LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

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-BP050323.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP015049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.446	7	10	19	rVB	23654	36361	1.14%	0.102%
2	3.746	58	61	66	rVB	13773	19268	0.60%	0.054%
3	3.899	83	87	89	rBV4	7912	9108	0.29%	0.026%
4	3.917	89	90	99	rVV2	13650	27257	0.85%	0.077%
5	4.005	100	105	111	rVV	63843	89858	2.81%	0.253%
6	4.075	115	117	120	rVV4	6645	6287	0.20%	0.018%
7	4.134	123	127	134	rVB	17539	29343	0.92%	0.083%
8	4.228	140	143	151	rVB	14144	21133	0.66%	0.060%
9	4.464	180	183	187	rVB4	13138	17452	0.55%	0.049%
10	4.664	211	217	224	rVB2	25479	50799	1.59%	0.143%
11	4.811	239	242	246	rVB2	14123	18441	0.58%	0.052%
12	5.193	301	307	314	rVB2	16349	34326	1.07%	0.097%
13	5.281	317	322	328	rBV2	20753	33252	1.04%	0.094%
14	5.805	408	411	415	rVB4	3289	5113	0.16%	0.014%
15	5.893	424	426	432	rVB7	2932	4717	0.15%	0.013%
16	6.164	467	472	476	rBV7	6893	12329	0.39%	0.035%
17	6.387	507	510	513	rBV5	2362	3314	0.10%	0.009%
18	6.705	562	564	569	rBV6	4198	6322	0.20%	0.018%
19	6.993	609	613	616	rBV6	3115	4991	0.16%	0.014%
20	7.116	630	634	638	rBV5	6577	9061	0.28%	0.026%
21	7.293	654	664	676	rBV	459876	756053	23.67%	2.130%
22	7.463	687	693	704	rVB	420434	649308	20.33%	1.829%
23	7.669	722	728	737	rBV	497699	807485	25.28%	2.275%
24	7.752	738	742	749	rVB3	10342	16840	0.53%	0.047%
25	7.828	752	755	759	rBV6	3504	5002	0.16%	0.014%
26	7.963	776	778	783	rVB6	2678	3454	0.11%	0.010%
27	8.146	801	809	820	rBV	979094	1591181	49.82%	4.483%
28	8.393	848	851	855	rBV6	2183	3762	0.12%	0.011%
29	8.540	872	876	882	rVB9	4315	5088	0.16%	0.014%
30	8.857	922	930	938	rBV	487326	828764	25.95%	2.335%
31	8.981	944	951	960	rVB	90589	149338	4.68%	0.421%
32	9.105	969	972	977	rBV7	2875	5610	0.18%	0.016%
33	9.322	1001	1009	1020	rBV	483433	800238	25.06%	2.255%
34	9.428	1020	1027	1032	rVV9	7969	16963	0.53%	0.048%
35	9.481	1032	1036	1041	rVB6	7632	12359	0.39%	0.035%
36	9.722	1073	1077	1083	rBV5	8056	12958	0.41%	0.037%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : JREE2

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-BP050323.MA.M
Title : SVOA CALIBRATION

37	9.857	1095	1100	1104	rBV8	3459	4942	0.15%	0.014%
38	10.052	1124	1133	1143	rBV	379358	634969	19.88%	1.789%
39	10.199	1152	1158	1165	rBV7	10112	27808	0.87%	0.078%
40	10.269	1167	1170	1171	rBV3	4022	4545	0.14%	0.013%
41	10.404	1190	1193	1200	rVB6	8744	16920	0.53%	0.048%
42	10.593	1218	1225	1238	rBV	623464	1058176	33.13%	2.981%
43	10.981	1278	1291	1298	rBV	1426714	2380620	74.54%	6.707%
44	11.116	1307	1314	1326	rBV	226517	431279	13.50%	1.215%
45	11.510	1376	1381	1389	rBV	6864	15618	0.49%	0.044%
46	11.757	1416	1423	1434	rBV9	15103	50766	1.59%	0.143%
47	12.016	1462	1467	1470	rBV7	3113	4041	0.13%	0.011%
48	12.216	1495	1501	1504	rBV5	7520	15449	0.48%	0.044%
49	12.293	1510	1514	1518	rBV6	2740	3519	0.11%	0.010%
50	12.451	1536	1541	1546	rBV4	8642	14292	0.45%	0.040%
51	12.516	1546	1552	1554	rBV7	2756	4727	0.15%	0.013%
52	12.575	1554	1562	1573	rBV	273090	477871	14.96%	1.346%
53	13.016	1635	1637	1639	rBV3	3744	4612	0.14%	0.013%
54	13.234	1670	1674	1678	rVB7	8900	12255	0.38%	0.035%
55	13.298	1680	1685	1687	rBV5	3362	4617	0.14%	0.013%
56	13.398	1698	1702	1704	rBV5	4825	7459	0.23%	0.021%
57	13.504	1714	1720	1723	rBV8	5580	9510	0.30%	0.027%
58	13.569	1726	1731	1734	rVV2	15797	29586	0.93%	0.083%
59	13.628	1737	1741	1746	rVB2	31855	48995	1.53%	0.138%
60	13.928	1788	1792	1795	rBV6	6714	9961	0.31%	0.028%
61	14.187	1830	1836	1853	rBV	1174392	1600509	50.12%	4.509%
62	14.310	1855	1857	1860	rVV4	5970	5939	0.19%	0.017%
63	14.481	1880	1886	1898	rBV2	1392708	2071299	64.86%	5.836%
64	14.616	1905	1909	1914	rVB7	16021	22656	0.71%	0.064%
65	14.663	1915	1917	1920	rBV3	5457	5638	0.18%	0.016%
66	14.787	1928	1938	1947	rBV	2078100	3142173	98.39%	8.853%
67	14.975	1964	1970	1982	rBV	191719	378460	11.85%	1.066%
68	15.181	2002	2005	2014	rVB9	23136	34458	1.08%	0.097%
69	15.781	2100	2107	2113	rBV	1750752	2521086	78.94%	7.103%
70	15.892	2121	2126	2132	rBV	227345	313418	9.81%	0.883%
71	16.139	2163	2168	2175	rBV	199560	269076	8.43%	0.758%
72	17.004	2312	2315	2322	rBV	69232	101050	3.16%	0.285%
73	17.539	2401	2406	2413	rBV	2260403	3193655	100.00%	8.998%
74	17.639	2418	2423	2434	rVB	1676721	2347977	73.52%	6.616%
75	18.398	2548	2552	2562	rBV	786867	1241948	38.89%	3.499%
76	19.622	2757	2760	2768	rBV	264613	383623	12.01%	1.081%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

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-BP050323.MA.M
Title : SVOA CALIBRATION

77	19.863	2796	2801	2807	rBV	1603736	2229704	69.82%	6.282%
78	20.357	2882	2885	2888	rVB4	212518	230315	7.21%	0.649%
79	21.622	3096	3100	3106	rVB2	1698520	2289577	71.69%	6.451%
80	24.039	3507	3511	3520	rVB2	900683	1733795	54.29%	4.885%

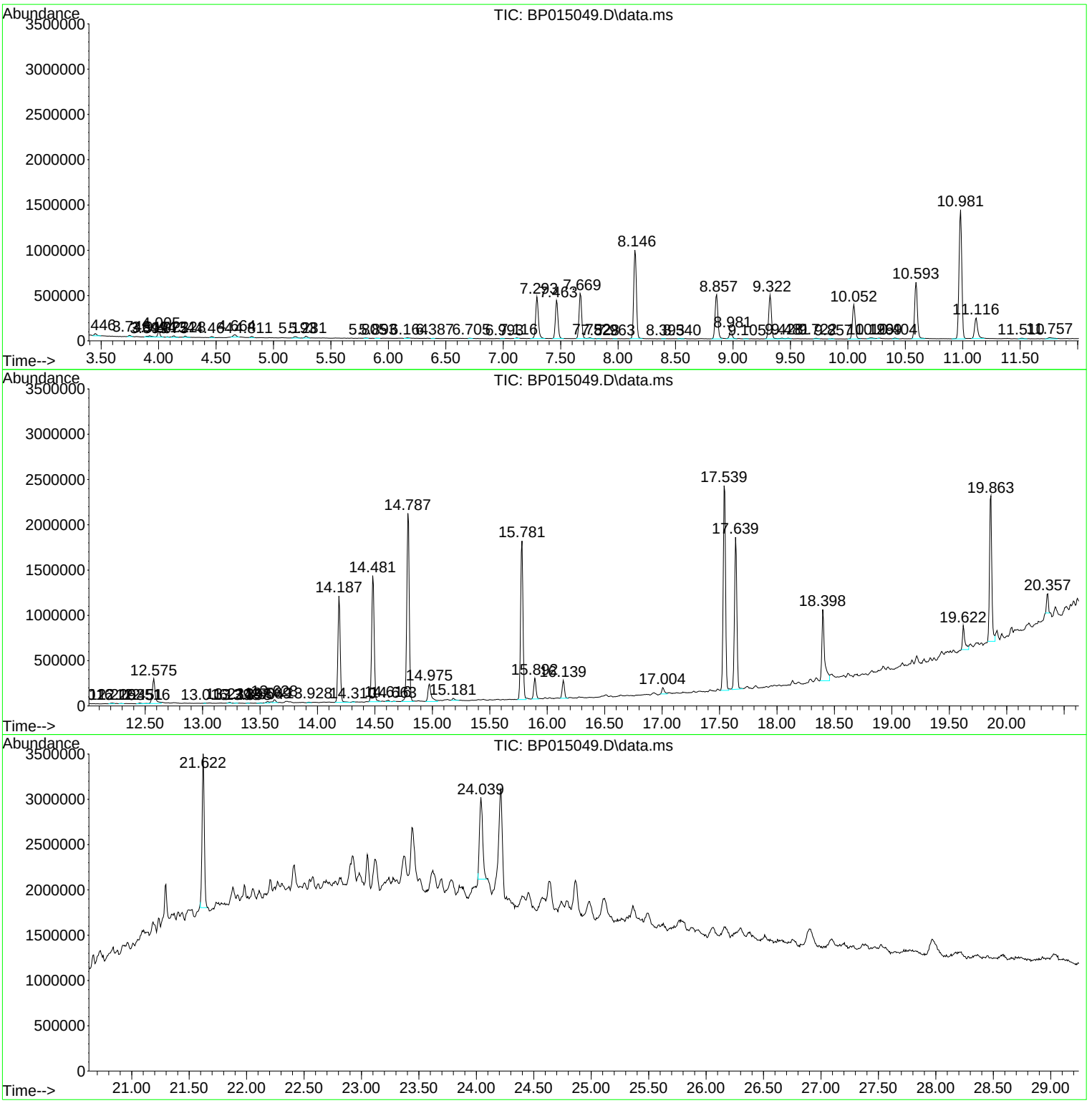
Sum of corrected areas: 35492028

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.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\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

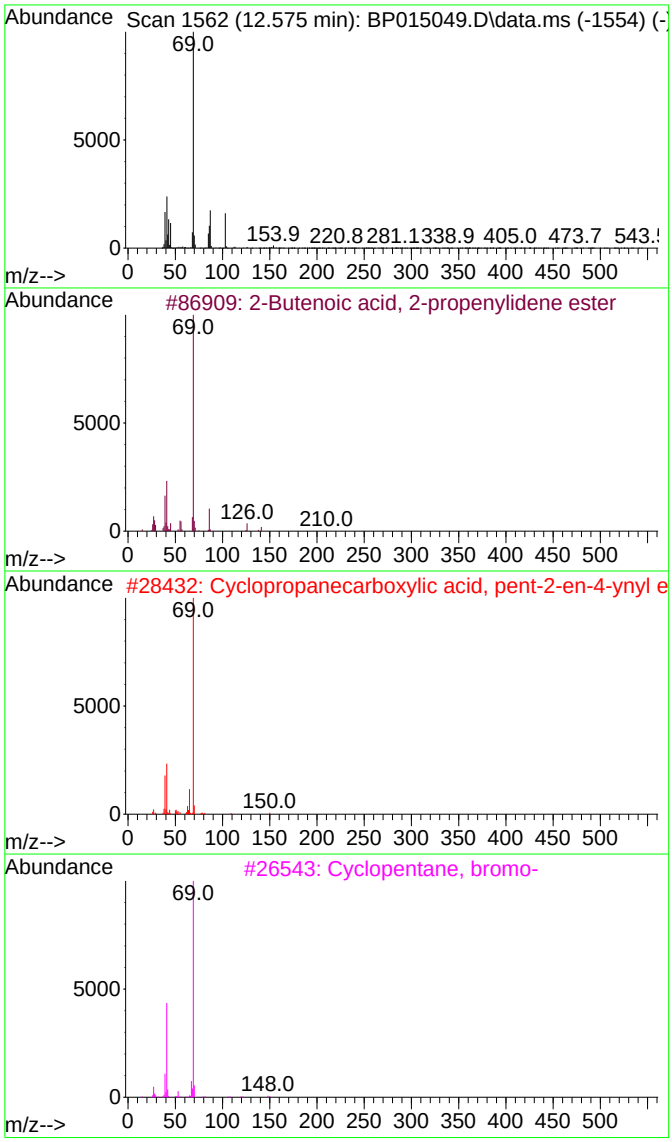
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

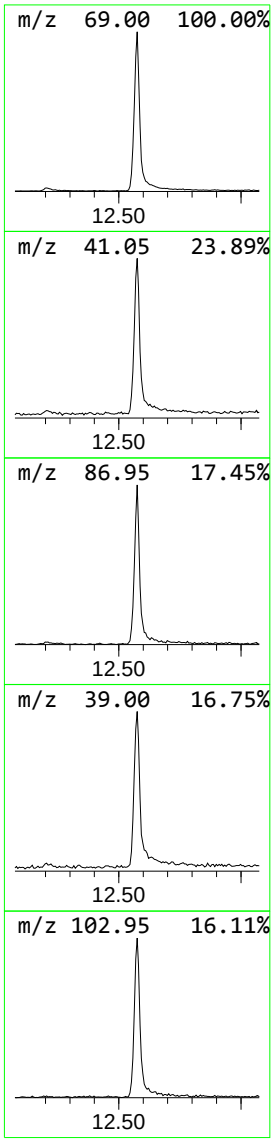
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	4.01 ng/ul	477871	Naphthalene-d8	10.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
2	Cyclopropanecarboxylic acid, pen...	150	C9H10O2	1010299-37-5	38
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	33
4	Oxazole	69	C3H3NO	000288-42-6	9
5	2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

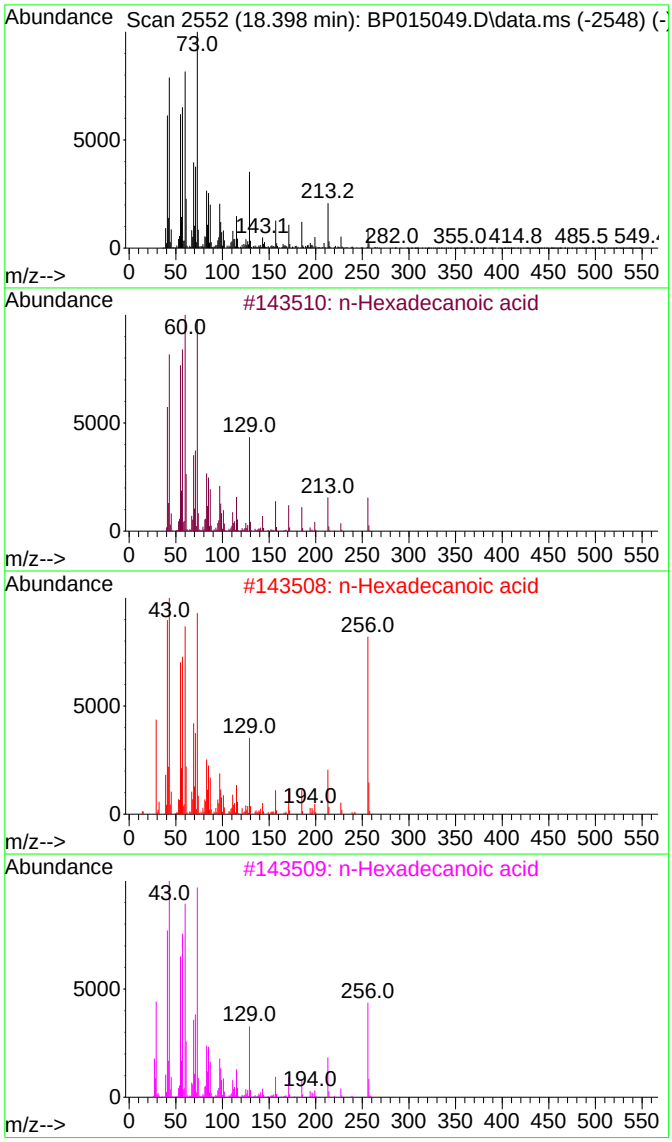
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

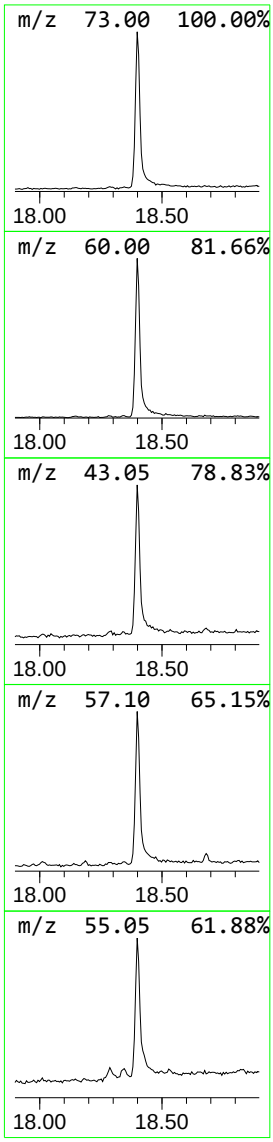
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	7.78 ng/ul	1241950	Phenanthrene-d10	17.539

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	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

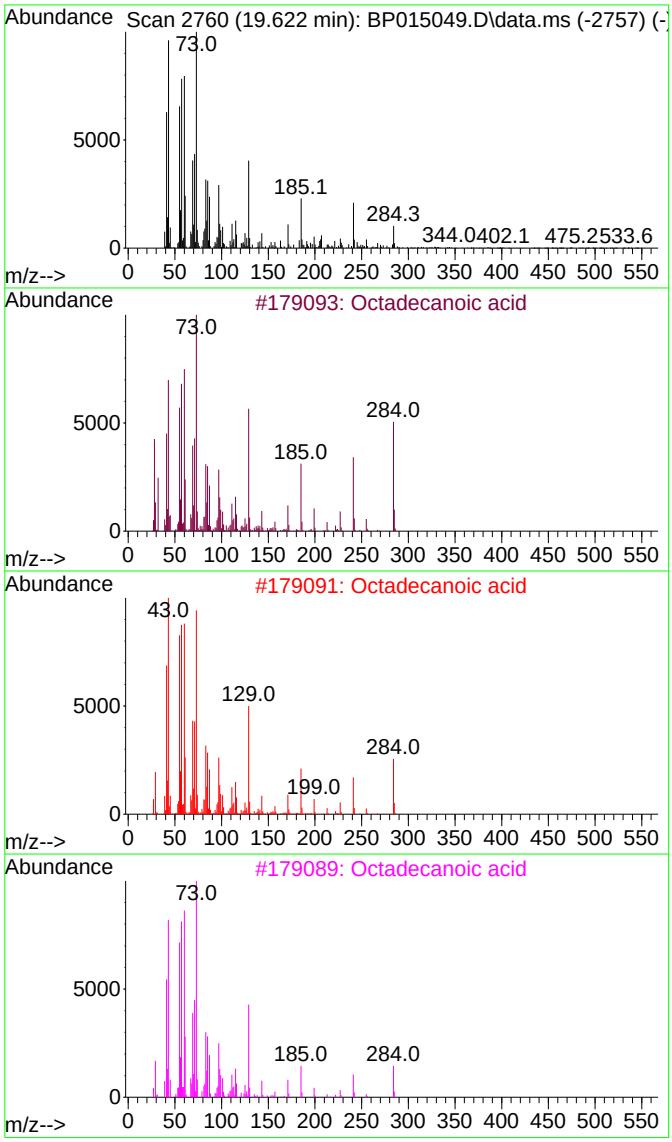
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

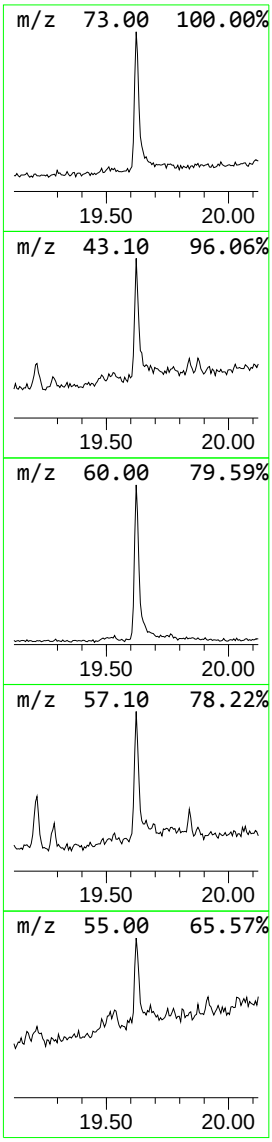
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.622	3.35 ng/ul	383623	Chrysene-d12	21.622

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	97
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

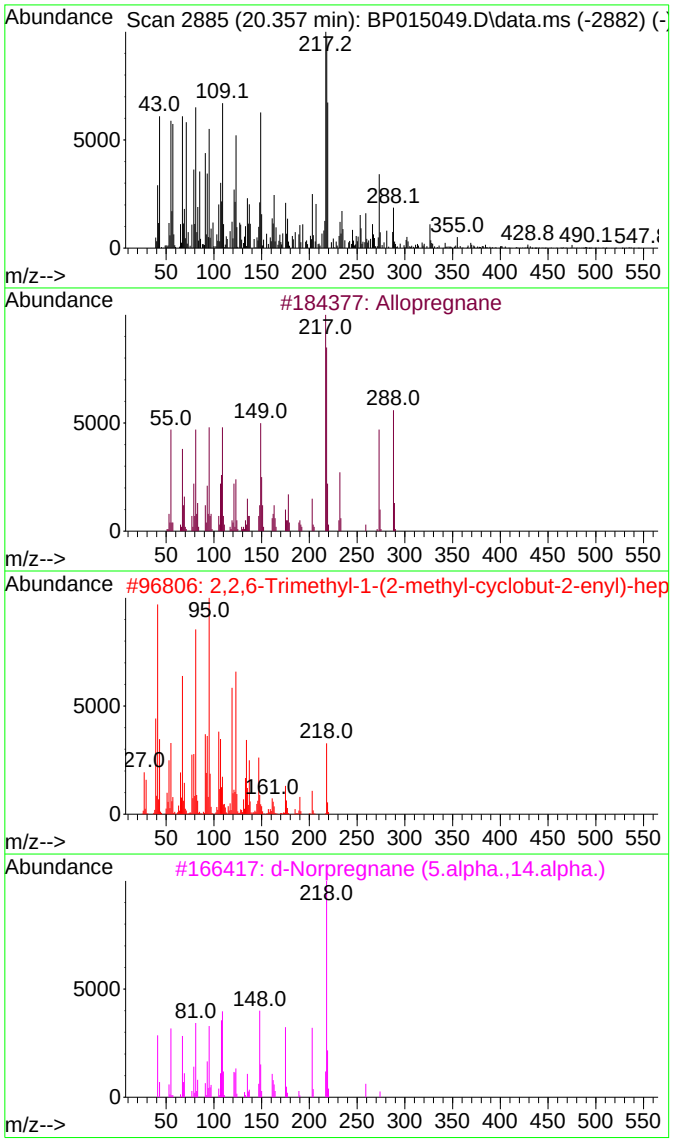
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

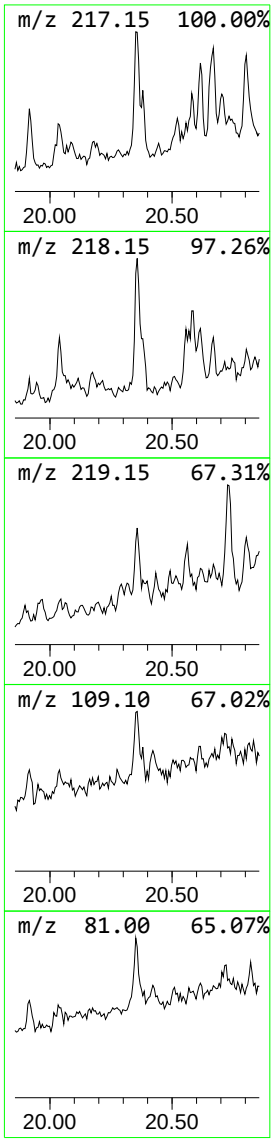
****

Peak Number 4 Allopregnane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.357	2.01 ng/ul	230315	Chrysene-d12	21.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allopregnane	288	C21H36	000641-85-0	72
2	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
3	d-Norpregnane (5.alpha.,14.alpha.)	274	C20H34	1000281-13-7	30
4	4-Bromo-2-fluoro-5-methylaniline...	217	C8H9BrFN	1000494-85-7	27
5	Allyl ionone 4	232	C16H24O	1000284-93-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015049.D
Acq On : 10 May 2023 18:50
Operator : CG/JU
Sample : 02591-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREE2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.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
unknown-01	12.575	4.0	ng/ul	477871	2	10.981	2380620	20.0
n-Hexadecanoic ...	18.398	7.8	ng/ul	1241950	4	17.539	3193660	20.0
Octadecanoic acid	19.622	3.4	ng/ul	383623	5	21.622	2289580	20.0
Allopregnane	20.357	2.0	ng/ul	230315	5	21.622	2289580	20.0