LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A4BY0

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-BP071024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP020968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	24	26	35	rVB6	11900	20174	0.54%	0.050%
2	3.246	40	44	49	rBV	36259	43528	1.17%	0.108%
3	3.528	88	92	105	rVB	70888	115898	3.12%	0.288%
4	3.681	116	118	128	rBV	30708	56204	1.51%	0.140%
5	3.758	128	131	139	rVB3	18796	29367	0.79%	0.073%
6	3.964	163	166	175	rVB	13641	20283	0.55%	0.050%
7	4.381	234	237	242	rVB2	8089	11683	0.31%	0.029%
8	4.469	249	252	257	rBV3	5232	7580	0.20%	0.019%
9	4.516	257	260	266	rVB2	12245	14515	0.39%	0.036%
10	4.752	296	300	303	rBV6	4627	6068	0.16%	0.015%
11	4.863	314	319	327	rBV	39862	59402	1.60%	0.148%
12	5.828	478	483	492	rVB2	7753	16551	0.45%	0.041%
13	6.352	566	572	574	rBV7	2856	4894	0.13%	0.012%
14	6.593	608	613	622	rVB7	3481	9436	0.25%	0.023%
15	6.810	642	650	656	rBV5	5068	10205	0.27%	0.025%
16	6.905	659	666	683	rBV	516346	960386	25.83%	2.390%
17	7.052	684	691	704	rVB	461843	735388	19.78%	1.830%
18	7.252	717	725	733	rBV	574492	1009751	27.16%	2.513%
19	7.699	792	801	810	rBV	631240	994383	26.75%	2.474%
20	7.775	810	814	819	rVB4	8390	16499	0.44%	0.041%
21	8.310	900	905	909	rBV7	3008	6543	0.18%	0.016%
22	8.416	914	923	938	rBV	562221	1125707	30.28%	2.801%
23	8.522	938	941	951	rVB10	8054	17996	0.48%	0.045%
24	8.857	986	998	1009	rBV	527186	924910	24.88%	2.301%
25	8.993	1016	1021	1026	rVB8	5151	10946	0.29%	0.027%
26	9.210	1051	1058	1064	rBV3	12691	21425	0.58%	0.053%
27	9.404	1083	1091	1102	rBV	53122	98224	2.64%	0.244%
28	9.557	1110	1117	1131	rBV	459306	804950	21.65%	2.003%
29	10.104	1202	1210	1228	rBV	604695	1222172	32.88%	3.041%
30	10.451	1261	1269	1284	rBV	817059	1370533	36.87%	3.410%
31	10.610	1288	1296	1307	rBV	334709	764708	20.57%	1.903%
32	10.993	1353	1361	1362	rBV7	15635	25646	0.69%	0.064%
33	11.134	1381	1385	1389	rVB6	4510	6984	0.19%	0.017%
34	11.204	1390	1397	1416	rBV2	67575	188498	5.07%	0.469%
35	11.528	1447	1452	1458	rVB6	6636	14160	0.38%	0.035%
36	11.681	1471	1478	1480	rVB7	4152	6923	0.19%	0.017%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

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-BP071024.MA.M
Title : SVOA CALIBRATION

37	11.722	1480	1485	1490	rVB9	2627	5251	0.14%	0.013%
38	11.857	1504	1508	1511	rBV5	5292	6855	0.18%	0.017%
39	11.957	1522	1525	1532	rVB7	4802	8663	0.23%	0.022%
40	12.040	1532	1539	1549	rVB4	15905	38108	1.03%	0.095%
41	12.457	1603	1610	1613	rBV9	4500	8235	0.22%	0.020%
42	12.592	1629	1633	1636	rBV6	4057	7005	0.19%	0.017%
43	12.640	1639	1641	1645	rVV5	4092	6003	0.16%	0.015%
44	12.722	1651	1655	1660	rBV8	5177	10595	0.29%	0.026%
45	12.828	1671	1673	1678	rVB5	6701	8518	0.23%	0.021%
46	12.910	1678	1687	1691	rBV5	12553	35388	0.95%	0.088%
47	13.063	1710	1713	1717	rBV6	11810	21509	0.58%	0.054%
48	13.722	1819	1825	1838	rBV	1153670	1897668	51.05%	4.722%
49	14.004	1864	1873	1884	rBV	1288357	2287183	61.52%	5.691%
50	14.128	1890	1894	1898	rVB2	35810	48715	1.31%	0.121%
51	14.263	1913	1917	1918	rBV4	14994	17078	0.46%	0.042%
52	14.304	1918	1924	1933	rVB	1139242	1847045	49.68%	4.596%
53	14.528	1955	1962	1966	rBV2	77823	176324	4.74%	0.439%
54	14.581	1966	1971	1979	rBV2	267991	552986	14.88%	1.376%
55	15.104	2056	2060	2065	rBV4	30725	48463	1.30%	0.121%
56	15.322	2091	2097	2112	rBV	1718625	2964641	79.75%	7.377%
57	15.481	2118	2124	2130	rBV	517724	748112	20.12%	1.862%
58	17.122	2397	2403	2408	rBV	1594580	2323325	62.50%	5.781%
59	17.222	2414	2420	2430	rBV2	1825670	3179454	85.53%	7.911%
60	18.057	2558	2562	2573	rBV2	249864	432623	11.64%	1.076%
61	18.227	2587	2591	2595	rBV2	71824	110571	2.97%	0.275%
62	19.257	2763	2766	2772	rVB	163939	228657	6.15%	0.569%
63	19.380	2784	2787	2794	rBV3	126257	295806	7.96%	0.736%
64	19.610	2820	2826	2833	rBV	2409581	3717538	100.00%	9.250%
65	20.692	3008	3010	3014	rVB	163674	155762	4.19%	0.388%
66	21.221	3096	3100	3109	rBV2	368747	637201	17.14%	1.586%
67	21.563	3153	3158	3165	rVB	1598257	2506056	67.41%	6.236%
68	24.615	3671	3677	3688	rVB2	966268	2407277	64.75%	5.990%
69	24.845	3709	3716	3726	rVB	1050419	2696794	72.54%	6.710%

Sum of corrected areas: 40187929

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
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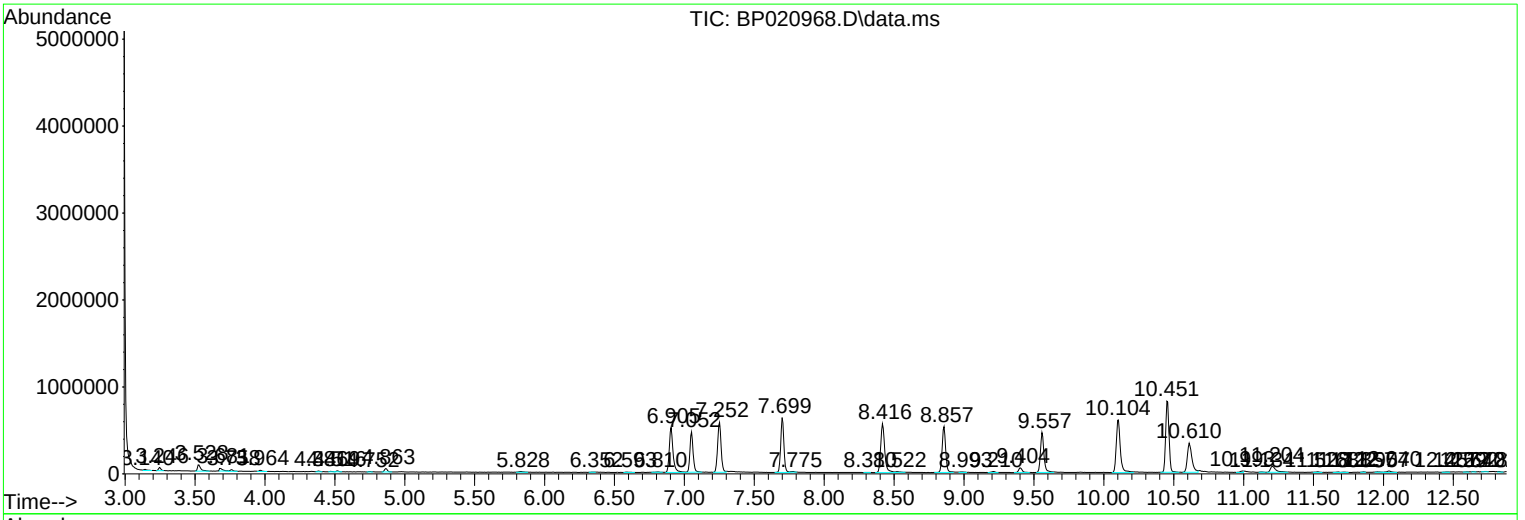
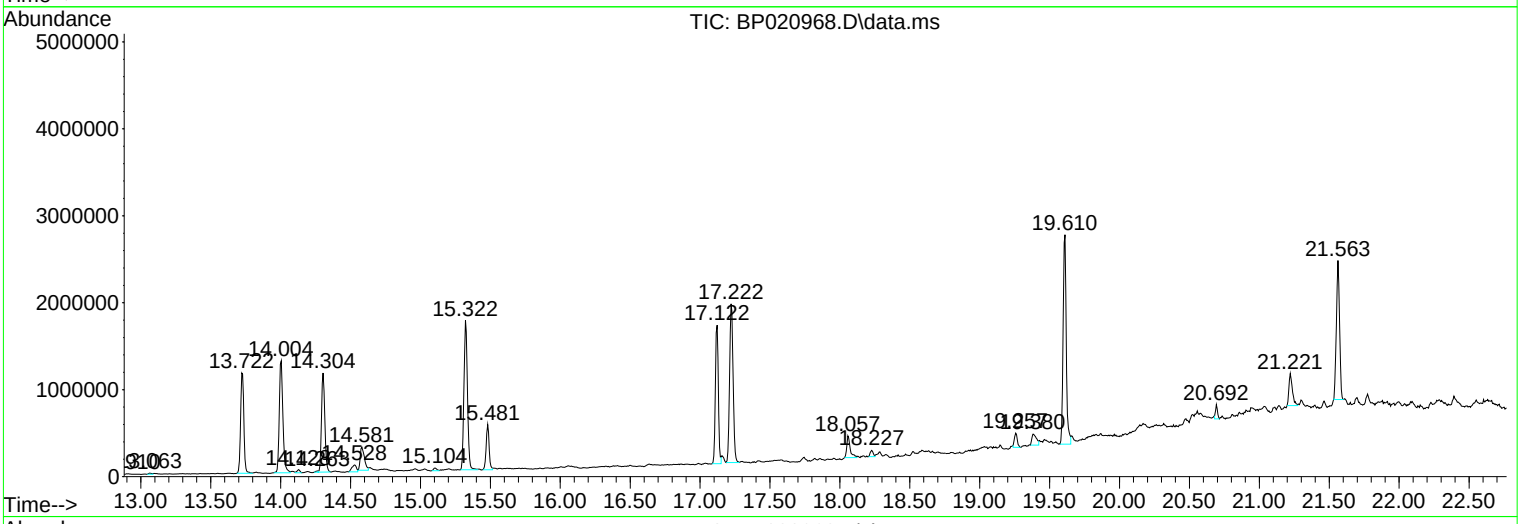
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

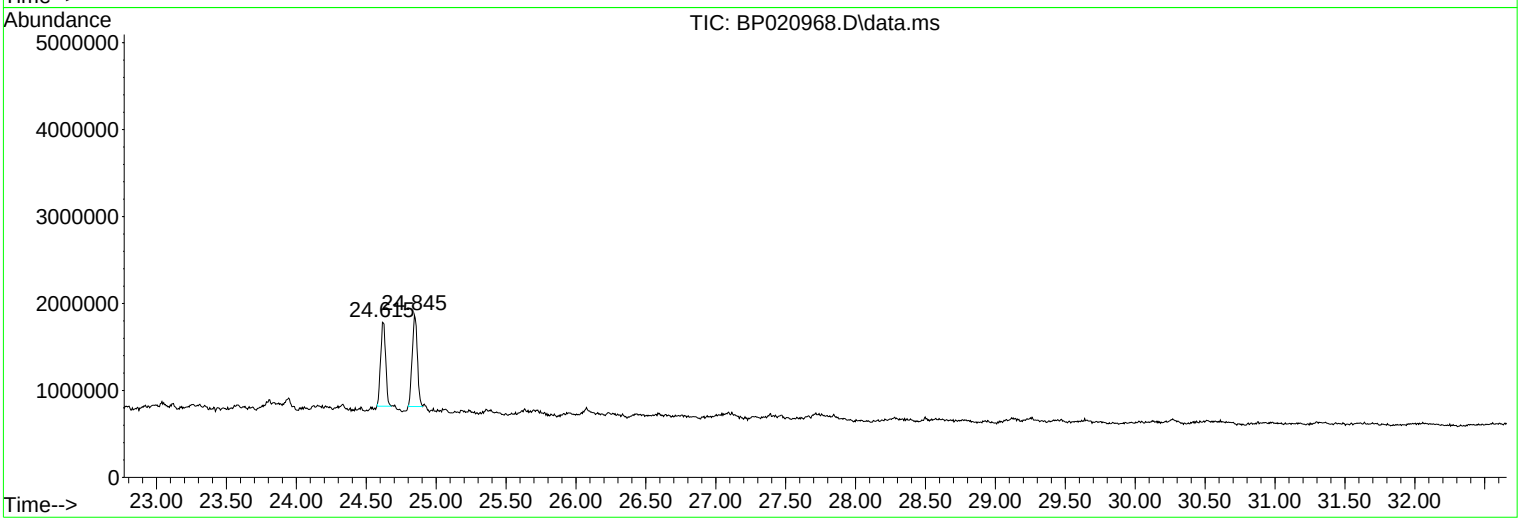
Instrument :
BNA_P
ClientSampleId :
A4BY0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.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\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

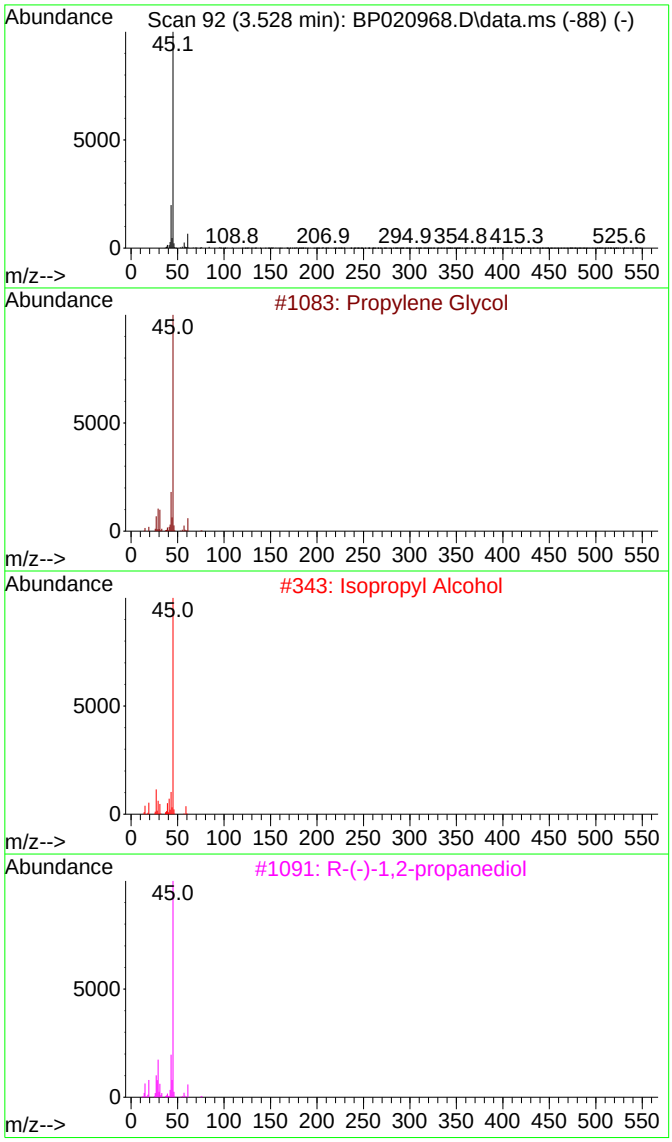
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

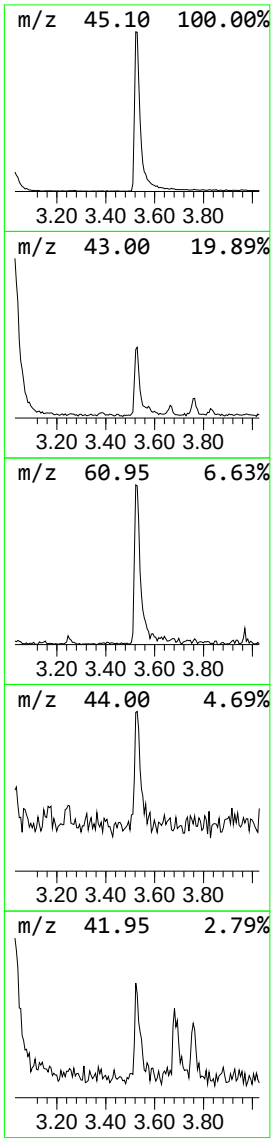
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.528	2.33 ng/ul	115898	1,4-Dichlorobenzene-d4	7.699

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

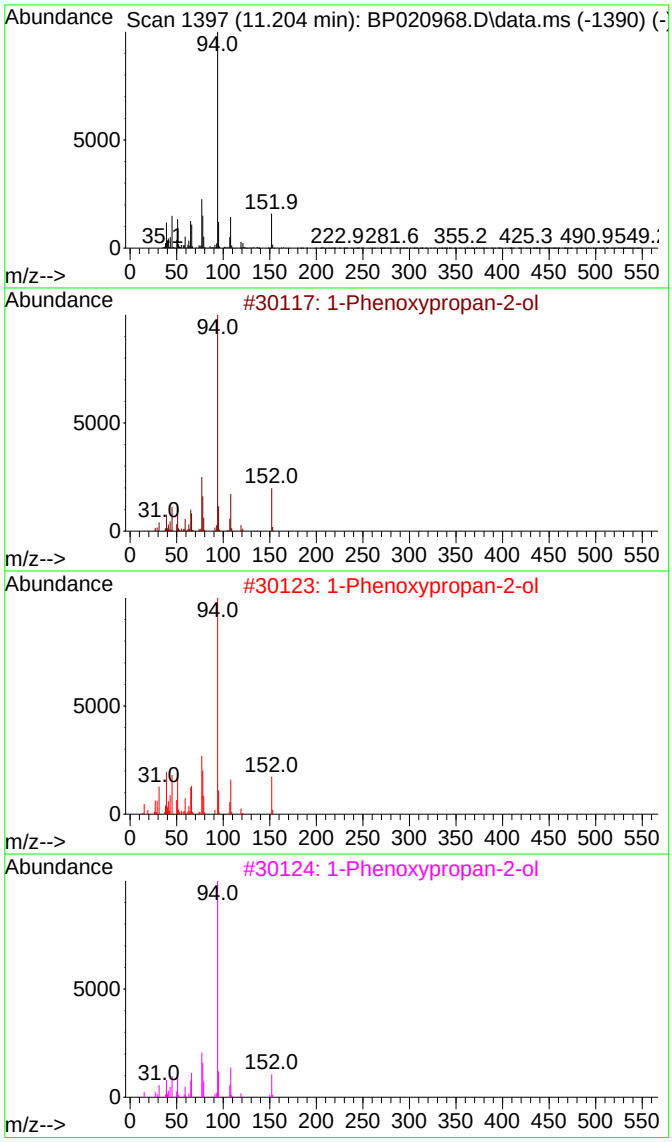
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

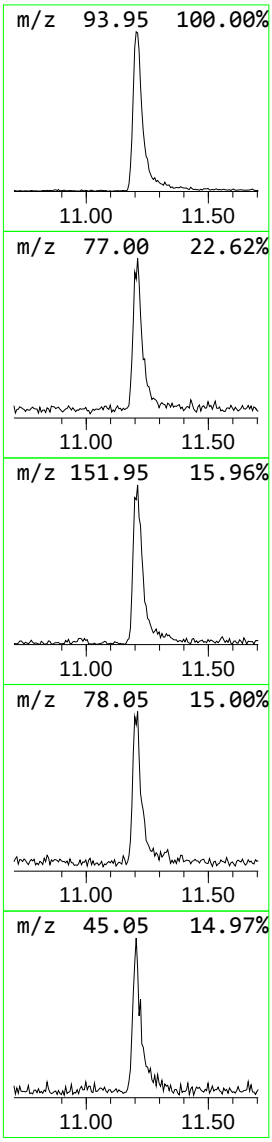
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	2.75 ng/ul	188498	Naphthalene-d8	10.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

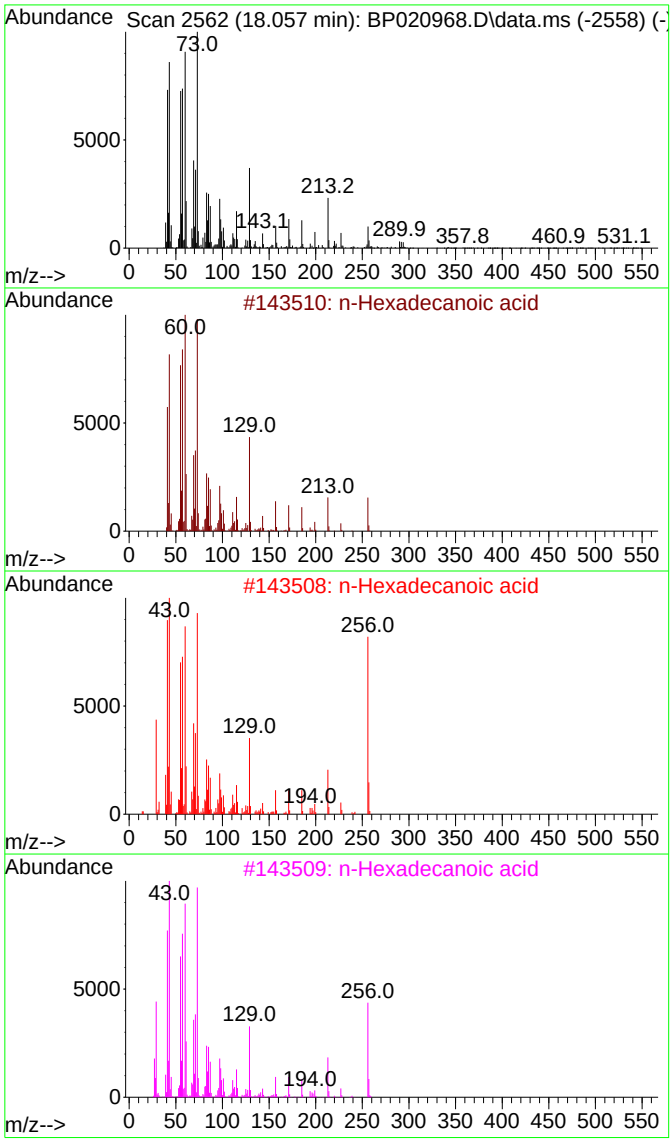
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

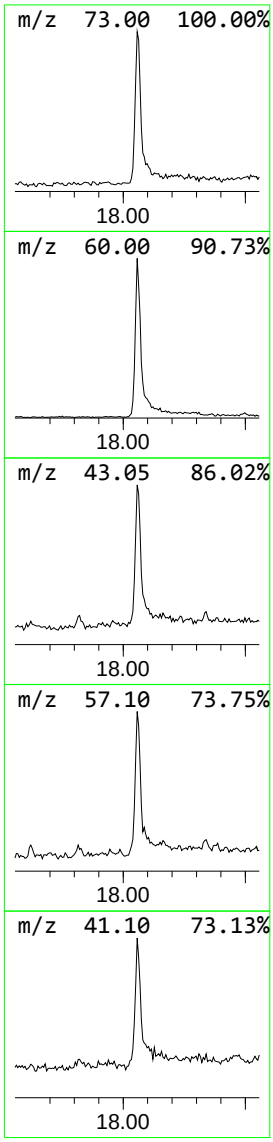
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	3.72 ng/ul	432623	Phenanthrene-d10	17.122

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





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Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

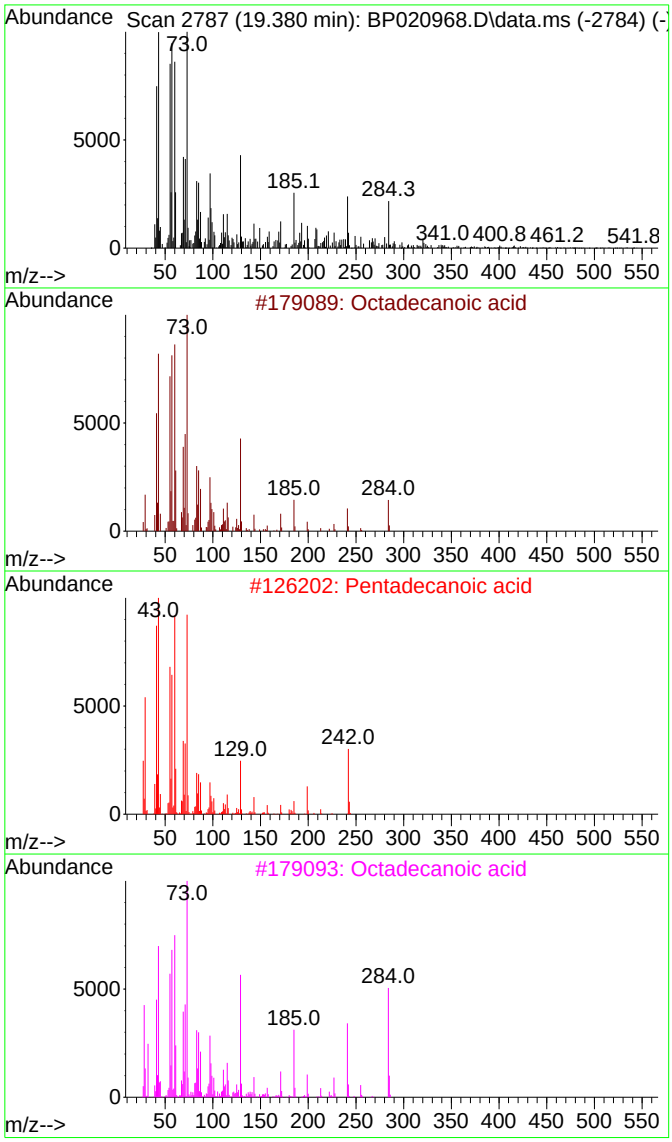
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

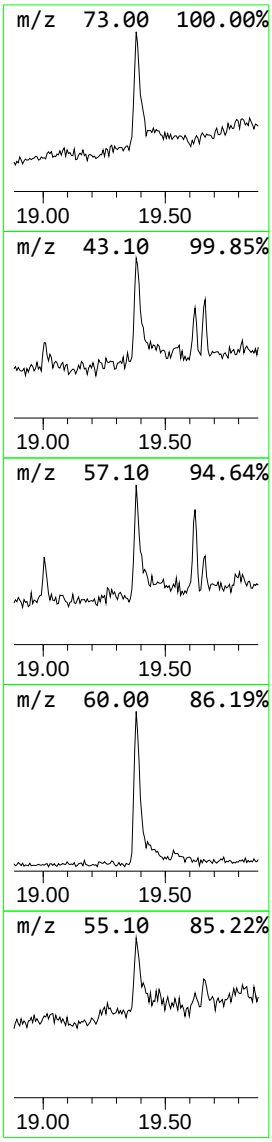
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.380	2.36 ng/ul	295806	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





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Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

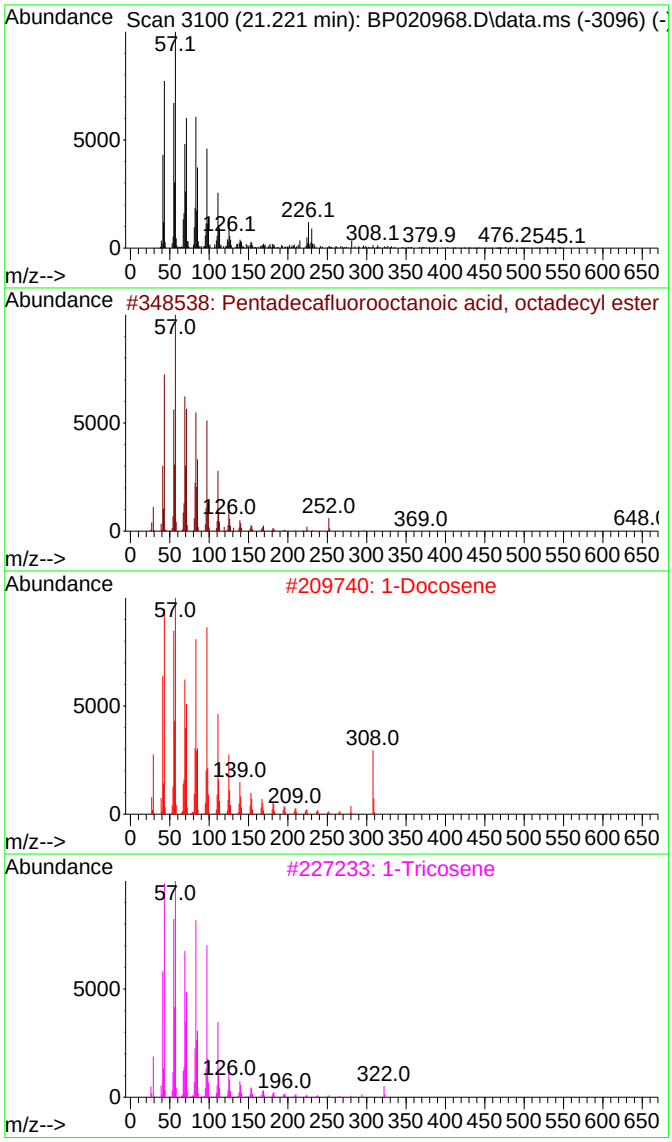
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

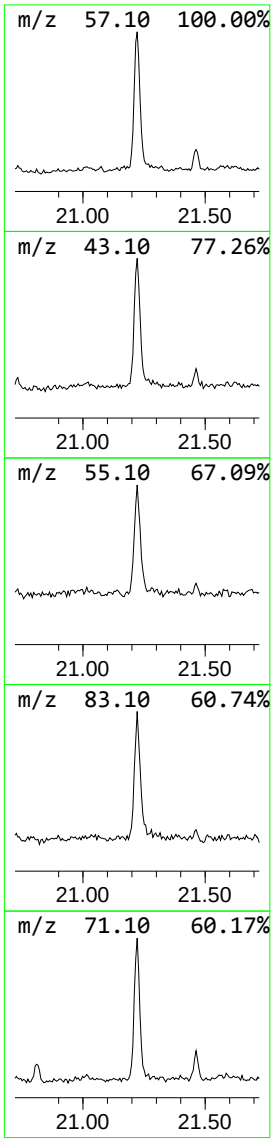
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	5.09 ng/ul	637201	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	1-Tricosene	322	C23H46	018835-32-0	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020968.D
Acq On : 15 Jul 2024 21:48
Operator : MA/JU
Sample : P3100-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BY0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.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
Propylene Glycol	3.528	2.3	ng/ul	115898	1	7.699	994383	20.0
1-Phenoxypropan...	11.204	2.8	ng/ul	188498	2	10.457	1370530	20.0
n-Hexadecanoic ...	18.057	3.7	ng/ul	432623	4	17.122	2323330	20.0
Octadecanoic acid	19.380	2.4	ng/ul	295806	5	21.563	2506060	20.0
Pentadecafluoro...	21.221	5.1	ng/ul	637201	5	21.563	2506060	20.0