LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110923\
Data File : BP018007.D
Acq On : 10 Nov 2023 01:46
Operator : MA/JU
Sample : 05082-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH354

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-BP110923.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018007.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.246	24	27	29	rBV	18390	17388	0.56%	0.064%
2	3.281	29	33	41	rVV	109684	141789	4.60%	0.523%
3	3.364	43	47	52	rVB	46040	58446	1.90%	0.216%
4	3.687	99	102	114	rBV	57477	100868	3.27%	0.372%
5	3.852	125	130	139	rBV2	35778	53740	1.74%	0.198%
6	3.975	149	151	155	rVB4	3866	4469	0.14%	0.016%
7	4.499	235	240	245	rBV4	21607	31797	1.03%	0.117%
8	4.881	301	305	308	rVB6	3883	5465	0.18%	0.020%
9	5.616	426	430	433	rVB6	3757	4822	0.16%	0.018%
10	5.728	440	449	459	rBV	273231	399409	12.95%	1.473%
11	5.934	482	484	489	rVB6	2989	4586	0.15%	0.017%
12	6.052	499	504	514	rVB	69367	109116	3.54%	0.402%
13	6.863	639	642	644	rBV4	4076	4171	0.14%	0.015%
14	7.034	665	671	679	rBV3	79018	188852	6.13%	0.696%
15	7.210	694	701	714	rBV	286098	477269	15.48%	1.760%
16	7.387	724	731	743	rBV	315494	534637	17.34%	1.972%
17	7.693	782	783	788	rVB5	3378	4221	0.14%	0.016%
18	7.863	804	812	826	rBV2	280508	547056	17.74%	2.018%
19	8.405	897	904	917	rBV	164466	258783	8.39%	0.954%
20	8.546	921	928	931	rVV	67752	105470	3.42%	0.389%
21	8.587	931	935	952	rVV	241911	460103	14.92%	1.697%
22	8.722	956	958	964	rVV6	5112	9178	0.30%	0.034%
23	8.928	987	993	994	rBV5	2248	3257	0.11%	0.012%
24	9.069	1010	1017	1034	rBV	387115	675719	21.92%	2.492%
25	9.287	1052	1054	1059	rVB6	3775	3115	0.10%	0.011%
26	9.446	1075	1081	1089	rBV2	17269	31385	1.02%	0.116%
27	9.646	1112	1115	1122	rBV9	2165	4497	0.15%	0.017%
28	9.722	1122	1128	1130	rBV7	3671	5245	0.17%	0.019%
29	9.781	1132	1138	1152	rVV	335250	593529	19.25%	2.189%
30	10.052	1176	1184	1192	rBV	110749	177433	5.75%	0.654%
31	10.310	1220	1228	1249	rBV	429785	813592	26.39%	3.001%
32	10.687	1285	1292	1308	rVB	371742	621967	20.17%	2.294%
33	10.863	1314	1322	1339	rBV	365647	714432	23.17%	2.635%
34	11.057	1350	1355	1363	rVV	5418	13245	0.43%	0.049%
35	11.475	1418	1426	1432	rBV5	7627	18301	0.59%	0.067%
36	11.716	1459	1467	1478	rBV	314554	514691	16.69%	1.898%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110923\
Data File : BP018007.D
Acq On : 10 Nov 2023 01:46
Operator : MA/JU
Sample : 05082-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH354

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-BP110923.MA.M
Title : SVOA CALIBRATION

37	11.869	1491	1493	1498	rBV6	2516	3800	0.12%	0.014%
38	12.287	1556	1564	1573	rBV8	7081	17483	0.57%	0.064%
39	12.504	1595	1601	1603	rBV6	2793	4760	0.15%	0.018%
40	12.634	1618	1623	1625	rBV6	3608	5753	0.19%	0.021%
41	12.669	1625	1629	1632	rVB5	3215	4863	0.16%	0.018%
42	13.004	1680	1686	1689	rBV8	3974	7479	0.24%	0.028%
43	13.110	1702	1704	1711	rVB8	2783	4162	0.13%	0.015%
44	13.375	1744	1749	1755	rBV4	14657	23354	0.76%	0.086%
45	13.957	1842	1848	1864	rVB	1067715	1494919	48.49%	5.513%
46	14.240	1889	1896	1910	rBV	1063631	1552848	50.36%	5.727%
47	14.422	1923	1927	1931	rBV7	4407	7253	0.24%	0.027%
48	14.540	1940	1947	1959	rVB	596841	856365	27.78%	3.158%
49	14.822	1987	1995	2004	rBV3	30154	91025	2.95%	0.336%
50	15.151	2048	2051	2056	rBV7	2500	3815	0.12%	0.014%
51	15.287	2067	2074	2078	rBV10	4051	9553	0.31%	0.035%
52	15.363	2082	2087	2092	rBV2	10702	17300	0.56%	0.064%
53	15.539	2108	2117	2128	rBV	1444687	2037224	66.07%	7.513%
54	15.692	2137	2143	2155	rBV	567378	812062	26.34%	2.995%
55	15.787	2155	2159	2163	rVB7	8106	12811	0.42%	0.047%
56	16.416	2263	2266	2272	rVB8	2637	4304	0.14%	0.016%
57	16.986	2360	2363	2365	rBV4	2793	3299	0.11%	0.012%
58	17.110	2379	2384	2390	rVB10	3338	5331	0.17%	0.020%
59	17.186	2392	2397	2402	rBV8	2600	5100	0.17%	0.019%
60	17.316	2412	2419	2430	rBV	782655	1107344	35.92%	4.084%
61	17.422	2430	2437	2453	rVV	1727758	2474831	80.27%	9.127%
62	17.739	2488	2491	2494	rBV5	2889	4326	0.14%	0.016%
63	17.945	2521	2526	2531	rVB9	3049	5725	0.19%	0.021%
64	18.063	2541	2546	2550	rBV7	2891	6019	0.20%	0.022%
65	18.163	2558	2563	2571	rBV2	43085	65751	2.13%	0.242%
66	18.251	2575	2578	2585	rVB	7382	13925	0.45%	0.051%
67	19.239	2742	2746	2751	rBV3	22254	34024	1.10%	0.125%
68	19.316	2755	2759	2763	rVB2	21472	32788	1.06%	0.121%
69	19.404	2770	2774	2783	rBV5	28906	49743	1.61%	0.183%
70	19.669	2813	2819	2827	rBV	2294801	2976905	96.55%	10.979%
71	21.445	3115	3121	3130	rBV	925771	1269400	41.17%	4.682%
72	23.792	3512	3520	3527	rVB	1535479	3083220	100.00%	11.371%
73	23.951	3541	3547	3559	rVB	620283	1293624	41.96%	4.771%

Sum of corrected areas: 27114531

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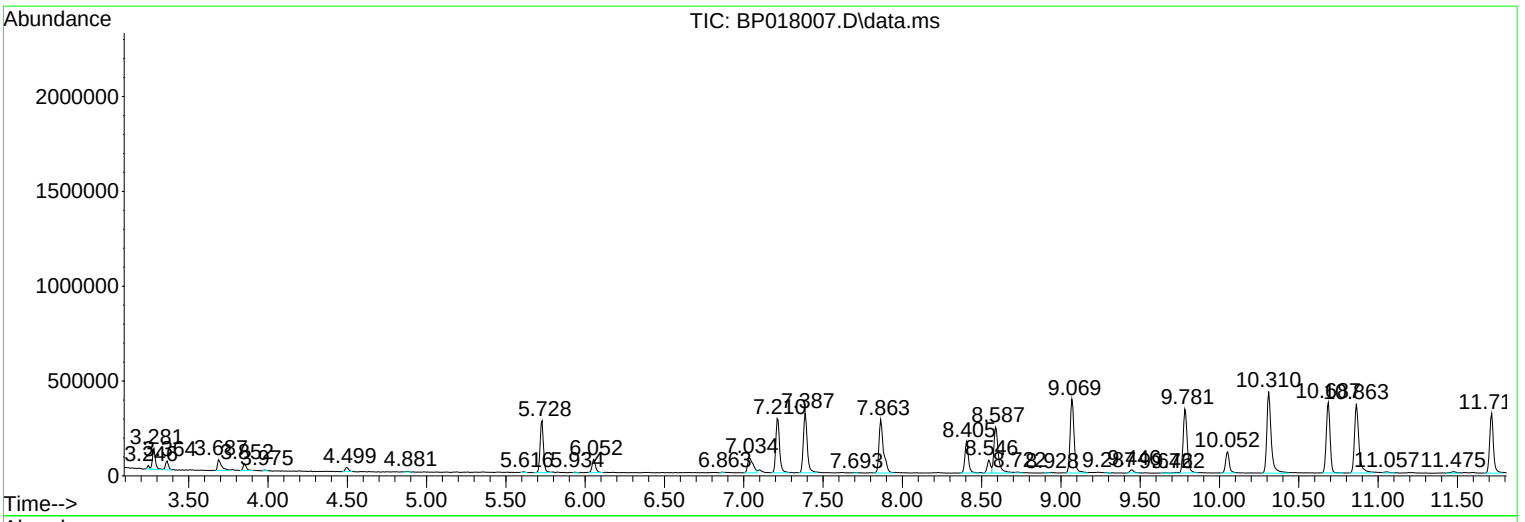
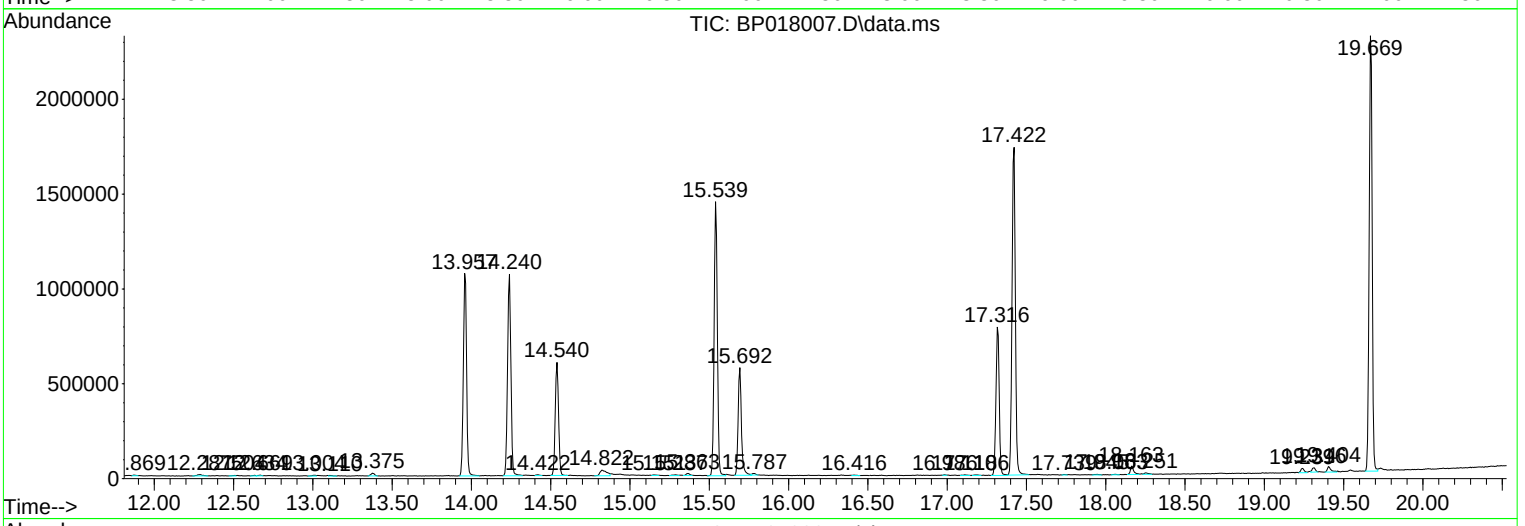
Misc :
ALS Vial : 13 Sample Multiplier: 1

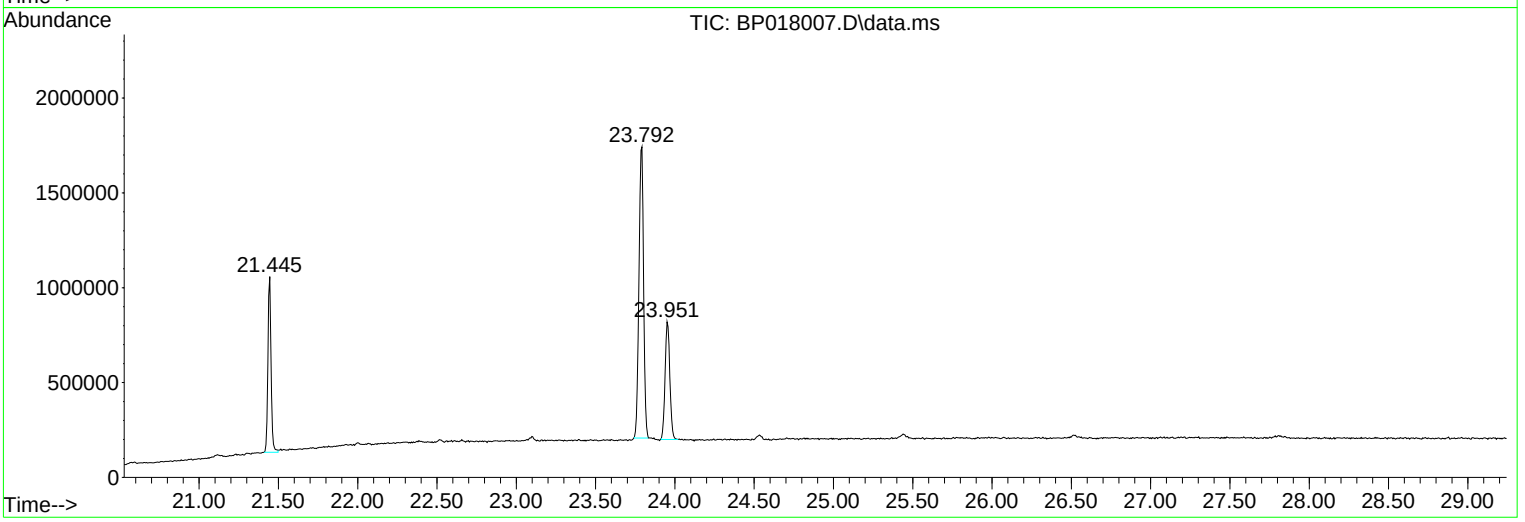
Instrument :
BNA_P
ClientSampleId :
BH354

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

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







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ClientSampleId :
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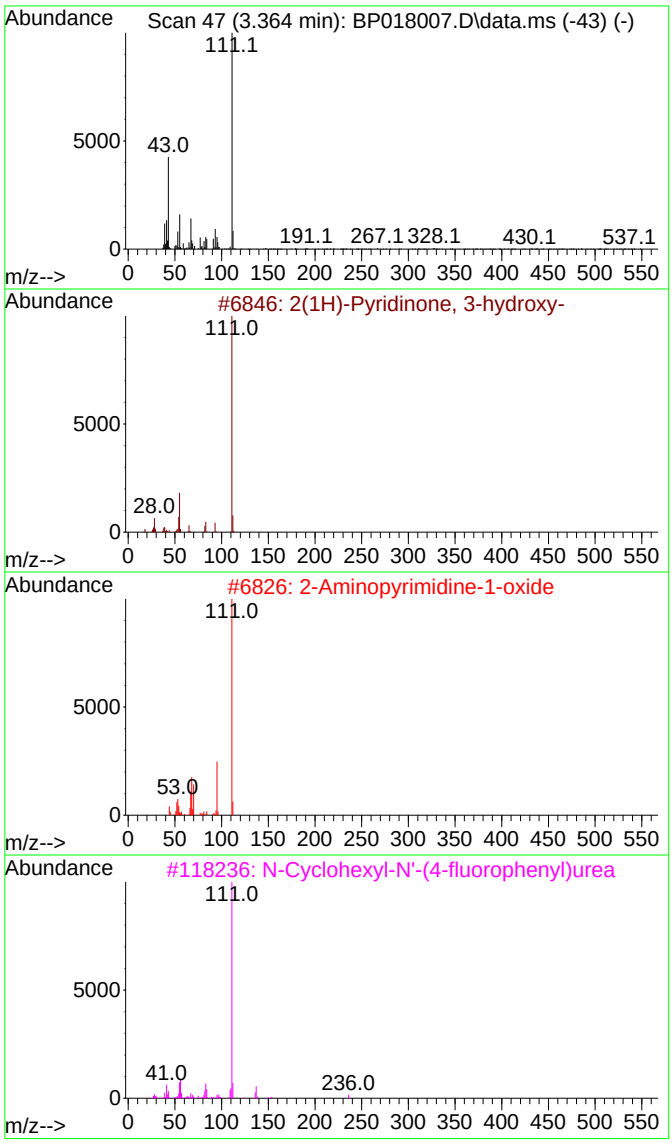
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

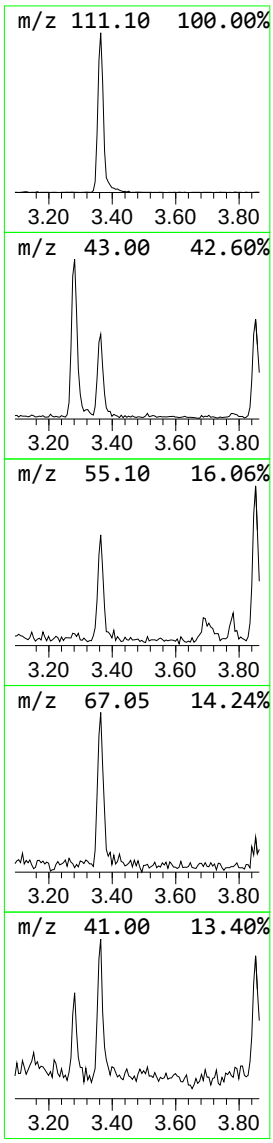
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2(1H)-Pyridinone, 3-hydroxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	2.14 ng/ul	58446	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	59
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	45
3	N-Cyclohexyl-N'-(4-fluorophenyl)...	236	C13H17FN2O	200058-85-1	45
4	Benzenamine, 3-fluoro-	111	C6H6FN	000372-19-0	42
5	Thiophene-2-carboxamide, N-(2-bu...	197	C10H15NOS	1000458-79-4	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110923\
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Operator : MA/JU
Sample : 05082-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH354

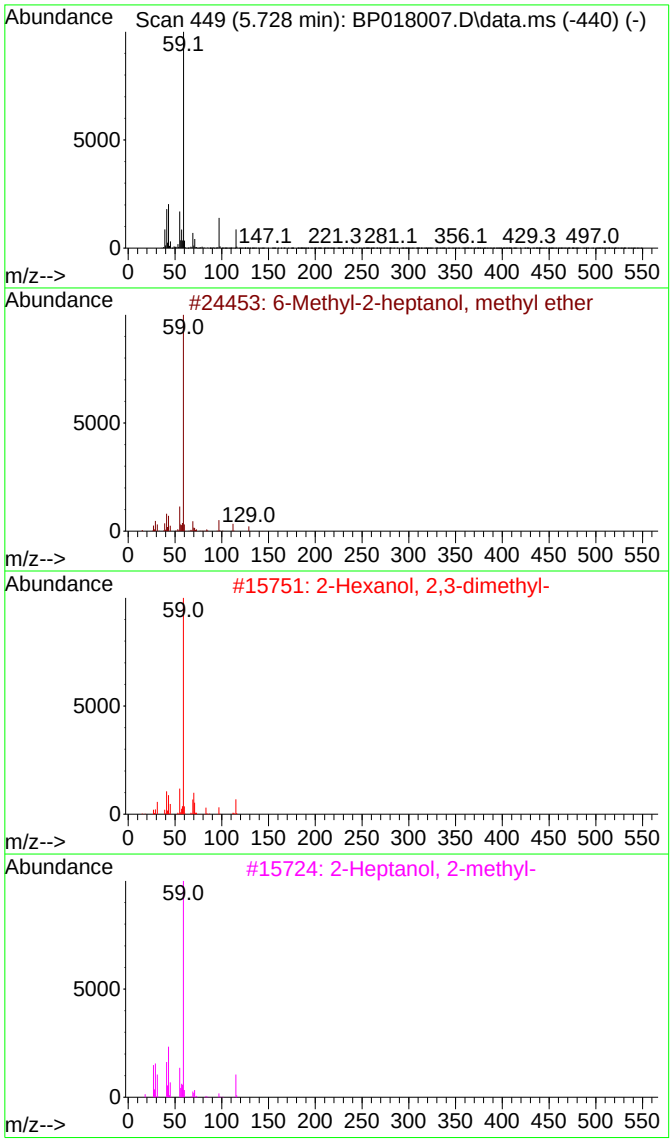
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

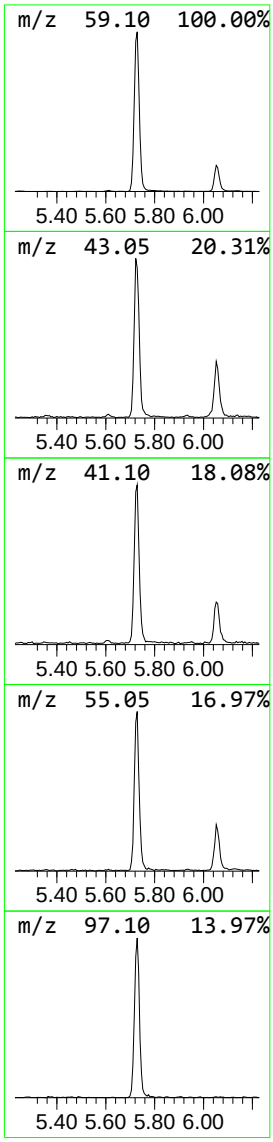
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 6-Methyl-2-heptanol, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	14.60 ng/ul	399409	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	56
2	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	56
3	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	56
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110923\
Data File : BP018007.D
Acq On : 10 Nov 2023 01:46
Operator : MA/JU
Sample : 05082-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH354

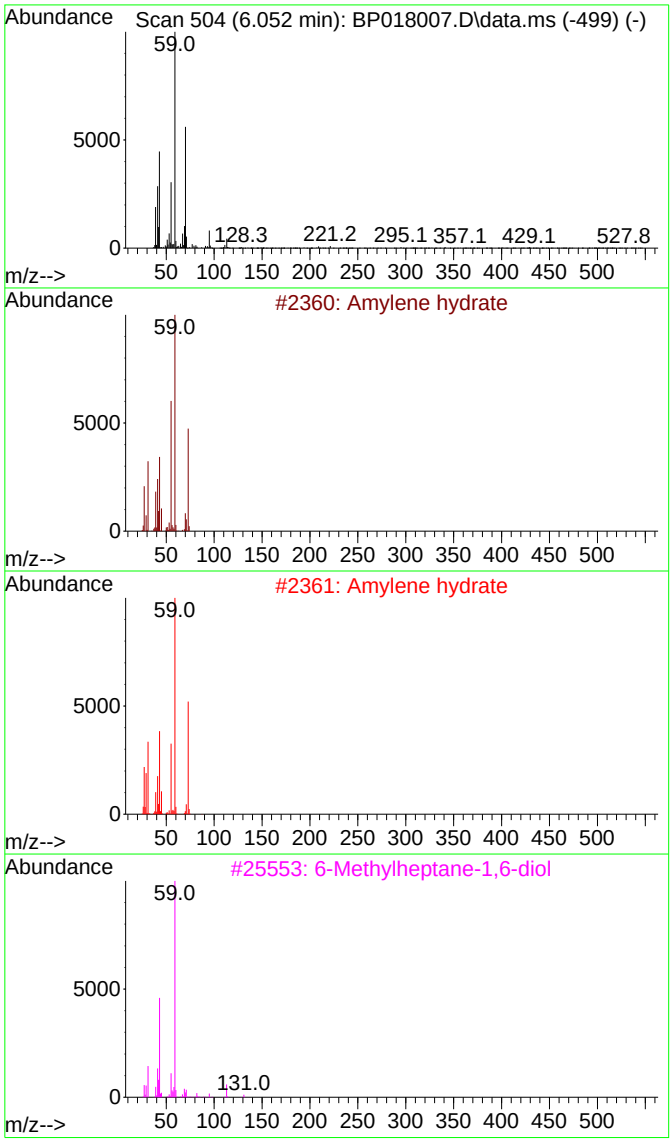
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

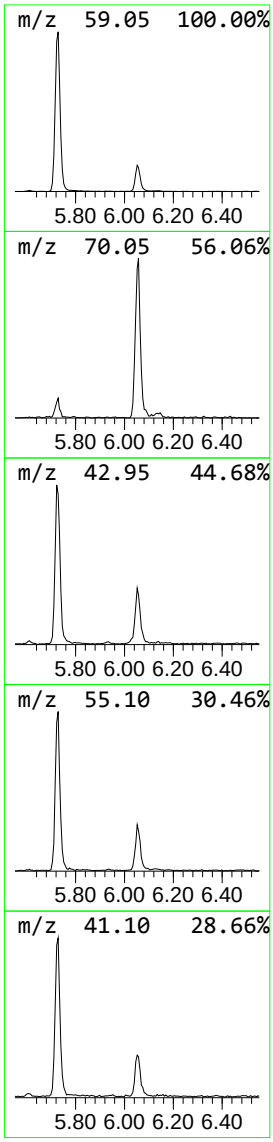
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.052	3.99 ng/ul	109116	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	38
2	Amylene hydrate	88	C5H12O	000075-85-4	37
3	6-Methylheptane-1,6-diol	146	C8H18O2	005392-57-4	33
4	Amylene hydrate	88	C5H12O	000075-85-4	32
5	.+/-.-trans-2-Cyclohexene-1,4-diol	114	C6H10O2	041513-32-0	30





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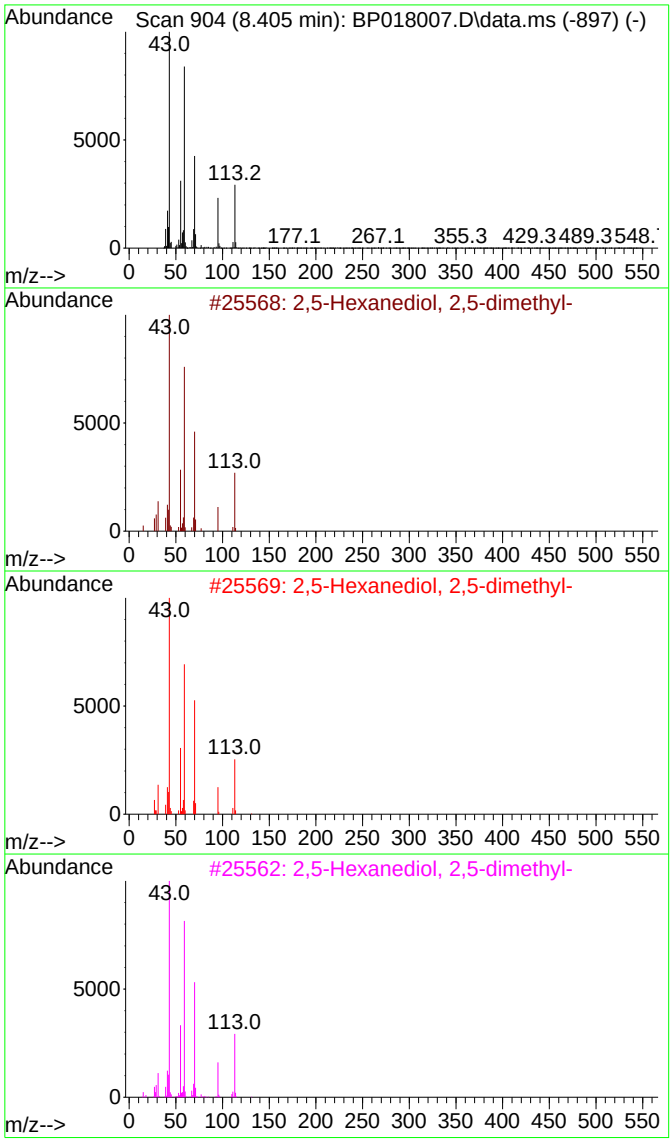
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

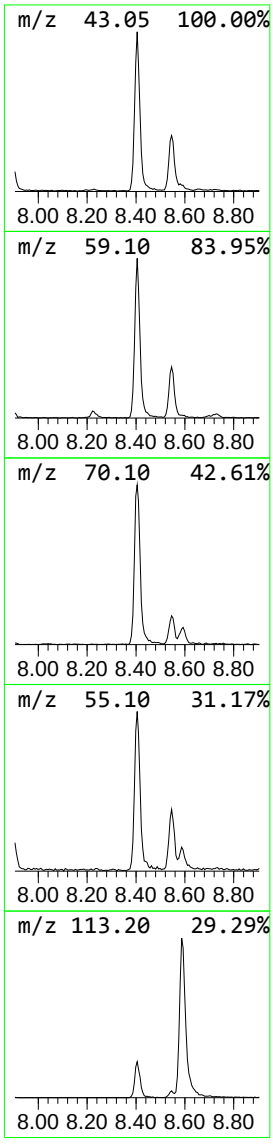
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,5-Hexanediol, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.405	9.46 ng/ul	258783	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	86
2	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	86
3	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	78
4	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	53
5	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	47





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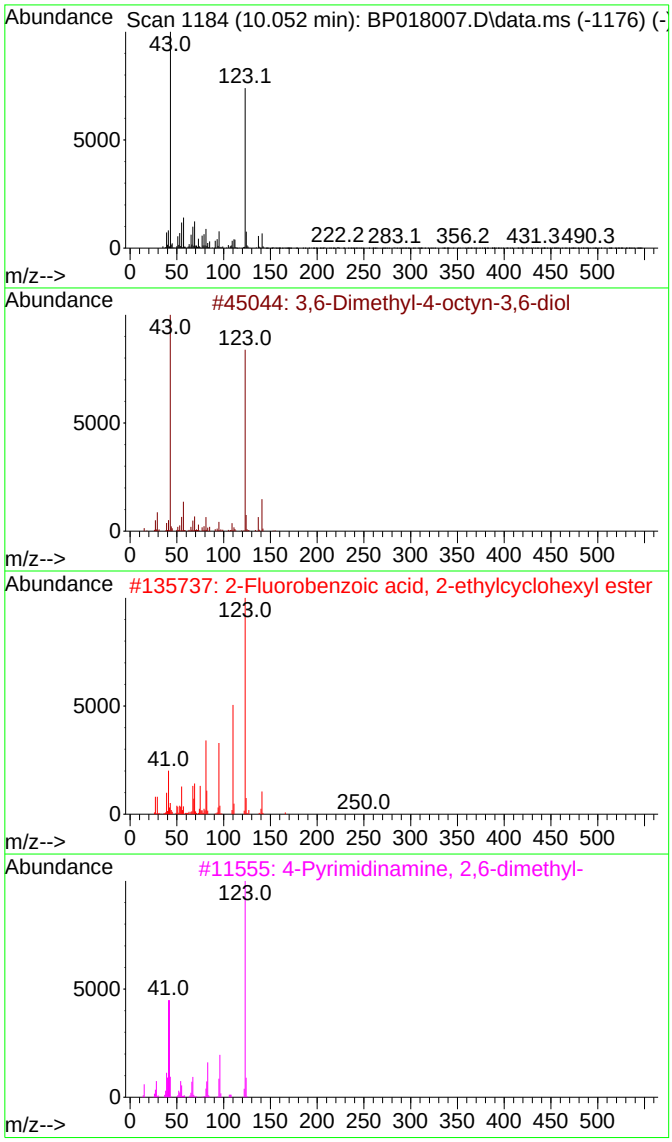
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

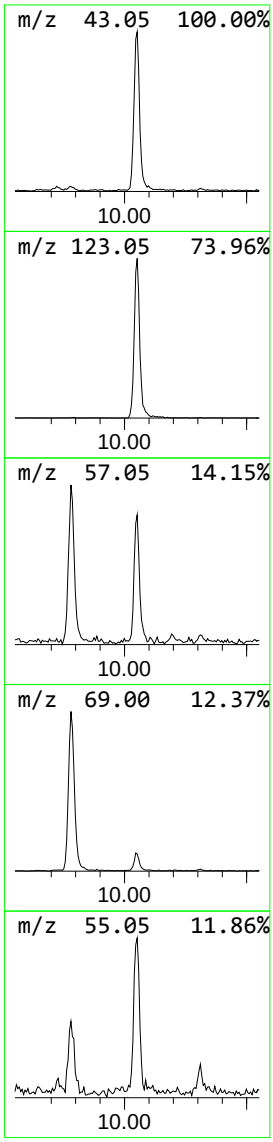
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3,6-Dimethyl-4-octyn-3,6-diol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.052	5.71 ng/ul	177433	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dimethyl-4-octyn-3,6-diol	170	C10H18O2	000078-66-0	83
2	2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000278-98-1	72
3	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	59
4	3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	59
5	Tetracosyl benzoate	458	C31H54O2	103569-99-9	59





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Sample : 05082-14
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.MA.M
Quant Title : SVOA CALIBRATION

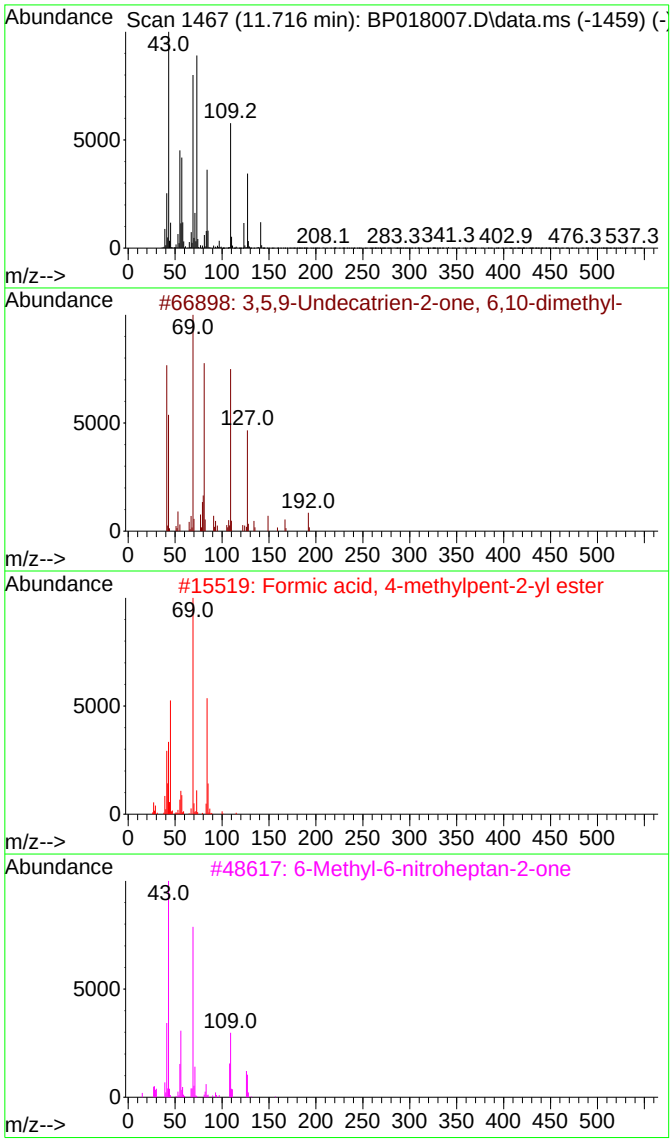
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

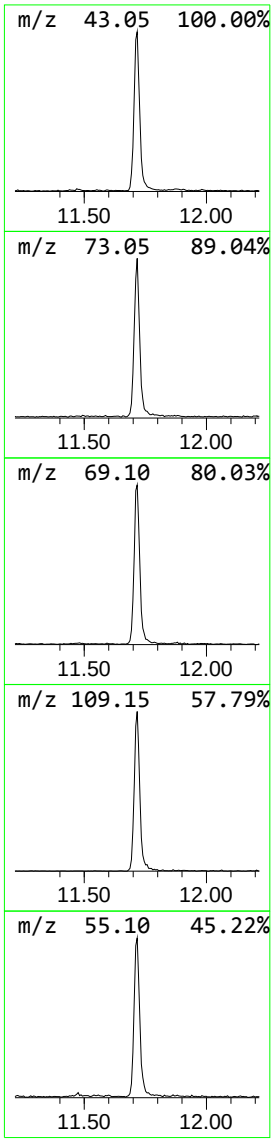
****

Peak Number 6 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	16.55 ng/ul	514691	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5,9-Undecatrien-2-one, 6,10-di...	192	C13H20O	000141-10-6	40
2	Formic acid, 4-methylpent-2-yl e...	130	C7H14O2	1000367-94-0	38
3	6-Methyl-6-nitroheptan-2-one	173	C8H15NO3	142963-25-5	37
4	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	35
5	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110923\
Data File : BP018007.D
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Instrument :
BNA_P
ClientSampleId :
BH354

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110923.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
2(1H)-Pyridinon...	3.364	2.1	ng/ul	58446	1	7.863	547056	20.0
6-Methyl-2-hept...	5.728	14.6	ng/ul	399409	1	7.863	547056	20.0
unknown-01	6.052	4.0	ng/ul	109116	1	7.863	547056	20.0
2,5-Hexanediol,...	8.405	9.5	ng/ul	258783	1	7.863	547056	20.0
3,6-Dimethyl-4-...	10.052	5.7	ng/ul	177433	2	10.687	621967	20.0
unknown-02	11.716	16.6	ng/ul	514691	2	10.687	621967	20.0