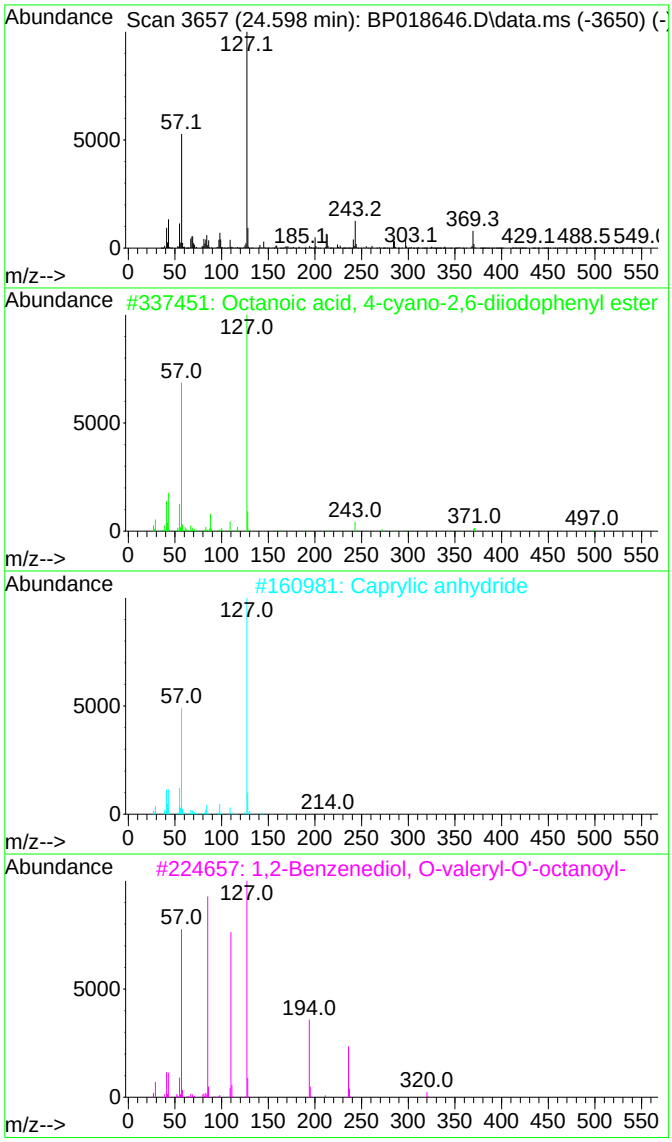
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

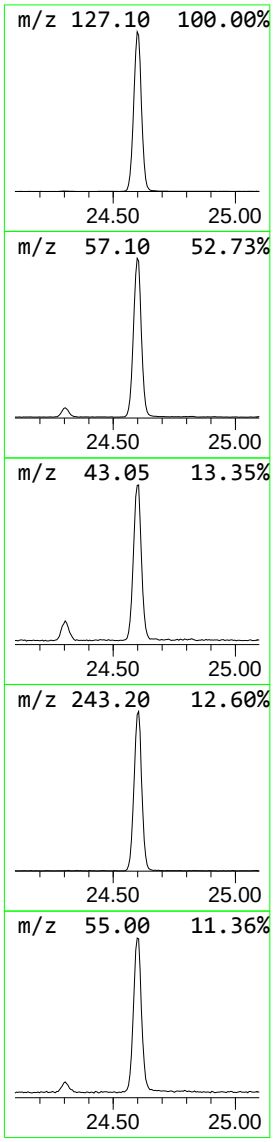
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octanoic acid, 4-cyano-2,6-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.598	28.47 ng/ul	6286300	Perylene-d12	23.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 4-cyano-2,6-diiod...	497	C15H17I2NO2	003861-47-0	53
2	Caprylic anhydride	270	C16H30O3	000623-66-5	53
3	1,2-Benzenediol, O-valeryl-O'-oc...	320	C19H28O4	1000329-77-5	53
4	4-Nitrophenyl caprylate	265	C14H19NO4	001956-10-1	53
5	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

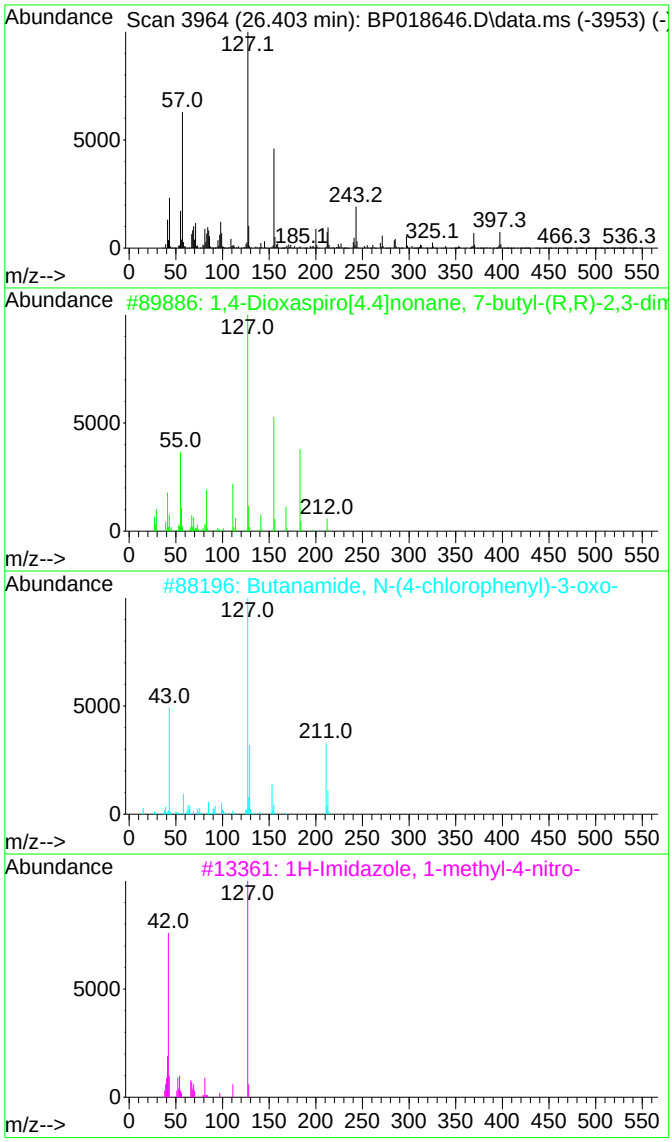
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

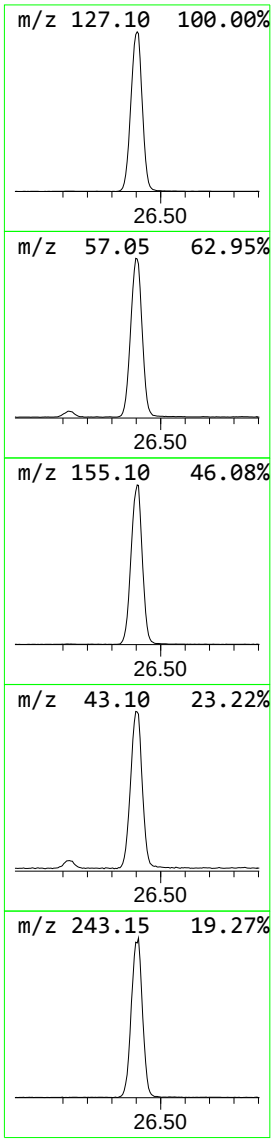
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,4-Dioxaspiro[4.4]nonane, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.404	55.69 ng/ul	12297600	Perylene-d12	23.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxaspiro[4.4]nonane, 7-but...	212	C13H24O2	104807-77-4	58
2	Butanamide, N-(4-chlorophenyl)-3...	211	C10H10ClNO2	000101-92-8	43
3	1H-Imidazole, 1-methyl-4-nitro-	127	C4H5N3O2	003034-41-1	38
4	2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	38
5	3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120423\
Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
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Sample : 05473-05
Misc :
ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AK6

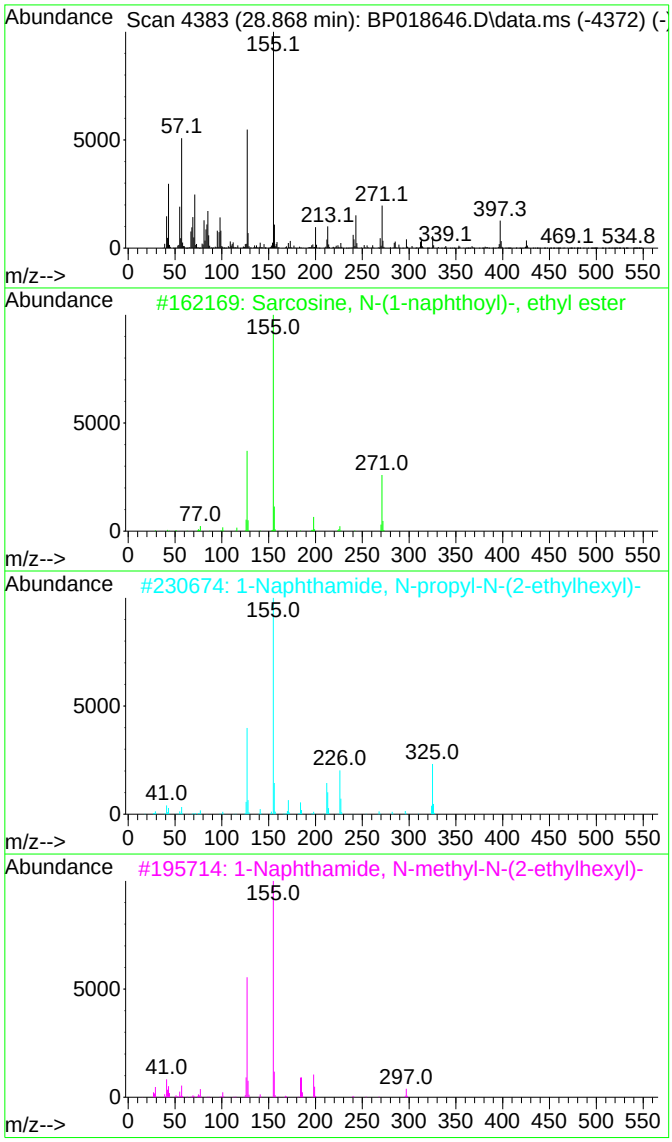
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

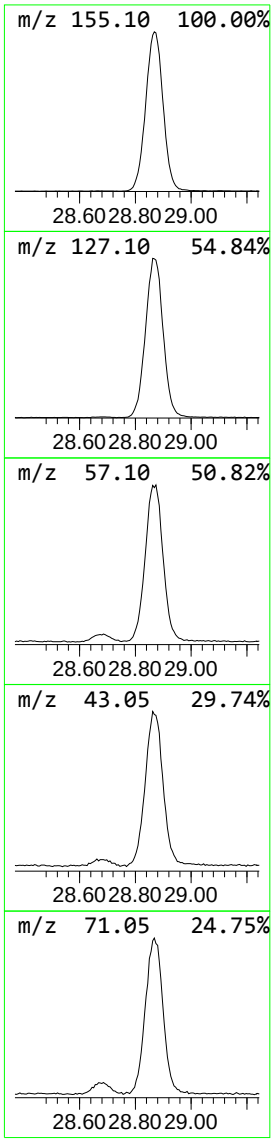
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Sarcosine, N-(1-naphthoyl)-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.868	33.14 ng/ul	7317270	Perylene-d12	23.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sarcosine, N-(1-naphthoyl)-, eth...	271	C16H17NO3	1000321-39-8	80
2	1-Naphthamide, N-propyl-N-(2-eth...	325	C22H31NO	1000438-07-1	62
3	1-Naphthamide, N-methyl-N-(2-eth...	297	C20H27NO	1000421-43-5	58
4	5-Amino-1-(quinolin-8-yl)-1,2,3-...	254	C12H10N6O	1000388-72-7	55
5	1-Naphthalenecarboxamide, N-(2-p...	317	C22H23NO	1000451-35-5	53





Tentatively Identified Compound (LSC) summary

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Data File : BP018646.D
Acq On : 06 Dec 2023 20:19
Operator : MA/JU
Sample : 05473-05
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ALS Vial : 83 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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
5-Fluoro-2-hydr...	21.510	2.5	ng/ul	488530	5	21.316	3985650	20.0
Allophanamide, ...	22.468	2.6	ng/ul	523009	5	21.316	3985650	20.0
Octanoic acid, ...	24.598	28.5	ng/ul	6286300	6	23.686	4416260	20.0
1,4-Dioxaspiro[...	26.404	55.7	ng/ul	12297600	6	23.686	4416260	20.0
Sarcosine, N-(1...	28.868	33.1	ng/ul	7317270	6	23.686	4416260	20.0