LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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: BP020972.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	41	44	52	rVB	38910	50333	1.23%	0.093%
2	3.528	88	92	104	rBV	83040	126225	3.07%	0.233%
3	3.664	112	115	129	rBV	397064	604894	14.73%	1.115%
4	3.969	163	167	171	rVB	11440	13405	0.33%	0.025%
5	4.328	226	228	234	rVB7	4463	6705	0.16%	0.012%
6	4.864	315	319	323	rBV	7442	11003	0.27%	0.020%
7	5.116	358	362	366	rBV5	4270	7470	0.18%	0.014%
8	5.828	479	483	491	rBV2	9610	16847	0.41%	0.031%
9	6.340	566	570	573	rBV6	3836	5835	0.14%	0.011%
10	6.787	640	646	647	rBV6	3824	5071	0.12%	0.009%
11	6.905	657	666	683	rBV	616615	1082534	26.36%	1.995%
12	7.040	683	689	704	rVB	479031	811534	19.76%	1.496%
13	7.246	717	724	734	rBV	673623	1114143	27.13%	2.054%
14	7.328	734	738	746	rVB	11137	23382	0.57%	0.043%
15	7.693	793	800	808	rBV	745525	1183461	28.82%	2.182%
16	7.763	808	812	822	rVB6	10237	25848	0.63%	0.048%
17	8.187	880	884	890	rVB9	2652	4213	0.10%	0.008%
18	8.410	915	922	936	rBV	757957	1335387	32.52%	2.462%
19	8.516	938	940	947	rVB8	5417	9012	0.22%	0.017%
20	8.846	987	996	1013	rBV	605914	1034320	25.19%	1.907%
21	8.993	1016	1021	1026	rVV8	6836	12161	0.30%	0.022%
22	9.199	1050	1056	1063	rVB2	12250	20023	0.49%	0.037%
23	9.399	1084	1090	1105	rVB2	48970	96518	2.35%	0.178%
24	9.552	1108	1116	1127	rBV	496910	896525	21.83%	1.653%
25	9.828	1155	1163	1166	rBV10	4470	9821	0.24%	0.018%
26	9.987	1185	1190	1196	rBV10	2857	6074	0.15%	0.011%
27	10.099	1201	1209	1226	rBV	657294	1395113	33.97%	2.572%
28	10.463	1258	1271	1282	rBV	1013901	1707267	41.57%	3.147%
29	10.610	1288	1296	1316	rBV	235203	509702	12.41%	0.940%
30	10.993	1355	1361	1368	rBV7	14710	31733	0.77%	0.058%
31	11.210	1391	1398	1411	rBV	70961	180672	4.40%	0.333%
32	11.851	1505	1507	1511	rVB4	4385	6154	0.15%	0.011%
33	11.957	1520	1525	1528	rBV5	4716	6564	0.16%	0.012%
34	12.051	1535	1541	1547	rVB4	12653	24415	0.59%	0.045%
35	12.287	1577	1581	1589	rVV5	3548	9356	0.23%	0.017%
36	12.604	1627	1635	1637	rBV9	2650	5502	0.13%	0.010%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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	12.722	1649	1655	1660	rBV9	5164	9510	0.23%	0.018%
38	12.816	1666	1671	1675	rBV7	4174	6830	0.17%	0.013%
39	13.034	1702	1708	1712	rBV9	2508	5695	0.14%	0.010%
40	13.116	1716	1722	1727	rVV5	9777	18615	0.45%	0.034%
41	13.169	1727	1731	1736	rVV8	4455	8755	0.21%	0.016%
42	13.263	1739	1747	1752	rBV8	9758	22158	0.54%	0.041%
43	13.487	1778	1785	1800	rBV	191055	573660	13.97%	1.057%
44	13.716	1818	1824	1833	rBV	1384878	1989058	48.43%	3.667%
45	13.792	1833	1837	1840	rVV5	10241	19924	0.49%	0.037%
46	13.834	1840	1844	1848	rVB7	14006	22438	0.55%	0.041%
47	13.957	1859	1865	1867	rBV3	18509	26046	0.63%	0.048%
48	14.010	1867	1874	1891	rVB	1558641	2458371	59.86%	4.532%
49	14.145	1891	1897	1900	rBV8	8235	13847	0.34%	0.026%
50	14.204	1902	1907	1913	rBV6	12063	20917	0.51%	0.039%
51	14.316	1916	1926	1933	rBV	1663202	2375075	57.83%	4.378%
52	14.522	1956	1961	1962	rBV	49099	60497	1.47%	0.112%
53	14.551	1962	1966	1968	rVV4	111603	190426	4.64%	0.351%
54	14.587	1968	1972	1989	rVV	359233	858161	20.90%	1.582%
55	14.716	1990	1994	2001	rVV3	52896	117855	2.87%	0.217%
56	14.775	2001	2004	2010	rVB2	40875	54260	1.32%	0.100%
57	14.863	2015	2019	2025	rVB	22790	36271	0.88%	0.067%
58	15.110	2057	2061	2065	rBV3	11482	19818	0.48%	0.037%
59	15.163	2066	2070	2075	rVB4	11884	15740	0.38%	0.029%
60	15.328	2087	2098	2109	rBV	2119561	3093761	75.33%	5.703%
61	15.463	2116	2121	2136	rBV	557825	869662	21.18%	1.603%
62	15.704	2154	2162	2167	rBV7	19209	47621	1.16%	0.088%
63	15.804	2176	2179	2182	rBV3	10852	13716	0.33%	0.025%
64	15.904	2191	2196	2203	rVB9	24399	48116	1.17%	0.089%
65	16.051	2217	2221	2228	rBV7	12819	31334	0.76%	0.058%
66	16.139	2230	2236	2242	rVB4	22137	40838	0.99%	0.075%
67	16.216	2246	2249	2254	rVB7	11273	17646	0.43%	0.033%
68	16.281	2257	2260	2263	rVV3	15424	17319	0.42%	0.032%
69	16.522	2295	2301	2309	rBV3	80556	188538	4.59%	0.348%
70	16.839	2350	2355	2363	rBV3	112705	183189	4.46%	0.338%
71	16.898	2363	2365	2371	rVB7	12370	22405	0.55%	0.041%
72	17.016	2381	2385	2392	rBV5	34337	58148	1.42%	0.107%
73	17.086	2393	2397	2398	rBV3	21702	29205	0.71%	0.054%
74	17.128	2398	2404	2410	rBV	1805948	2849251	69.38%	5.252%
75	17.228	2415	2421	2426	rBV	2345729	3236622	78.81%	5.966%
76	17.528	2468	2472	2478	rBV5	37020	54870	1.34%	0.101%

LSC Area Percent Report

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Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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

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

77	17.675	2492	2497	2503	rVB2	22947	45816	1.12%	0.084%
78	17.804	2516	2519	2524	rVB2	39322	54181	1.32%	0.100%
79	17.933	2537	2541	2547	rVB4	30236	47630	1.16%	0.088%
80	17.992	2547	2551	2555	rBV	123972	165841	4.04%	0.306%
81	18.045	2555	2560	2571	rBV	831643	1311071	31.92%	2.417%
82	18.357	2609	2613	2617	rBV4	64426	111351	2.71%	0.205%
83	18.739	2676	2678	2681	rBV4	25554	30855	0.75%	0.057%
84	19.010	2721	2724	2726	rBV	48748	56604	1.38%	0.104%
85	19.222	2754	2760	2762	rBV2	111587	220464	5.37%	0.406%
86	19.251	2762	2765	2780	rVV	228730	549347	13.38%	1.013%
87	19.386	2784	2788	2800	rVV	239339	366270	8.92%	0.675%
88	19.604	2819	2825	2833	rBV	2991355	4106795	100.00%	7.570%
89	21.210	3094	3098	3105	rVB	667117	1017556	24.78%	1.876%
90	21.551	3151	3156	3162	rVB	2152444	3159586	76.94%	5.824%
91	22.433	3303	3306	3318	rVB	434677	822514	20.03%	1.516%
92	23.939	3557	3562	3569	rVB	375189	828307	20.17%	1.527%
93	24.627	3670	3679	3690	rVB	1340765	3963805	96.52%	7.307%
94	24.851	3710	3717	3727	rBV	1349329	3085136	75.12%	5.687%
95	28.921	4401	4409	4425	rVB	579871	2190415	53.34%	4.038%

Sum of corrected areas: 54248934

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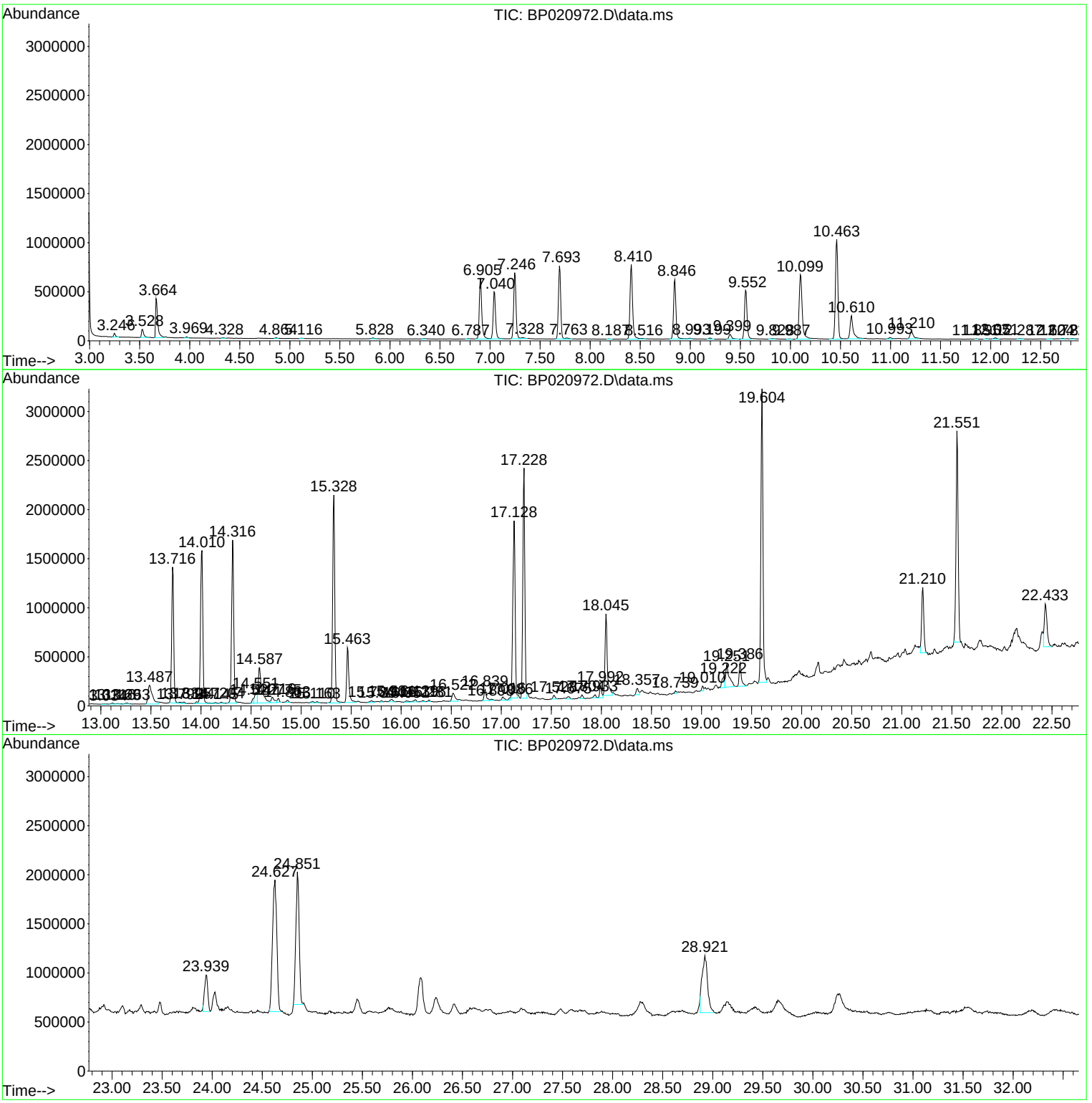
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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 : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
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Instrument :
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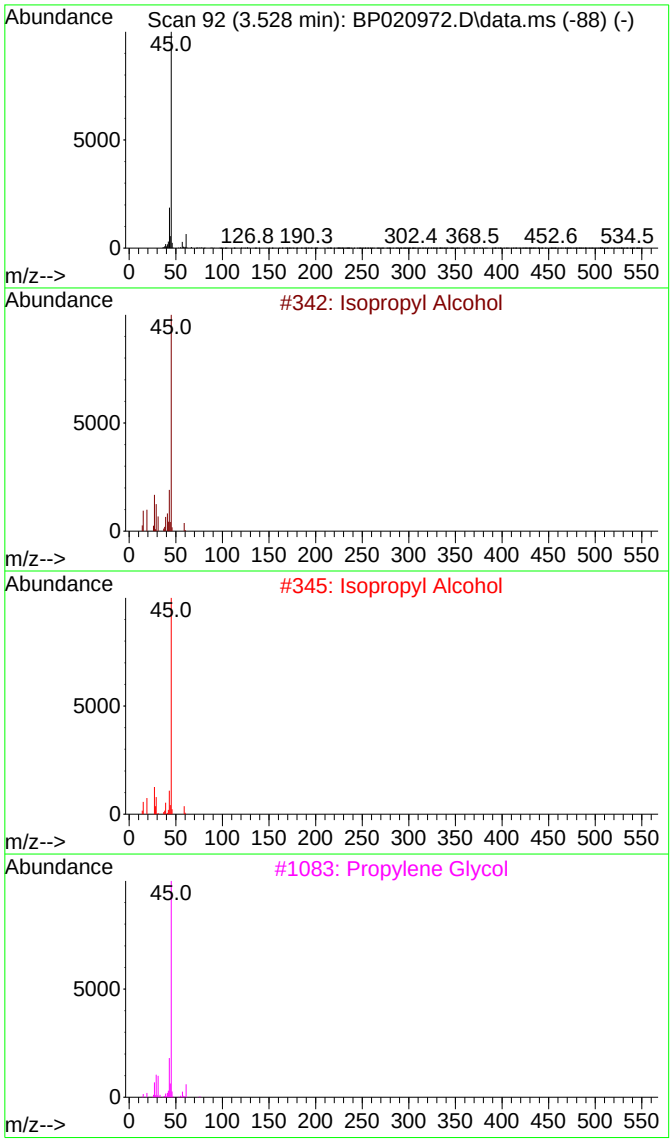
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

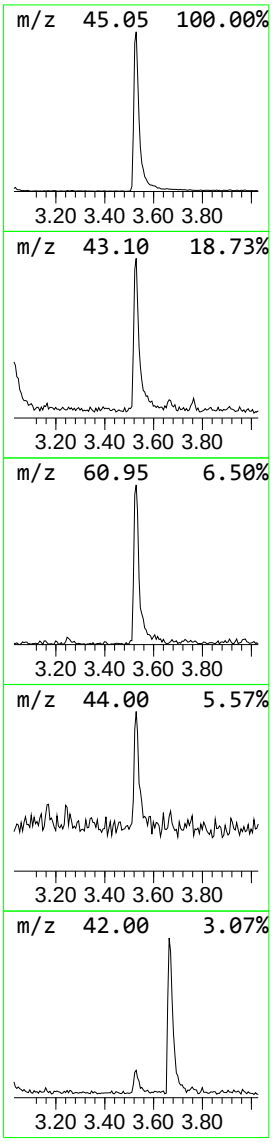
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Isopropyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.528	2.13 ng/ul	126225	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

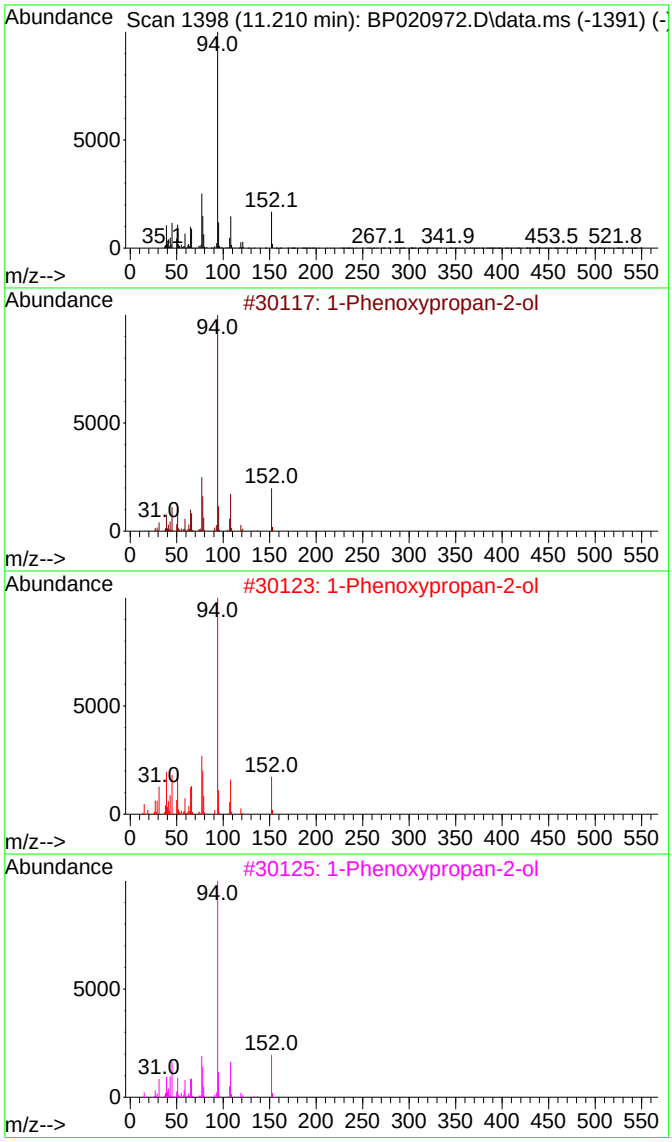
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

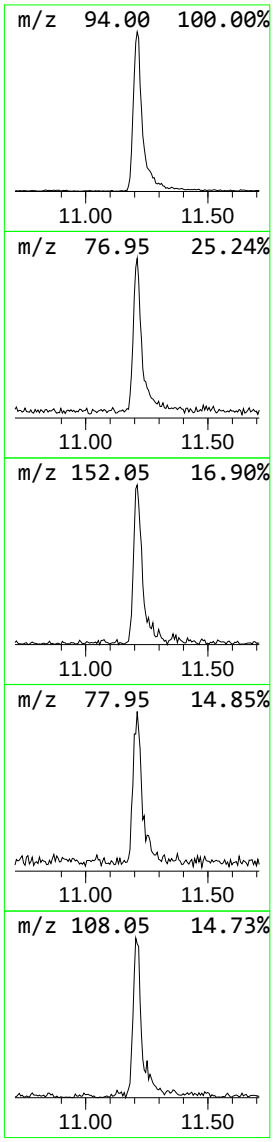
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.210	2.12 ng/ul	180672	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	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

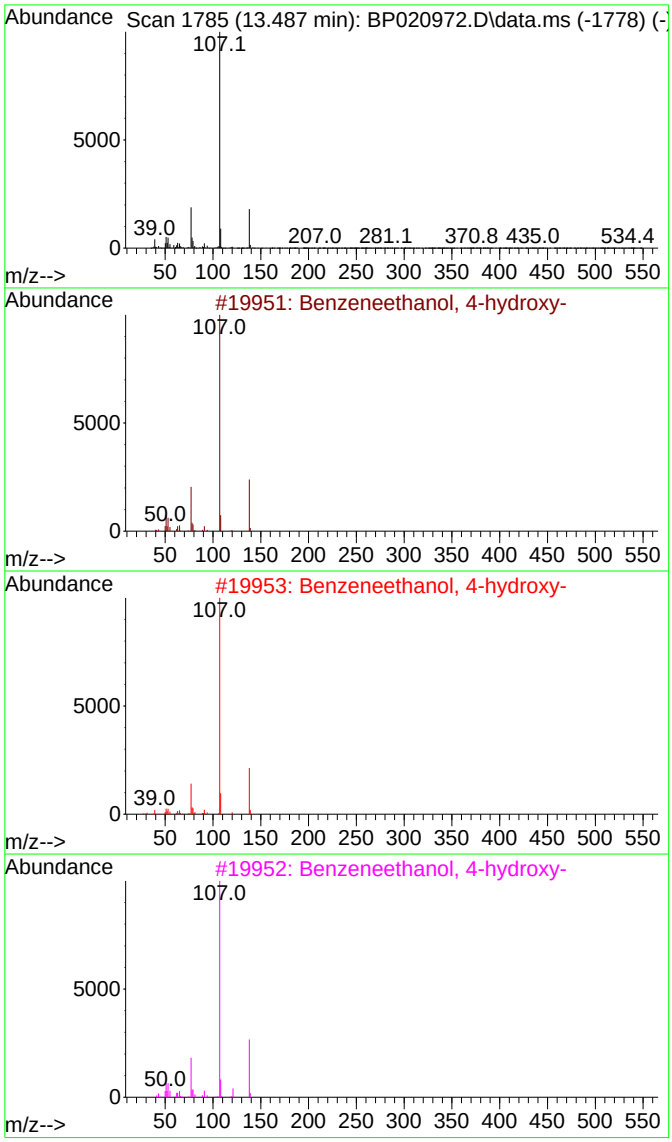
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

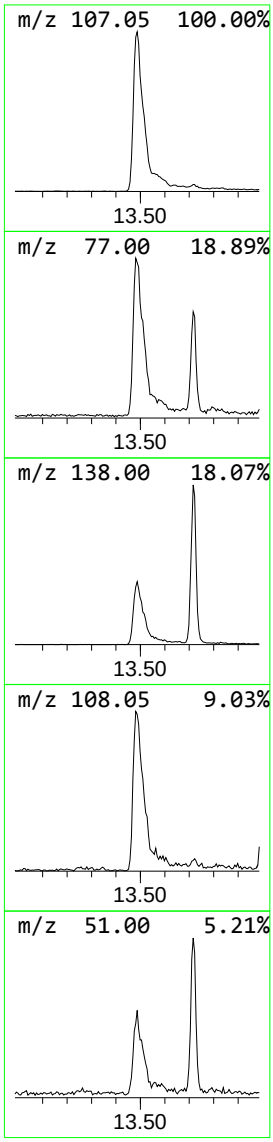
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzeneethanol, 4-hydroxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.487	4.83 ng/ul	573660	Acenaphthene-d10	14.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	94
2	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	91
3	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	91
4	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	86
5	Phenol, 4-propyl-	136	C9H12O	000645-56-7	72





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Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

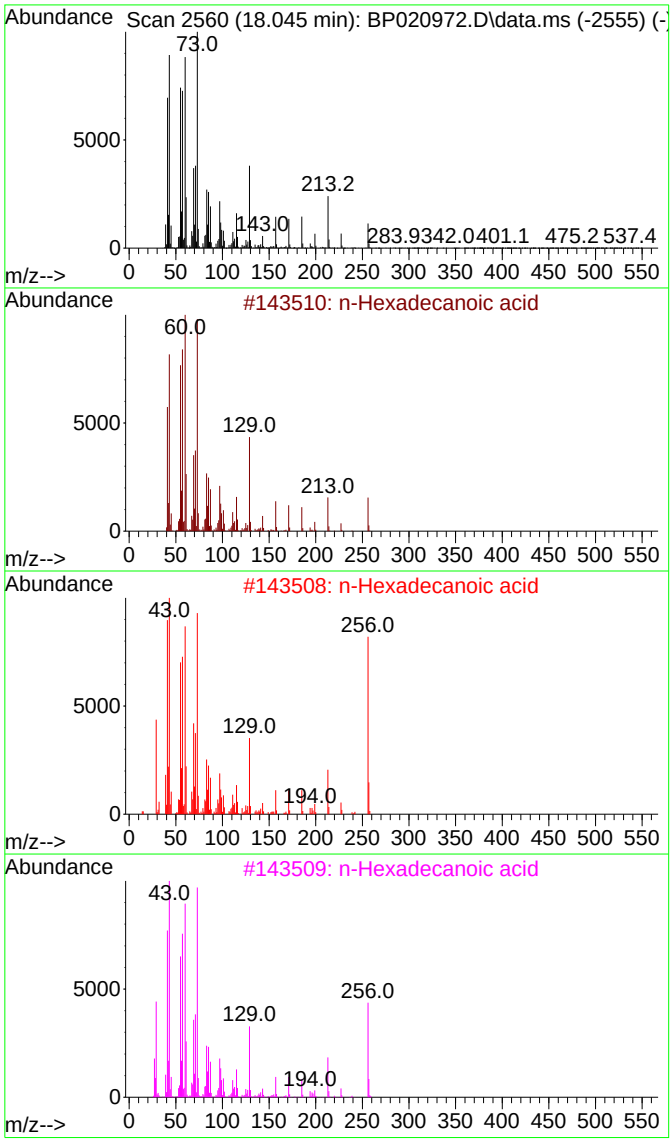
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

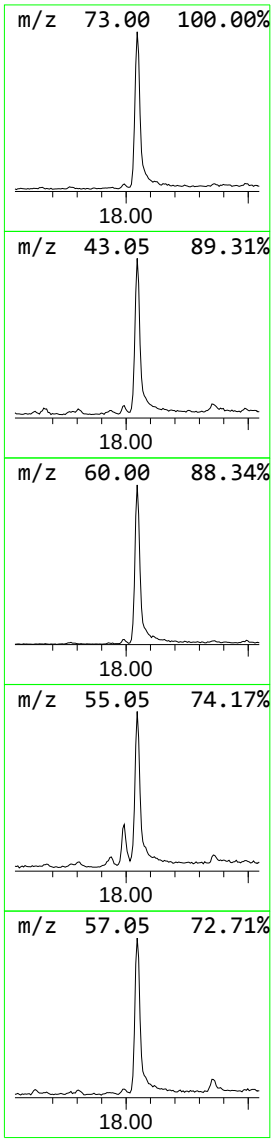
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	9.20 ng/ul	1311070	Phenanthrene-d10	17.128

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	97
5	Tridecanoic acid	214	C13H26O2	000638-53-9	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

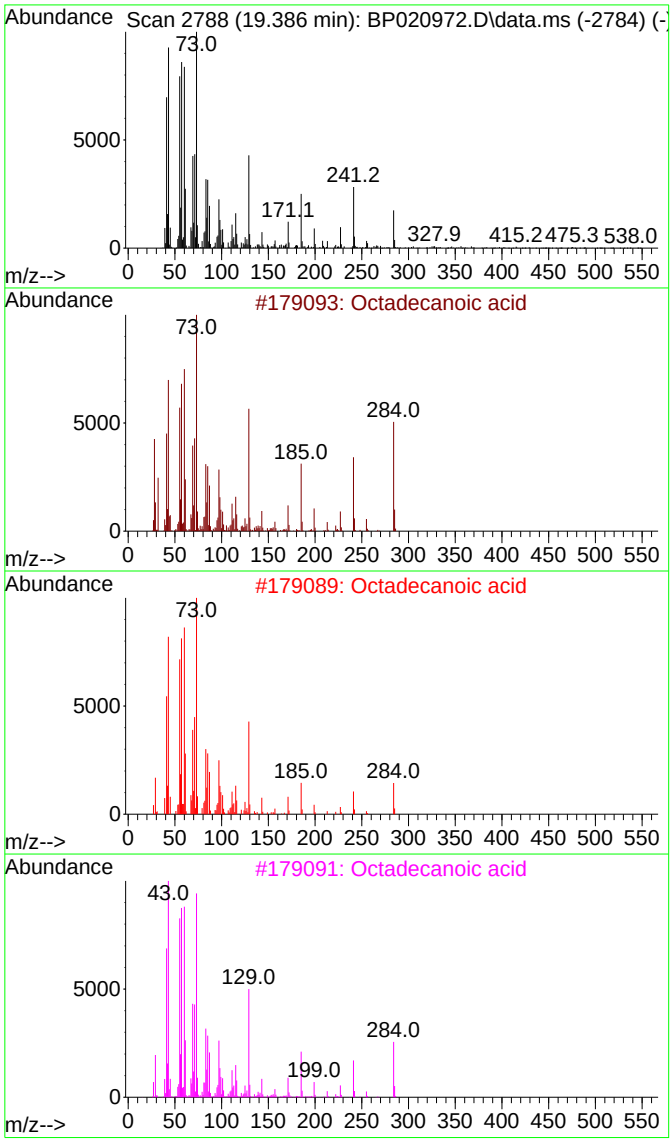
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

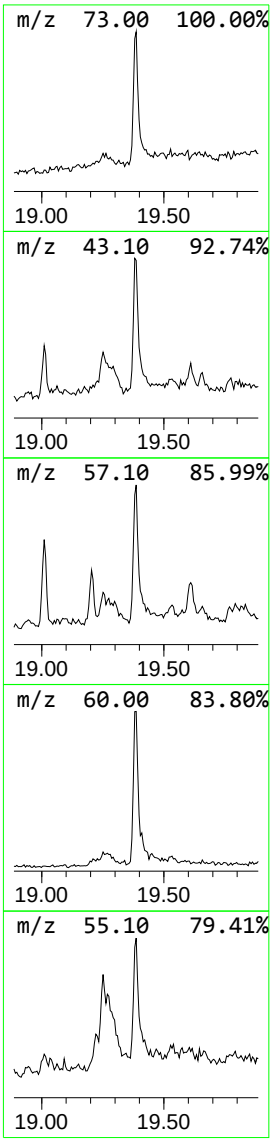
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	2.32 ng/ul	366270	Chrysene-d12	21.551

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	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

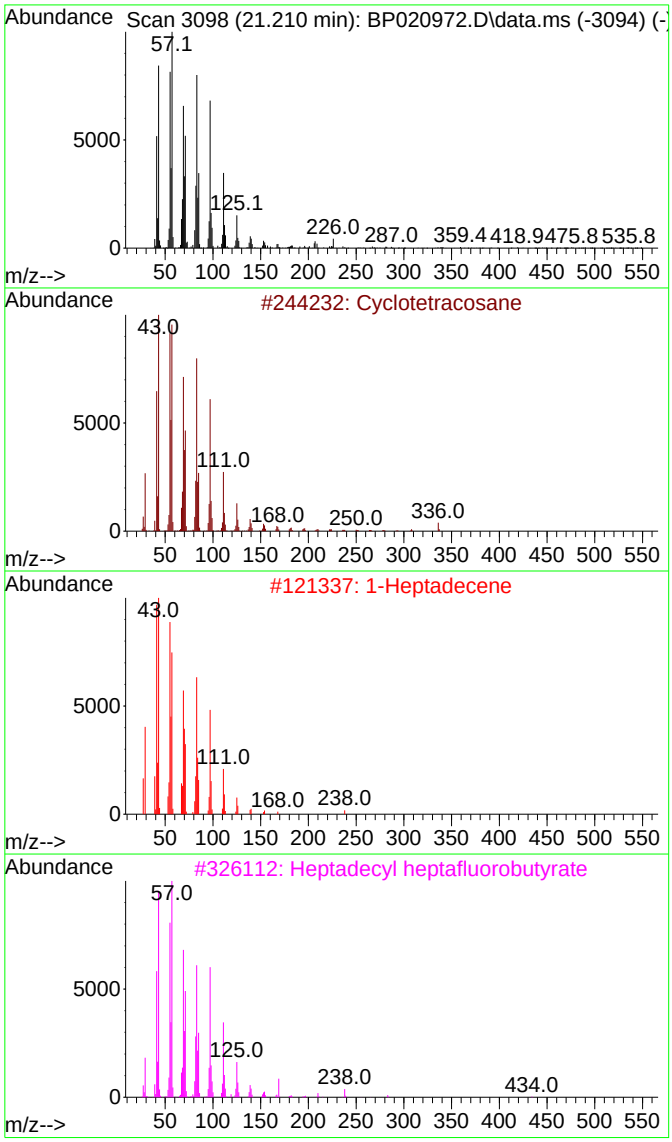
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

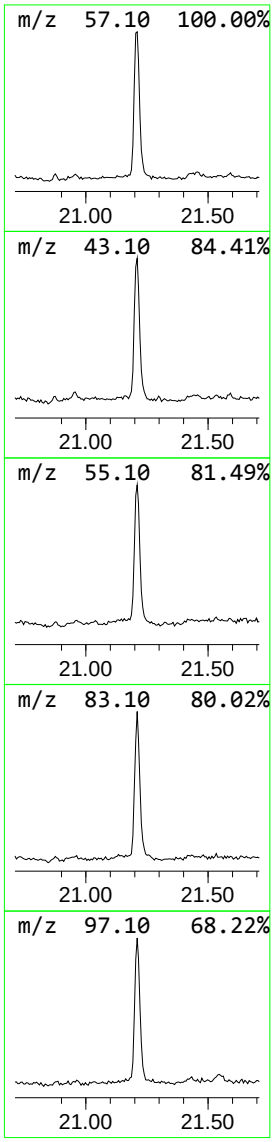
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Cyclic21.210 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.210	6.44 ng/ul	1017560	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	97
2	1-Heptadecene	238	C17H34	006765-39-5	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

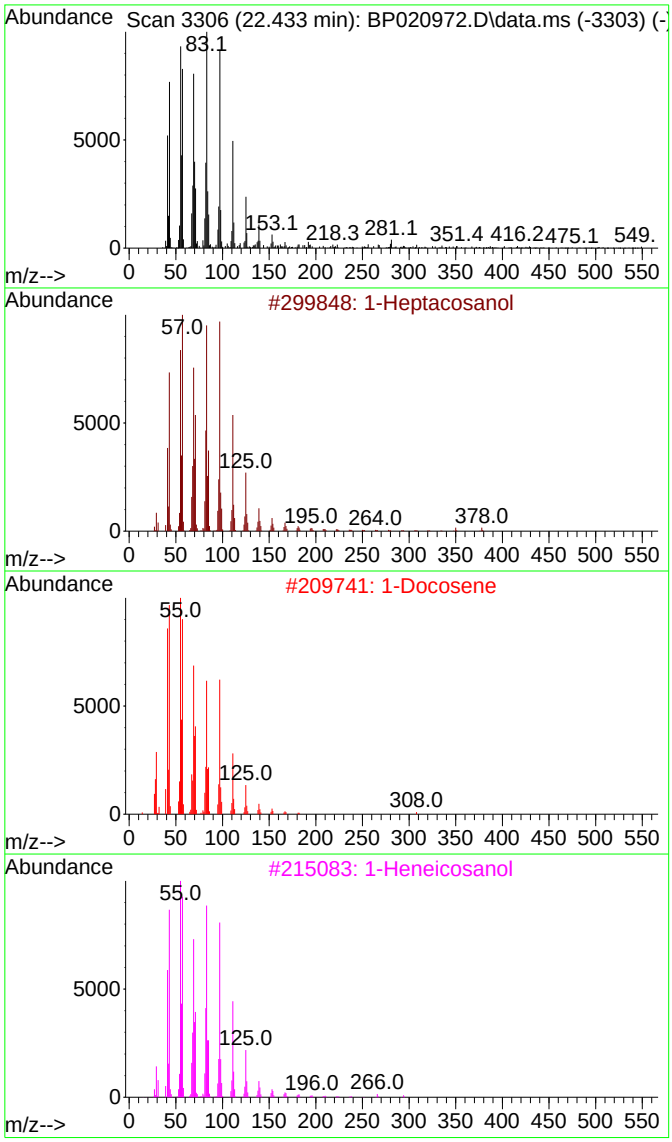
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

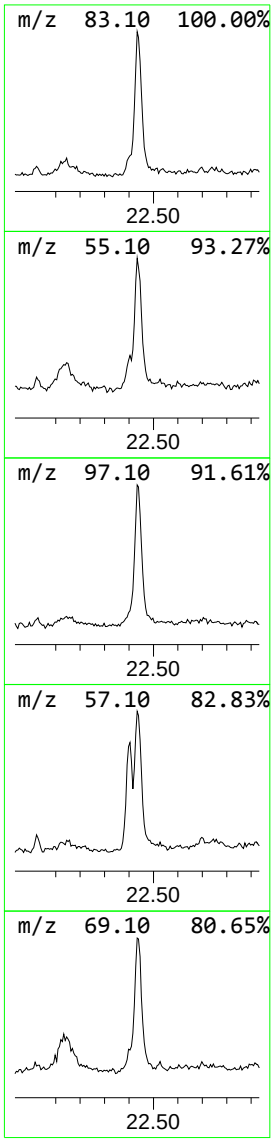
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.433	5.21 ng/ul	822514	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	1-Docosene	308	C22H44	001599-67-3	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

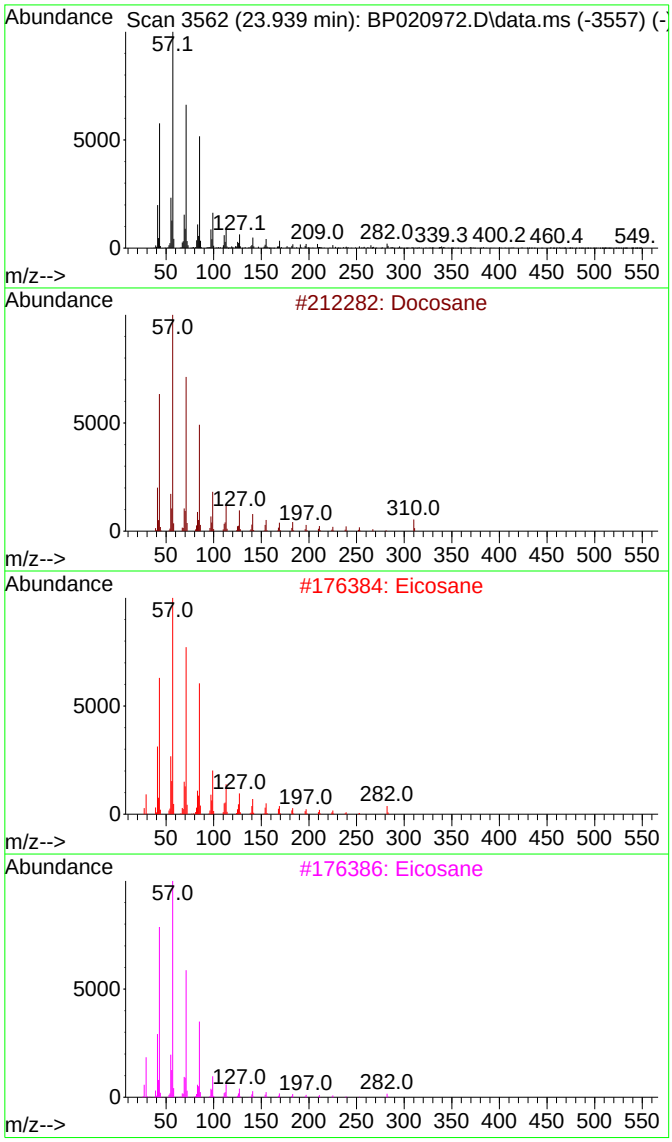
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

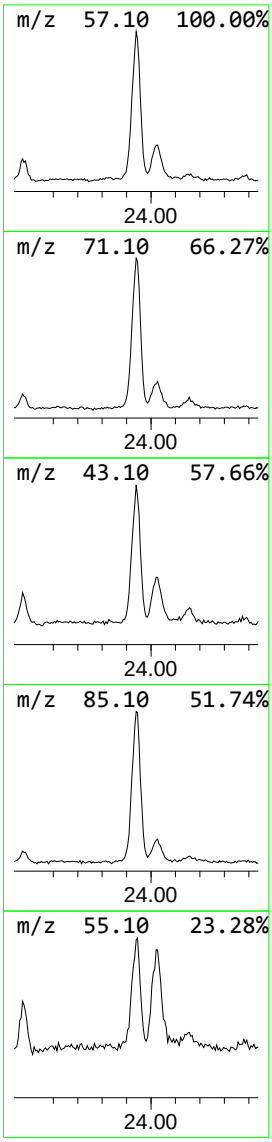
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.939	5.37 ng/ul	828307	Perylene-d12	24.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	98
2	Eicosane	282	C20H42	000112-95-8	93
3	Eicosane	282	C20H42	000112-95-8	93
4	Tetracosane	338	C24H50	000646-31-1	93
5	Tetracosane	338	C24H50	000646-31-1	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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

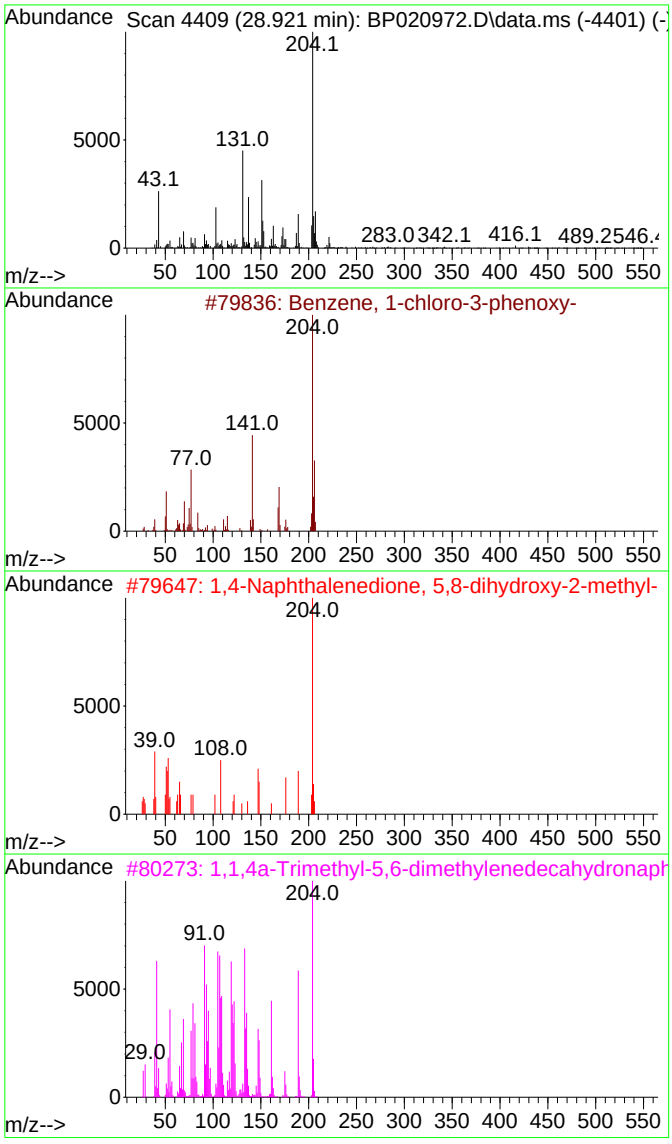
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

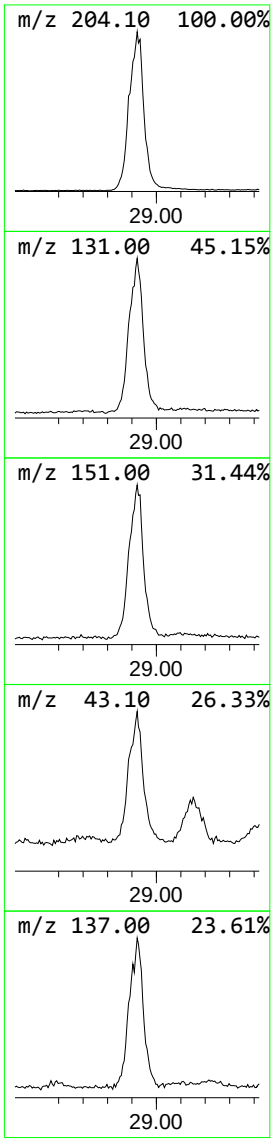
****

Peak Number 10 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.921	14.20 ng/ul	2190420	Perylene-d12	24.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-chloro-3-phenoxy-	204	C12H9ClO	006452-49-9	43
2	1,4-Naphthalenedione, 5,8-dihydr...	204	C11H8O4	014554-09-7	43
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	42
4	8-Nitro-7-methoxyisoquinoline	204	C10H8N2O3	063485-75-6	38
5	Benzene, 1-bromo-2-(methylthio)-	202	C7H7BrS	019614-16-5	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071524\
Data File : BP020972.D
Acq On : 16 Jul 2024 00:42
Operator : MA/JU
Sample : P3100-21
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4D38

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
Isopropyl Alcohol	3.528	2.1	ng/ul	126225	1	7.693	1183460	20.0
1-Phenoxypropan...	11.210	2.1	ng/ul	180672	2	10.463	1707270	20.0
Benzeneethanol,...	13.487	4.8	ng/ul	573660	3	14.316	2375080	20.0
n-Hexadecanoic ...	18.045	9.2	ng/ul	1311070	4	17.128	2849250	20.0
Octadecanoic acid	19.386	2.3	ng/ul	366270	5	21.551	3159590	20.0
(DEL) Alkane: C...	21.210	6.4	ng/ul	1017560	5	21.551	3159590	20.0
1-Heptacosanol	22.433	5.2	ng/ul	822514	5	21.551	3159590	20.0
(DEL) Alkane: S...	23.939	5.4	ng/ul	828307	6	24.851	3085140	20.0
unknown-01	28.921	14.2	ng/ul	2190420	6	24.851	3085140	20.0