LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

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-BP100724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP022272.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.228	37	41	48	rVB	16339	23941	0.80%	0.075%
2	3.499	83	87	96	rBV	39047	56175	1.88%	0.176%
3	3.640	107	111	126	rBV	179137	273264	9.16%	0.857%
4	3.964	162	166	171	rVB2	9048	12438	0.42%	0.039%
5	4.864	315	319	326	rVB4	3621	6670	0.22%	0.021%
6	5.840	479	485	487	rBV5	2145	3016	0.10%	0.009%
7	6.322	563	567	572	rVV7	1854	3571	0.12%	0.011%
8	6.734	634	637	643	rBV7	4110	7624	0.26%	0.024%
9	6.893	656	664	674	rBV	237068	422143	14.15%	1.323%
10	7.046	684	690	698	rBV	187860	288895	9.68%	0.906%
11	7.252	718	725	732	rBV	250859	396716	13.30%	1.244%
12	7.316	732	736	748	rVB	21314	45722	1.53%	0.143%
13	7.705	794	802	810	rBV	381531	587967	19.71%	1.843%
14	7.775	810	814	819	rVB7	3875	5374	0.18%	0.017%
15	8.399	913	920	937	rBV	335674	545862	18.30%	1.711%
16	8.840	988	995	1008	rBV	224486	401878	13.47%	1.260%
17	9.005	1020	1023	1034	rVB5	11880	19745	0.66%	0.062%
18	9.263	1062	1067	1071	rVB6	2793	3824	0.13%	0.012%
19	9.399	1085	1090	1100	rBV2	17196	33431	1.12%	0.105%
20	9.557	1110	1117	1130	rBV	189462	341305	11.44%	1.070%
21	9.969	1181	1187	1194	rBV2	18368	31966	1.07%	0.100%
22	10.093	1200	1208	1220	rBV	338153	587435	19.69%	1.841%
23	10.463	1260	1271	1283	rBV	453572	811160	27.19%	2.543%
24	10.599	1283	1294	1311	rBV	283211	519115	17.40%	1.627%
25	10.999	1358	1362	1373	rVB9	6885	14784	0.50%	0.046%
26	11.199	1386	1396	1404	rBV	39532	82464	2.76%	0.259%
27	11.481	1438	1444	1449	rBV10	2541	5661	0.19%	0.018%
28	11.957	1522	1525	1529	rBV3	2544	4011	0.13%	0.013%
29	12.046	1534	1540	1547	rVV3	6435	11955	0.40%	0.037%
30	12.846	1670	1676	1681	rVB8	4709	7723	0.26%	0.024%
31	13.140	1716	1726	1728	rBV8	3288	6073	0.20%	0.019%
32	13.204	1733	1737	1740	rVV6	3284	4785	0.16%	0.015%
33	13.269	1744	1748	1755	rVB9	5423	9923	0.33%	0.031%
34	13.716	1816	1824	1834	rBV	654548	995163	33.35%	3.120%
35	13.804	1836	1839	1842	rVB5	6958	7884	0.26%	0.025%
36	13.998	1859	1872	1886	rBV	729098	1089433	36.51%	3.415%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

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-BP100724.MA.M
Title : SVOA CALIBRATION

37	14.304	1916	1924	1932	rBV	754170	1231071	41.26%	3.859%
38	14.534	1955	1963	1975	rBV2	1457150	2973783	99.67%	9.322%
39	14.716	1991	1994	1995	rBV3	4149	4377	0.15%	0.014%
40	15.234	2078	2082	2088	rBV2	12265	22681	0.76%	0.071%
41	15.316	2088	2096	2103	rVV	991874	1475575	49.46%	4.626%
42	15.451	2113	2119	2132	rBV	296517	443208	14.85%	1.389%
43	15.587	2136	2142	2149	rVB6	15361	28078	0.94%	0.088%
44	15.687	2153	2159	2168	rVB3	21123	43336	1.45%	0.136%
45	15.798	2172	2178	2181	rBV8	4050	7514	0.25%	0.024%
46	15.887	2189	2193	2202	rBV8	6158	14685	0.49%	0.046%
47	16.092	2221	2228	2231	rBV5	9085	14920	0.50%	0.047%
48	16.204	2243	2247	2251	rBV5	6677	12269	0.41%	0.038%
49	16.316	2264	2266	2273	rVB5	7114	10945	0.37%	0.034%
50	16.510	2296	2299	2305	rBV7	10523	15859	0.53%	0.050%
51	16.634	2318	2320	2323	rBV4	3029	3691	0.12%	0.012%
52	16.839	2351	2355	2357	rBV5	3527	5949	0.20%	0.019%
53	16.928	2368	2370	2376	rVB6	12693	15444	0.52%	0.048%
54	16.986	2376	2380	2383	rBV6	11308	14508	0.49%	0.045%
55	17.022	2383	2386	2387	rBV3	4298	4806	0.16%	0.015%
56	17.110	2394	2401	2407	rBV	1078402	1682696	56.40%	5.275%
57	17.157	2407	2409	2413	rVV3	40954	49671	1.66%	0.156%
58	17.216	2413	2419	2429	rVB	1121064	1706070	57.18%	5.348%
59	17.298	2429	2433	2439	rBV8	17360	38183	1.28%	0.120%
60	17.586	2480	2482	2485	rVB3	6962	5226	0.18%	0.016%
61	17.716	2501	2504	2510	rVB5	17104	30967	1.04%	0.097%
62	17.816	2518	2521	2525	rBV6	10384	13504	0.45%	0.042%
63	18.045	2554	2560	2570	rBV	510634	800203	26.82%	2.508%
64	18.498	2633	2637	2640	rBV5	15266	23622	0.79%	0.074%
65	18.628	2656	2659	2661	rBV3	15075	19156	0.64%	0.060%
66	18.945	2710	2713	2718	rBV6	18464	37145	1.24%	0.116%
67	19.039	2722	2729	2732	rBV7	43721	74981	2.51%	0.235%
68	19.239	2758	2763	2768	rBV	74852	118504	3.97%	0.371%
69	19.380	2783	2787	2797	rBV	243873	377267	12.64%	1.183%
70	19.586	2817	2822	2831	rBV	1647991	2409689	80.76%	7.554%
71	19.657	2832	2834	2840	rVB2	44045	53399	1.79%	0.167%
72	19.869	2867	2870	2877	rVB4	45336	65071	2.18%	0.204%
73	20.145	2913	2917	2920	rBV6	82720	122743	4.11%	0.385%
74	20.186	2921	2924	2927	rVB	70192	80875	2.71%	0.254%
75	20.522	2978	2981	2984	rBV	89872	86812	2.91%	0.272%
76	20.692	3007	3010	3014	rVB	111286	138584	4.64%	0.434%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

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-BP100724.MA.M
Title : SVOA CALIBRATION

77	21.216	3095	3099	3108	rVB	285634	451942	15.15%	1.417%
78	21.545	3149	3155	3161	rBV	1466964	2392563	80.19%	7.500%
79	22.416	3301	3303	3315	rVB5	117309	238566	8.00%	0.748%
80	23.104	3415	3420	3438	rVB2	598515	1299247	43.55%	4.073%
81	24.604	3667	3675	3694	rVB	1128570	2983582	100.00%	9.353%
82	24.827	3704	3713	3724	rVB	921479	2587799	86.73%	8.112%

Sum of corrected areas: 31899862

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
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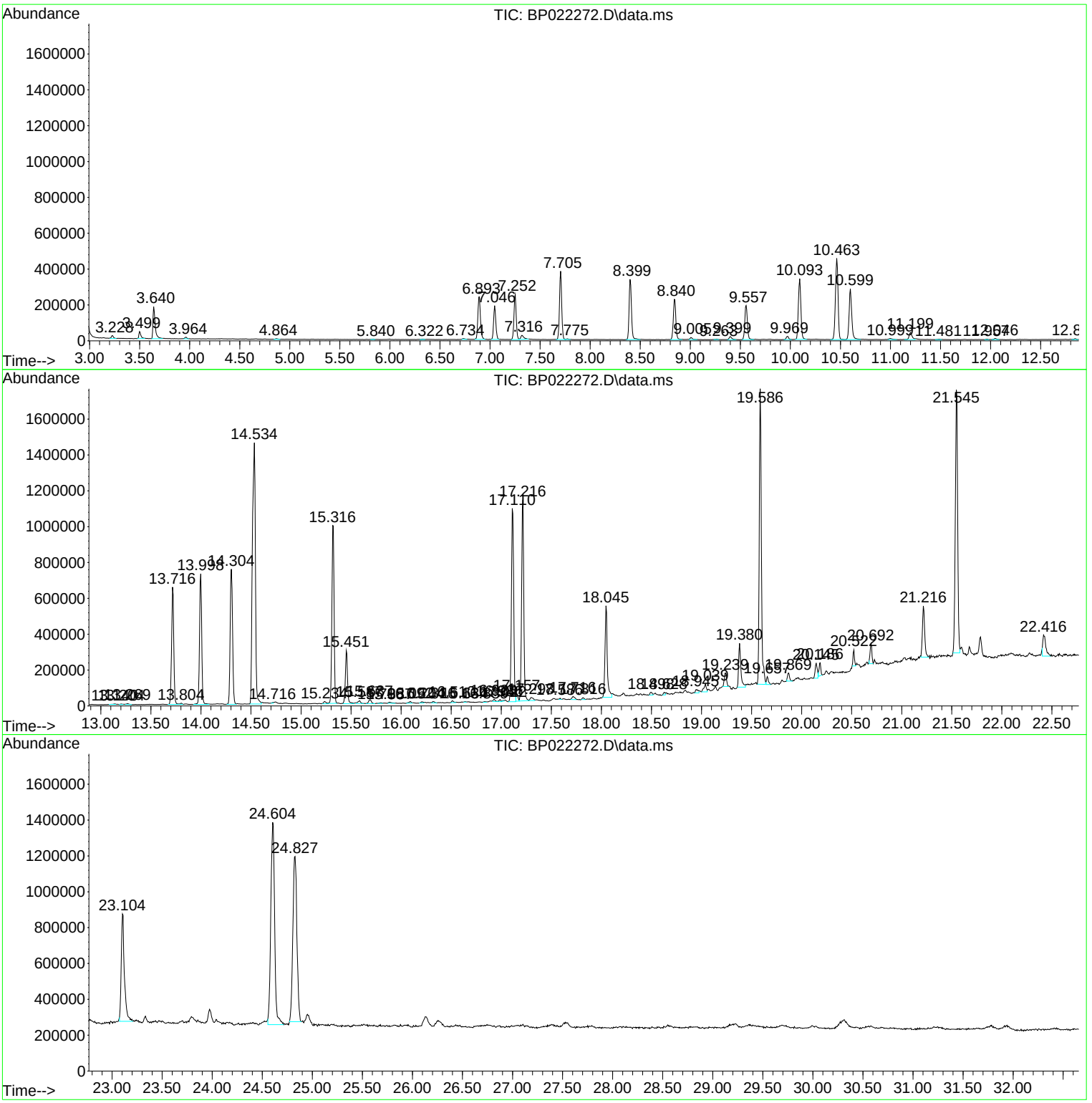
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

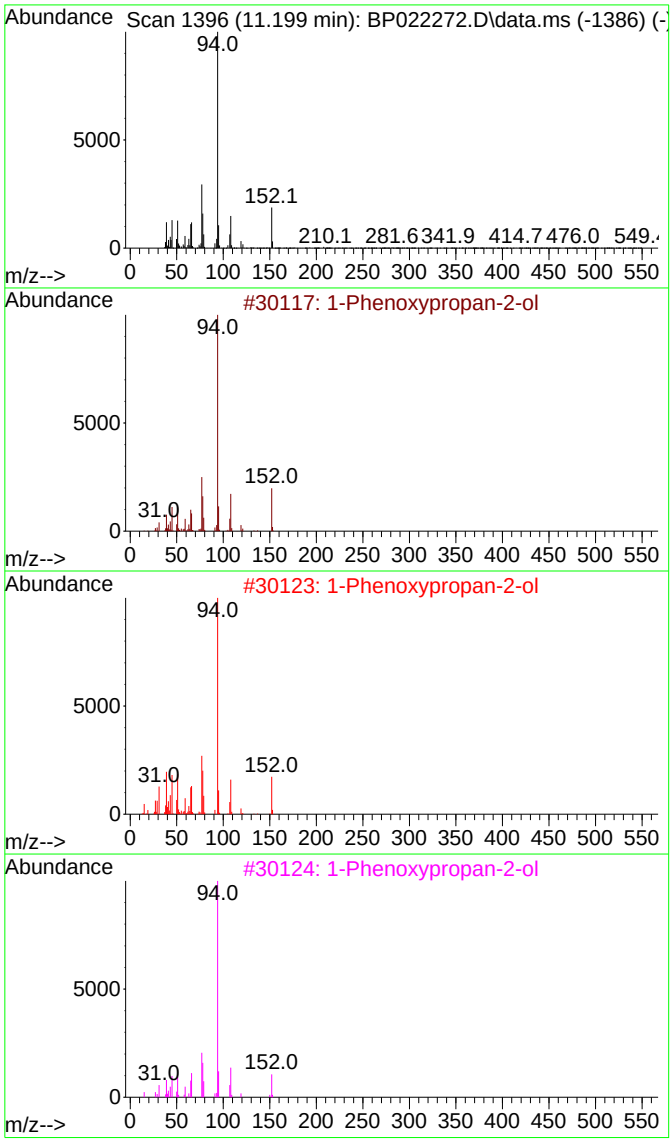
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

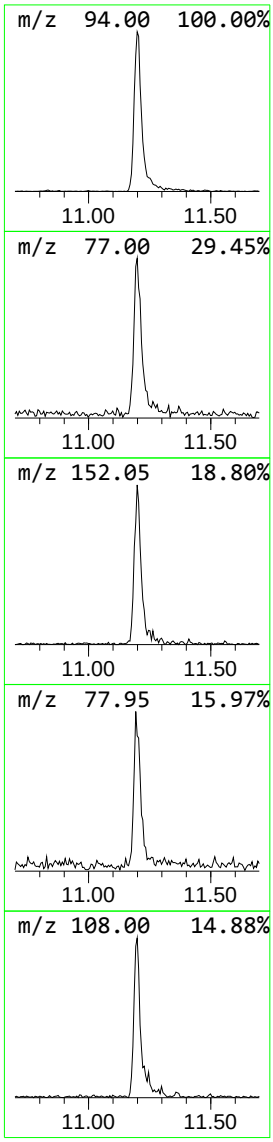
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.199	2.03 ng/ul	82464	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

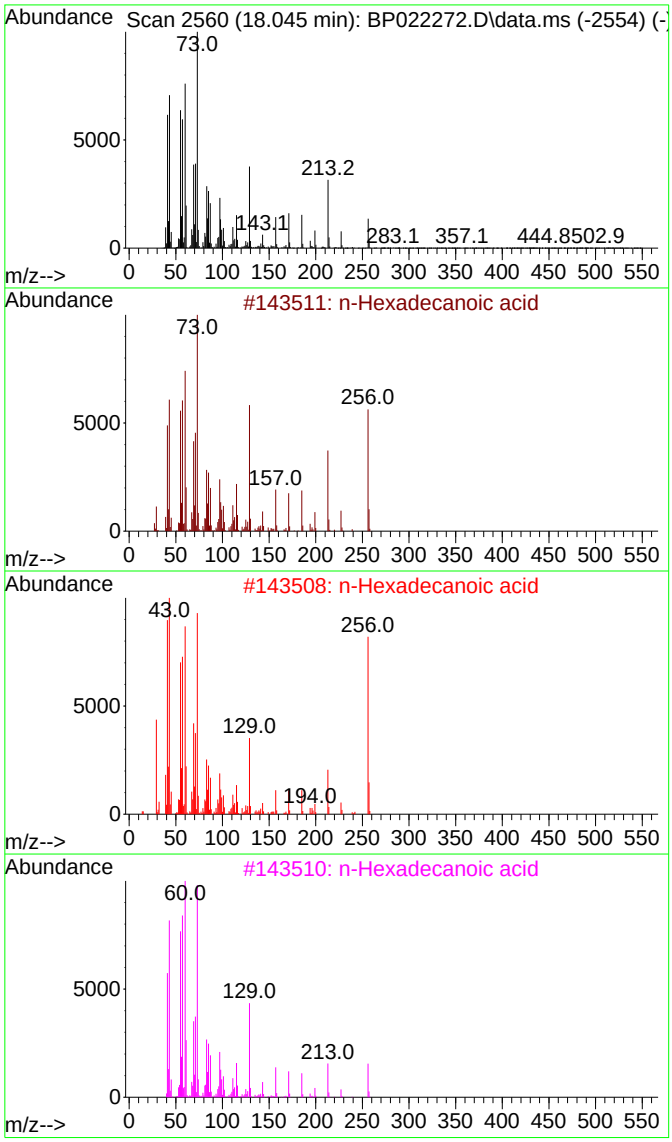
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

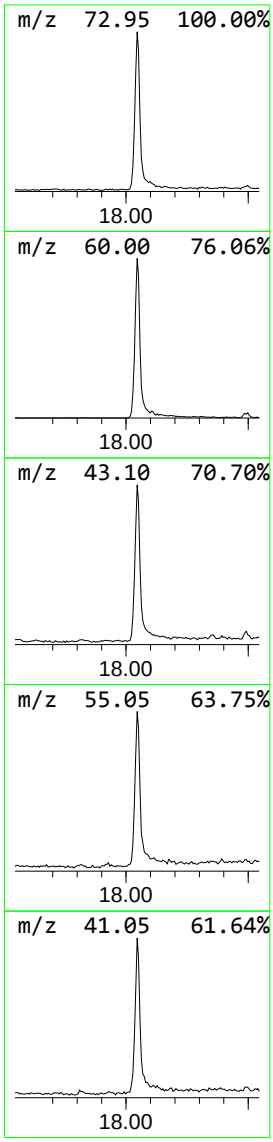
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	9.51 ng/ul	800203	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

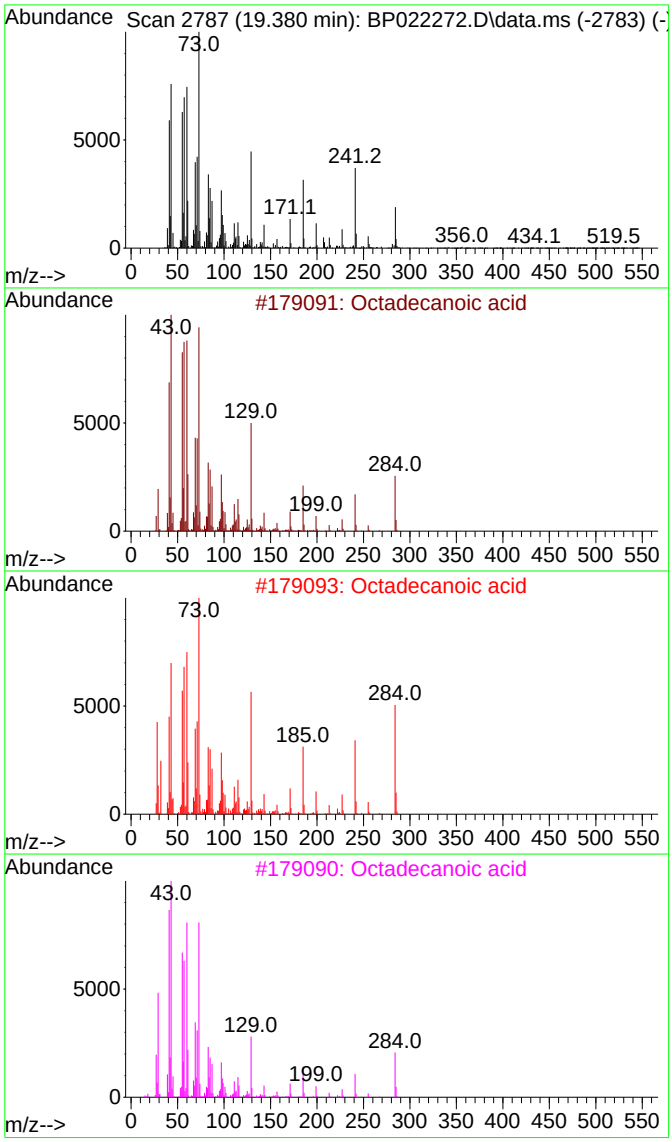
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

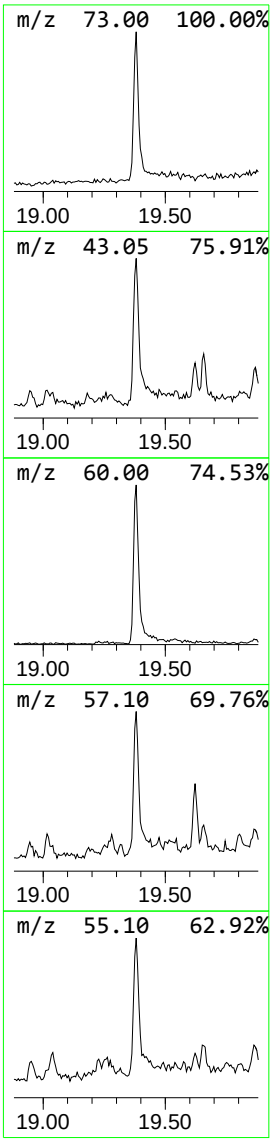
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.381	3.15 ng/ul	377267	Chrysene-d12	21.545

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, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	93
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

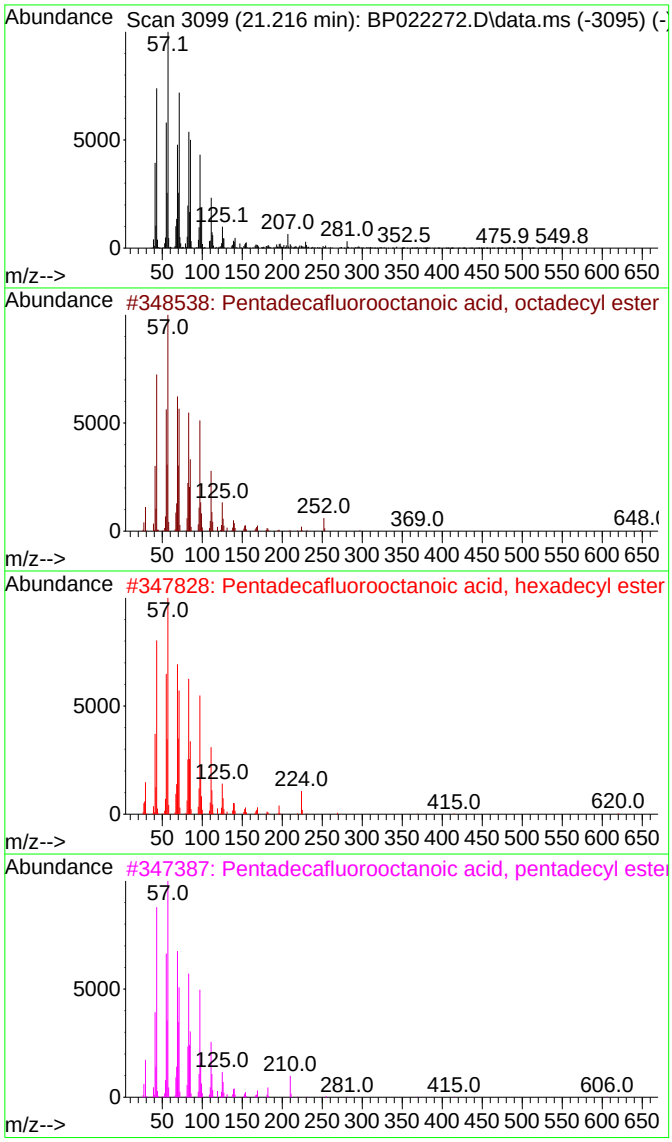
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

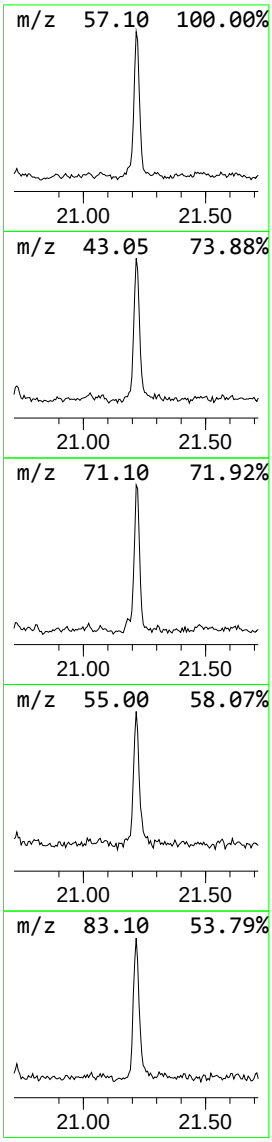
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.216	3.78 ng/ul	451942	Chrysene-d12	21.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	90
3	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	90
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5	1-Docosene	308	C22H44	001599-67-3	78





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Data File : BP022272.D
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Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

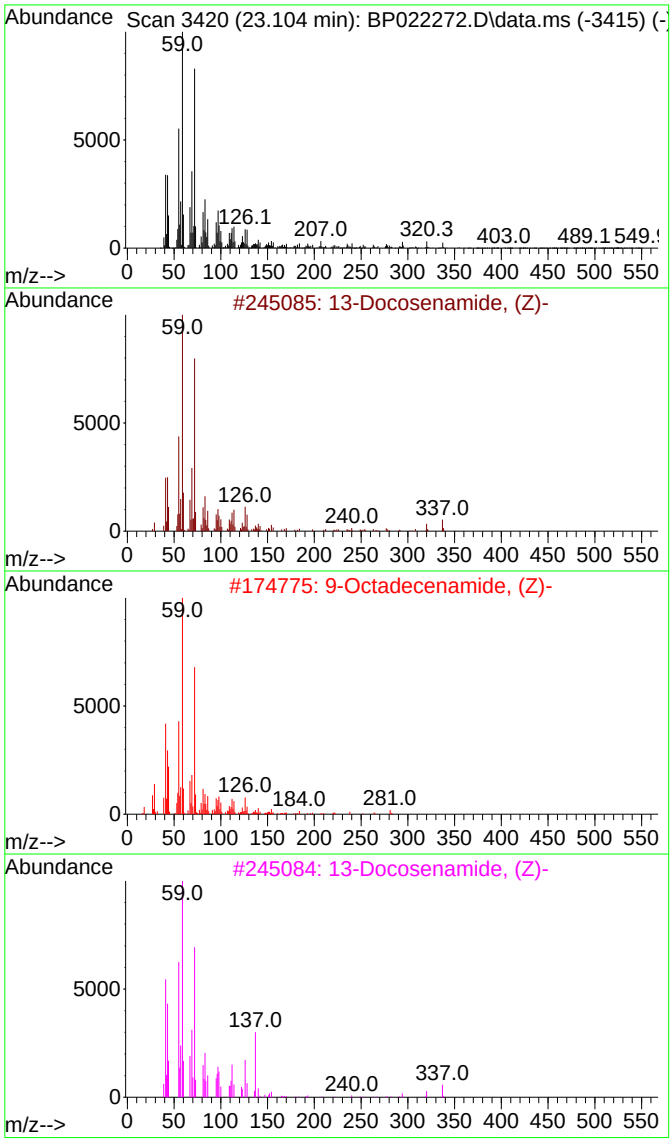
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

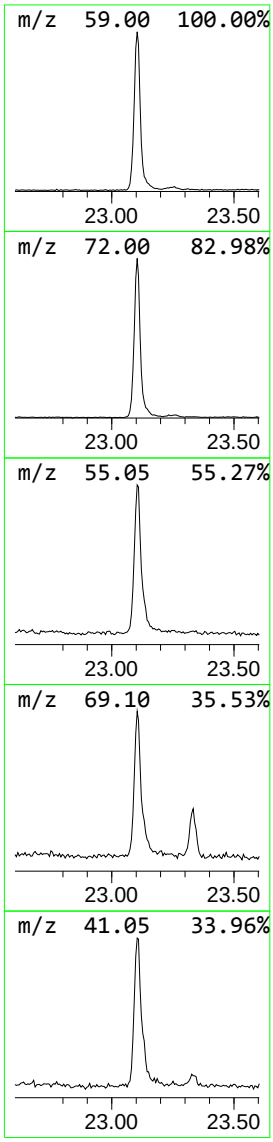
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.104	10.86 ng/ul	1299250	Chrysene-d12	21.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100824\
Data File : BP022272.D
Acq On : 08 Oct 2024 15:26
Operator : RC/JU
Sample : P4162-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4ES6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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
1-Phenoxypropan...	11.199	2.0	ng/ul	82464	2	10.463	811160	20.0
n-Hexadecanoic ...	18.045	9.5	ng/ul	800203	4	17.110	1682700	20.0
Octadecanoic acid	19.381	3.1	ng/ul	377267	5	21.545	2392560	20.0
Pentadecafluoro...	21.216	3.8	ng/ul	451942	5	21.545	2392560	20.0
13-Docosenamide...	23.104	10.9	ng/ul	1299250	5	21.545	2392560	20.0