LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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: BP019106.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	23	27	32	rBV	36798	44326	1.34%	0.160%
2	3.540	74	77	82	rVB2	7682	11354	0.34%	0.041%
3	3.664	94	98	110	rBV	243128	365937	11.04%	1.317%
4	3.893	133	137	142	rBV3	7349	9903	0.30%	0.036%
5	3.987	149	153	158	rBV	12174	17472	0.53%	0.063%
6	4.364	214	217	220	rVB5	3463	3714	0.11%	0.013%
7	4.911	306	310	315	rVB2	6866	10741	0.32%	0.039%
8	5.122	338	346	351	rBV	25098	39184	1.18%	0.141%
9	5.899	471	478	483	rBV	10327	19856	0.60%	0.071%
10	6.993	661	664	672	rVB7	3318	7527	0.23%	0.027%
11	7.146	684	690	703	rVB	319285	505404	15.25%	1.819%
12	7.346	718	724	731	rBV3	12235	23767	0.72%	0.086%
13	7.428	734	738	747	rBV	12581	23616	0.71%	0.085%
14	7.811	796	803	812	rBV	582605	930416	28.07%	3.349%
15	7.893	812	817	824	rVB4	13084	26245	0.79%	0.094%
16	8.163	858	863	868	rVB3	6750	10082	0.30%	0.036%
17	8.540	921	927	932	rBV8	8318	17725	0.53%	0.064%
18	8.969	992	1000	1013	rBV	329795	553054	16.68%	1.990%
19	9.134	1025	1028	1037	rVB10	4597	9526	0.29%	0.034%
20	9.375	1065	1069	1079	rVB2	18848	33318	1.01%	0.120%
21	9.546	1092	1098	1107	rBV	50587	84169	2.54%	0.303%
22	9.693	1120	1123	1130	rBV7	6015	12168	0.37%	0.044%
23	10.240	1211	1216	1226	rVB4	12548	28663	0.86%	0.103%
24	10.469	1250	1255	1260	rVB9	3474	4553	0.14%	0.016%
25	10.605	1271	1278	1287	rBV	707331	1210585	36.52%	4.357%
26	10.752	1294	1303	1312	rBV	414037	736202	22.21%	2.650%
27	10.987	1340	1343	1347	rVB5	3510	5208	0.16%	0.019%
28	11.169	1369	1374	1382	rVB9	10071	20237	0.61%	0.073%
29	11.357	1400	1406	1423	rBV	80238	186097	5.61%	0.670%
30	11.757	1470	1474	1480	rBV6	6473	10393	0.31%	0.037%
31	11.869	1487	1493	1501	rVB4	7201	14031	0.42%	0.050%
32	12.028	1514	1520	1524	rBV3	7453	12251	0.37%	0.044%
33	12.122	1528	1536	1539	rVV10	2361	5083	0.15%	0.018%
34	12.193	1539	1548	1555	rVV3	8982	17849	0.54%	0.064%
35	12.834	1655	1657	1661	rBV5	2971	4198	0.13%	0.015%
36	12.928	1671	1673	1680	rVV6	3633	5885	0.18%	0.021%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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	12.987	1680	1683	1690	rVV9	2882	5631	0.17%	0.020%
38	13.075	1690	1698	1703	rVV8	9230	20200	0.61%	0.073%
39	13.128	1705	1707	1712	rVB5	3129	3641	0.11%	0.013%
40	13.269	1727	1731	1738	rVB	18682	26449	0.80%	0.095%
41	13.346	1738	1744	1750	rBV7	9115	18023	0.54%	0.065%
42	13.757	1809	1814	1825	rBV8	11516	25360	0.77%	0.091%
43	13.863	1825	1832	1847	rVV	706214	1009020	30.44%	3.631%
44	13.963	1847	1849	1854	rVB6	3506	5273	0.16%	0.019%
45	14.140	1868	1879	1894	rBV	861856	1348775	40.69%	4.854%
46	14.345	1911	1914	1917	rVB4	6500	6481	0.20%	0.023%
47	14.445	1920	1931	1940	rBV	1044011	1573307	47.46%	5.662%
48	14.669	1959	1969	1982	rBV	172306	406119	12.25%	1.462%
49	15.104	2036	2043	2045	rVV8	2082	4402	0.13%	0.016%
50	15.245	2063	2067	2069	rBV4	3460	4222	0.13%	0.015%
51	15.292	2072	2075	2083	rVB5	6407	10804	0.33%	0.039%
52	15.440	2093	2100	2118	rBV	1189105	1791877	54.05%	6.449%
53	15.581	2120	2124	2131	rVB10	3303	8055	0.24%	0.029%
54	15.675	2136	2140	2144	rBV5	5792	10340	0.31%	0.037%
55	15.857	2168	2171	2175	rBV6	2345	4510	0.14%	0.016%
56	16.010	2192	2197	2201	rBV8	5137	9337	0.28%	0.034%
57	16.163	2217	2223	2230	rBV9	7297	16495	0.50%	0.059%
58	16.222	2232	2233	2238	rVB5	5755	6570	0.20%	0.024%
59	16.328	2245	2251	2254	rBV7	3841	7860	0.24%	0.028%
60	16.798	2329	2331	2335	rVB5	2640	3575	0.11%	0.013%
61	16.957	2354	2358	2361	rBV4	8253	11313	0.34%	0.041%
62	17.116	2382	2385	2391	rBV8	6470	10068	0.30%	0.036%
63	17.198	2392	2399	2409	rBV	1278513	1929920	58.22%	6.946%
64	17.292	2409	2415	2427	rVV2	1363994	2026726	61.14%	7.294%
65	17.698	2481	2484	2487	rBV5	5685	5761	0.17%	0.021%
66	17.875	2510	2514	2518	rVB2	11692	14435	0.44%	0.052%
67	18.086	2546	2550	2557	rBV3	45497	65531	1.98%	0.236%
68	18.369	2596	2598	2603	rBV6	7691	12002	0.36%	0.043%
69	18.498	2617	2620	2626	rBV4	21265	27457	0.83%	0.099%
70	19.116	2721	2725	2729	rVB3	19825	27583	0.83%	0.099%
71	19.181	2733	2736	2739	rBV	18038	27110	0.82%	0.098%
72	19.328	2758	2761	2766	rBV6	12525	16014	0.48%	0.058%
73	19.533	2791	2796	2802	rBV	2091842	2646702	79.84%	9.526%
74	21.010	3042	3047	3055	rBV2	264502	526497	15.88%	1.895%
75	21.286	3089	3094	3101	rBV	1976831	2499177	75.39%	8.995%
76	22.510	3299	3302	3313	rVB	253177	351549	10.60%	1.265%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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

77	23.486	3462	3468	3483	rVB2	1658694	3315019	100.00%	11.931%
78	23.639	3488	3494	3510	rVB	1409832	2925475	88.25%	10.529%

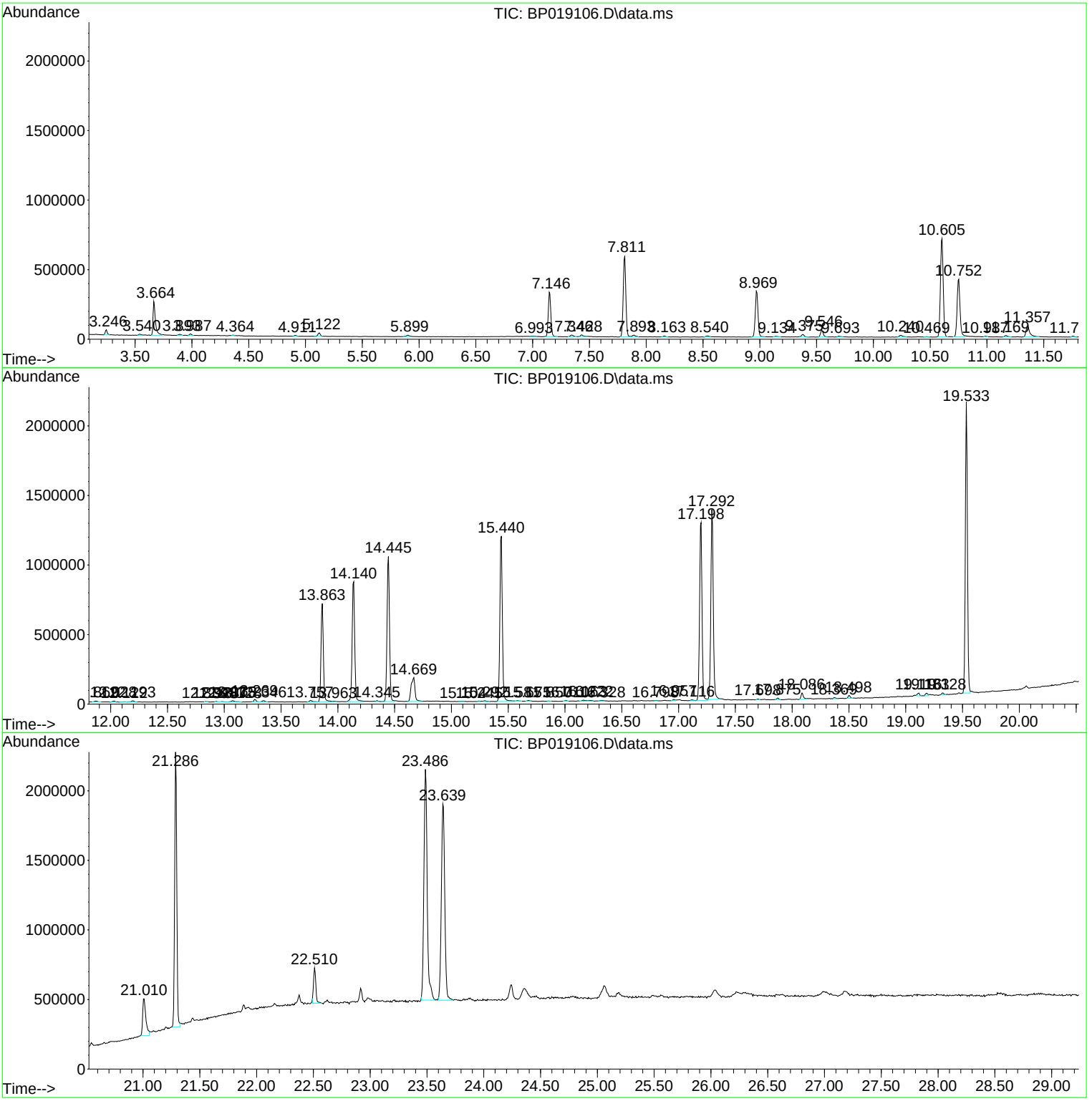
Sum of corrected areas: 27785404

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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

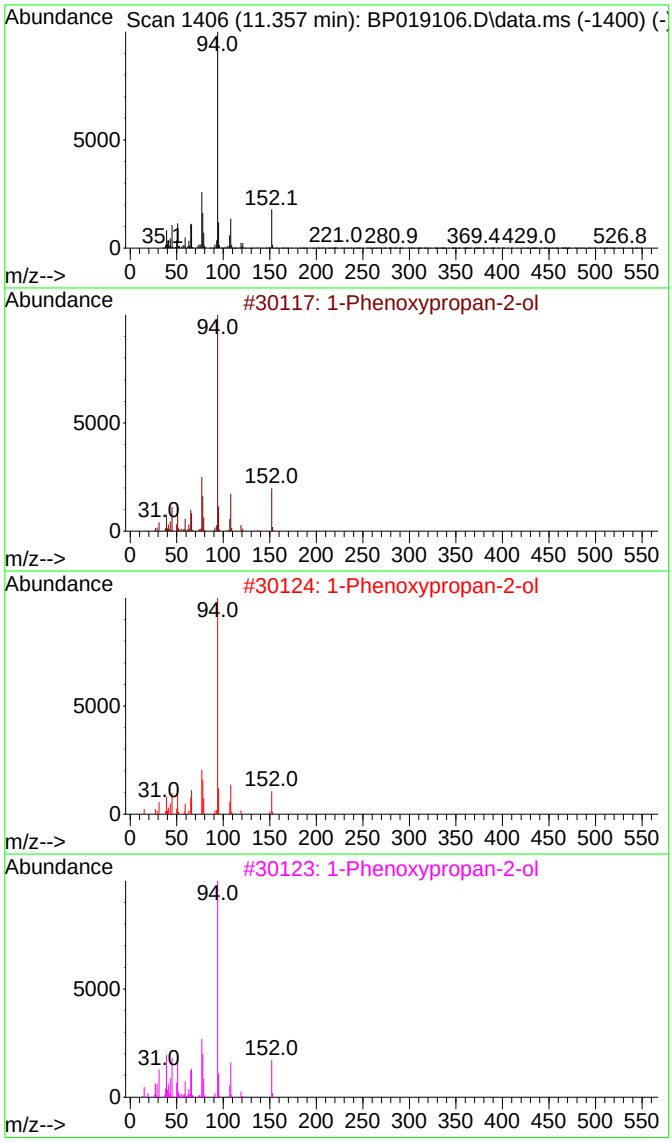
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

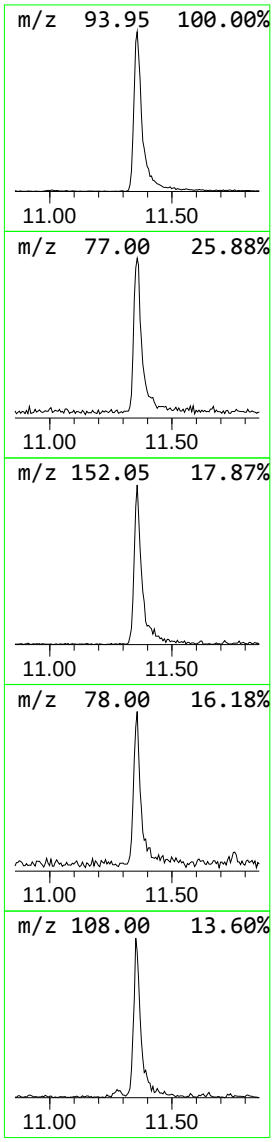
****

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.357	3.07 ng/ul	186097	Naphthalene-d8	10.605

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	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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

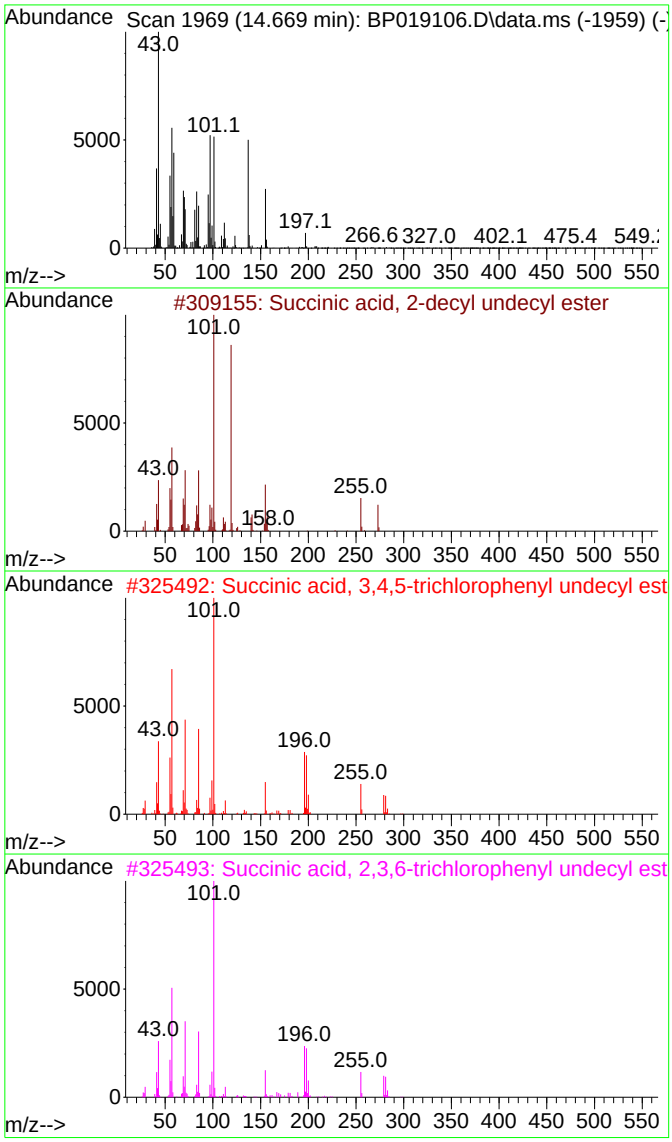
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

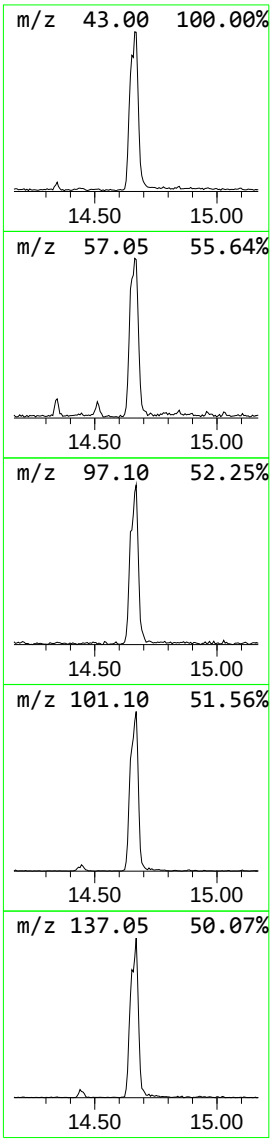
****

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.669	5.16 ng/ul	406119	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-decyl undecyl e...	412	C25H48O4	1000349-43-1	22
2	Succinic acid, 3,4,5-trichloroph...	450	C21H29Cl3O4	1000349-64-7	14
3	Succinic acid, 2,3,6-trichloroph...	450	C21H29Cl3O4	1010349-71-2	14
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
5	Succinic acid, 3-hexyl nonyl ester	328	C19H36O4	1000349-44-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

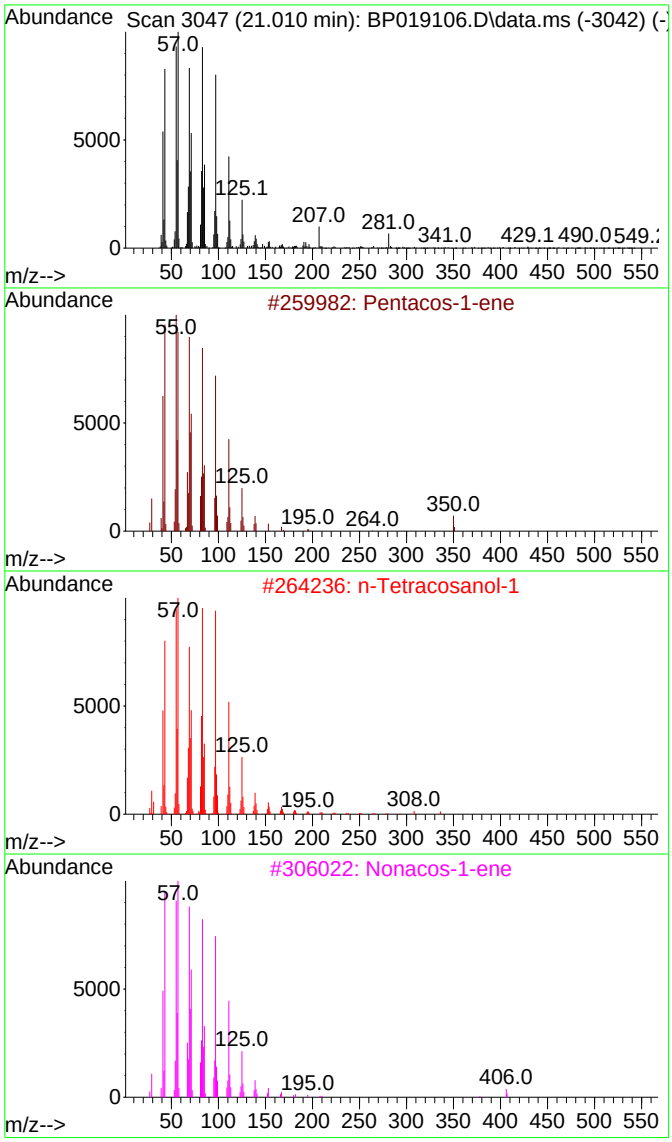
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

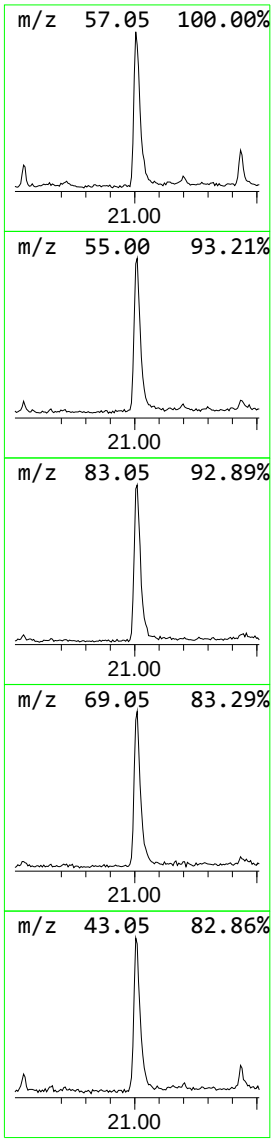
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	4.21 ng/ul	526497	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0Q55

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

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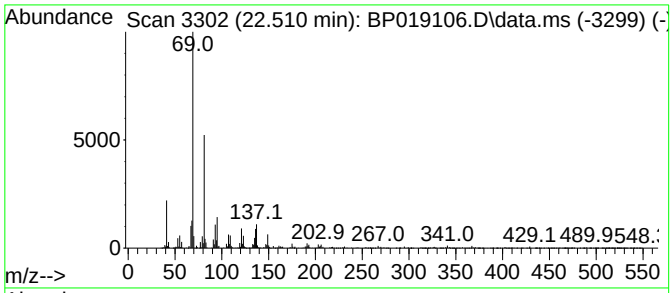
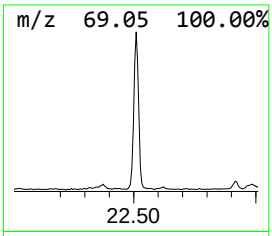
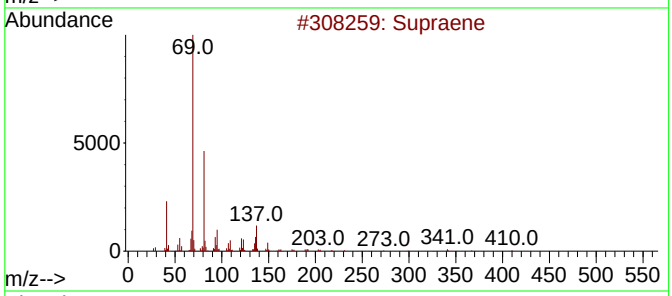
Peak Number 4 Supraene Concentration Rank 4

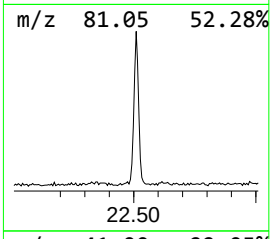
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.510	2.40 ng/ul	351549	Perylene-d12	23.639

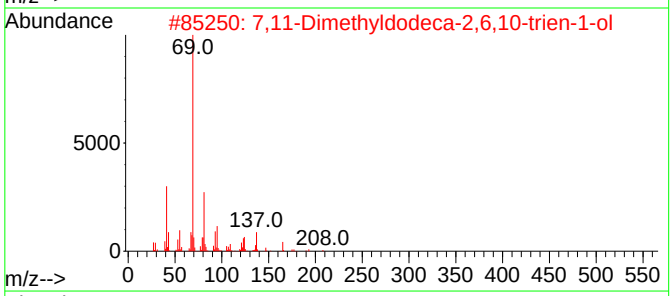
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4	(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	64
5	Supraene	410	C30H50	007683-64-9	64

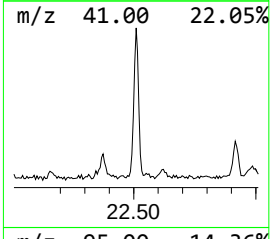


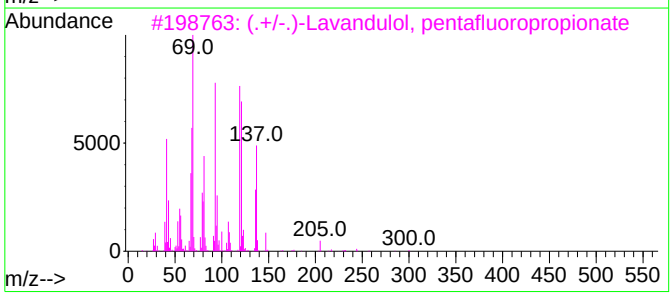


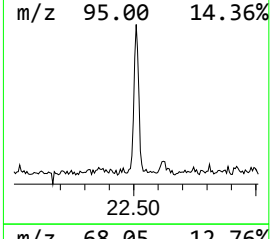


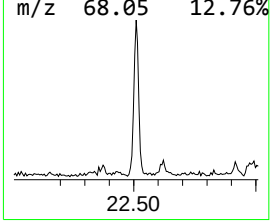












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122623\
Data File : BP019106.D
Acq On : 27 Dec 2023 04:32
Operator : MA/JU
Sample : 05988-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0Q55

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
1-Phenoxypropan...	11.357	3.1	ng/ul	186097	2	10.605	1210590	20.0
unknown-01	14.669	5.2	ng/ul	406119	3	14.445	1573310	20.0
(DEL) Alkane: S...	21.010	4.2	ng/ul	526497	5	21.286	2499180	20.0
Supraene	22.510	2.4	ng/ul	351549	6	23.639	2925480	20.0