LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	22	26	35	rVB	140110	201982	1.25%	0.141%
2	3.628	72	75	83	rVB	50003	74597	0.46%	0.052%
3	3.770	96	99	112	rBV	699715	1033087	6.41%	0.720%
4	3.870	113	116	125	rVV	98879	141010	0.87%	0.098%
5	3.946	126	129	132	rVV4	15921	24228	0.15%	0.017%
6	3.999	134	138	145	rVB	75182	110829	0.69%	0.077%
7	4.099	151	155	159	rVB	39029	53501	0.33%	0.037%
8	4.475	215	219	223	rVB6	16616	25554	0.16%	0.018%
9	4.664	248	251	256	rVB6	18193	20940	0.13%	0.015%
10	5.040	309	315	326	rVB	515381	745336	4.62%	0.520%
11	5.134	328	331	335	rVB4	13743	16644	0.10%	0.012%
12	6.934	630	637	641	rBV8	18383	36687	0.23%	0.026%
13	7.111	658	667	685	rVB	2212390	3714223	23.04%	2.589%
14	7.281	690	696	705	rBV	1865810	2850231	17.68%	1.987%
15	7.481	722	730	739	rBV	2262456	3547048	22.01%	2.473%
16	7.569	741	745	753	rVB3	23556	42416	0.26%	0.030%
17	7.952	803	810	818	rBV	2090432	3339360	20.72%	2.328%
18	8.016	818	821	827	rVB5	16266	25601	0.16%	0.018%
19	8.663	922	931	942	rBV	2147050	3426820	21.26%	2.389%
20	8.787	947	952	960	rVB	102170	173357	1.08%	0.121%
21	9.122	1002	1009	1019	rBV	2161145	3485861	21.63%	2.430%
22	9.228	1024	1027	1032	rVV6	13633	22254	0.14%	0.016%
23	9.281	1032	1036	1042	rVB6	16681	29147	0.18%	0.020%
24	9.528	1071	1078	1084	rBV	64067	101369	0.63%	0.071%
25	9.846	1125	1132	1144	rBV	1810141	3011736	18.69%	2.100%
26	9.999	1151	1158	1164	rVV7	15760	42784	0.27%	0.030%
27	10.063	1167	1169	1178	rVB6	15649	28757	0.18%	0.020%
28	10.387	1216	1224	1238	rBV	2714165	4520484	28.05%	3.151%
29	10.546	1244	1251	1258	rVB	12151	24785	0.15%	0.017%
30	10.769	1281	1289	1296	rBV	2905153	4815516	29.88%	3.357%
31	10.904	1305	1312	1326	rBV	2035299	3605435	22.37%	2.513%
32	11.304	1375	1380	1384	rBV7	11486	22955	0.14%	0.016%
33	11.552	1416	1422	1430	rBV6	22794	54637	0.34%	0.038%
34	12.022	1495	1502	1506	rBV5	10470	17212	0.11%	0.012%
35	12.175	1522	1528	1535	rVB6	14801	24791	0.15%	0.017%
36	12.263	1538	1543	1545	rBV6	10827	17671	0.11%	0.012%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

37	12.293	1545	1548	1552	rVV4	11094	18574	0.12%	0.013%
38	12.351	1552	1558	1563	rVV2	48971	82583	0.51%	0.058%
39	13.204	1698	1703	1710	rVB10	14150	28259	0.18%	0.020%
40	13.410	1730	1738	1744	rVB2	47539	74554	0.46%	0.052%
41	13.487	1744	1751	1755	rBV5	15000	28543	0.18%	0.020%
42	13.916	1820	1824	1829	rVB8	18673	27231	0.17%	0.019%
43	14.004	1831	1839	1849	rBV	4517968	6245128	38.75%	4.354%
44	14.122	1855	1859	1863	rVB6	15121	22724	0.14%	0.016%
45	14.234	1874	1878	1881	rBV6	12981	21595	0.13%	0.015%
46	14.293	1881	1888	1898	rVV	5327073	7668764	47.58%	5.346%
47	14.481	1916	1920	1924	rVB4	18683	23185	0.14%	0.016%
48	14.598	1932	1940	1948	rBV	4100203	6105309	37.88%	4.256%
49	14.793	1967	1973	1987	rBV	1477840	2367613	14.69%	1.651%
50	14.893	1987	1990	1994	rVV3	35157	58056	0.36%	0.040%
51	14.951	1996	2000	2004	rVV4	36975	67063	0.42%	0.047%
52	15.010	2004	2010	2020	rVB6	84045	165051	1.02%	0.115%
53	15.375	2068	2072	2077	rBV5	16379	38028	0.24%	0.027%
54	15.434	2080	2082	2085	rVB3	21378	19923	0.12%	0.014%
55	15.592	2101	2109	2115	rBV	6388882	9293371	57.66%	6.479%
56	15.645	2115	2118	2123	rVV5	28959	42654	0.26%	0.030%
57	15.710	2123	2129	2140	rVV	1564075	2178273	13.51%	1.519%
58	15.828	2145	2149	2156	rVB4	33732	61188	0.38%	0.043%
59	15.957	2166	2171	2175	rVB	68516	94991	0.59%	0.066%
60	16.298	2227	2229	2237	rVB7	20909	37795	0.23%	0.026%
61	16.369	2237	2241	2248	rVB10	9552	17133	0.11%	0.012%
62	16.481	2257	2260	2264	rVB4	20051	27727	0.17%	0.019%
63	16.739	2300	2304	2312	rVB4	16060	32971	0.20%	0.023%
64	16.887	2324	2329	2334	rBV2	59888	86145	0.53%	0.060%
65	17.092	2361	2364	2369	rBV4	17483	22987	0.14%	0.016%
66	17.234	2385	2388	2390	rBV4	23246	28462	0.18%	0.020%
67	17.351	2402	2408	2415	rVV	4476034	6374349	39.55%	4.444%
68	17.451	2419	2425	2434	rVV2	5831879	8307208	51.54%	5.791%
69	17.539	2435	2440	2449	rVB3	173862	289779	1.80%	0.202%
70	17.728	2469	2472	2479	rVB6	43061	65571	0.41%	0.046%
71	18.010	2516	2520	2523	rVB5	25789	34718	0.22%	0.024%
72	18.110	2533	2537	2541	rBV7	22933	32577	0.20%	0.023%
73	18.163	2543	2546	2551	rBV5	31155	45151	0.28%	0.031%
74	18.222	2551	2556	2566	rBV	668358	976875	6.06%	0.681%
75	18.633	2622	2626	2633	rVB	360416	389406	2.42%	0.271%
76	18.704	2635	2638	2641	rVB5	37656	47268	0.29%	0.033%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

77	19.110	2703	2707	2714	rBV6	58751	99719	0.62%	0.070%
78	19.257	2729	2732	2737	rVB3	95074	129215	0.80%	0.090%
79	19.328	2739	2744	2747	rBV	107983	209630	1.30%	0.146%
80	19.451	2762	2765	2773	rBV	142420	217453	1.35%	0.152%
81	19.680	2799	2804	2816	rBV	7313631	9461562	58.70%	6.596%
82	21.127	3046	3050	3060	rBV	1266606	1674120	10.39%	1.167%
83	21.333	3082	3085	3090	rVB	205860	210498	1.31%	0.147%
84	21.439	3098	3103	3114	rVB	4395823	5832665	36.19%	4.066%
85	23.133	3388	3391	3397	rVB	454348	638895	3.96%	0.445%
86	23.757	3491	3497	3514	rVB2	4713825	10069910	62.48%	7.020%
87	23.921	3518	3525	3534	rVB2	3189538	6606687	40.99%	4.606%
88	24.539	3627	3630	3638	rVB	660173	1198968	7.44%	0.836%
89	28.509	4295	4305	4322	rVB2	4215707	16117699	100.00%	11.236%

Sum of corrected areas: 143444648

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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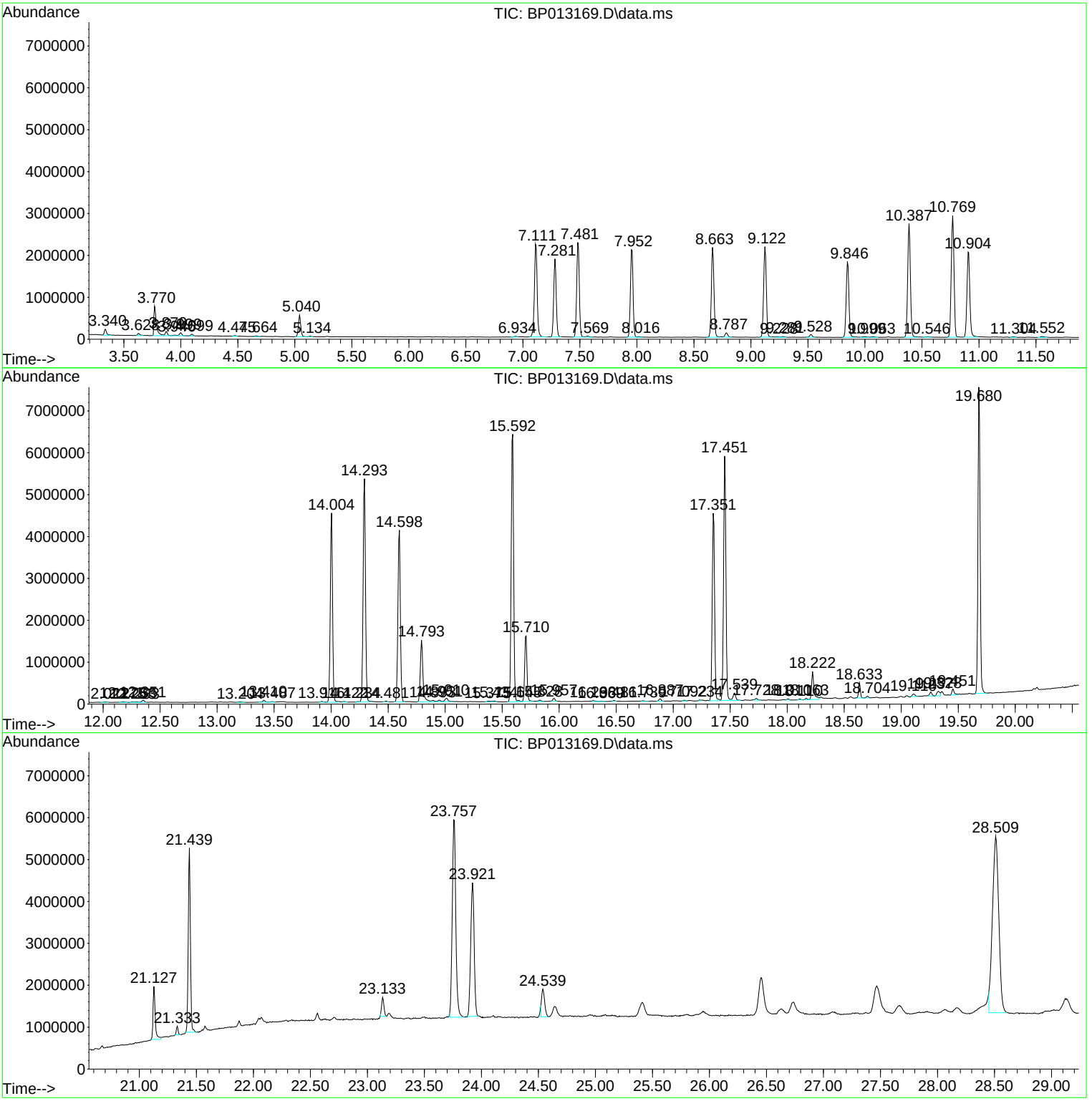
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

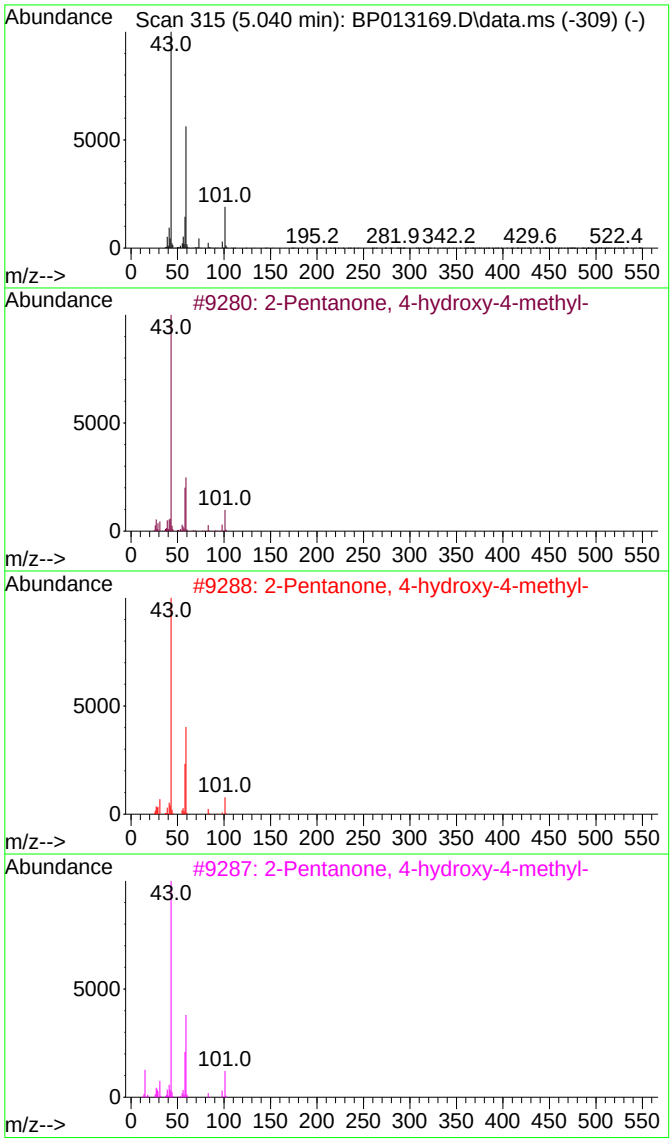
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

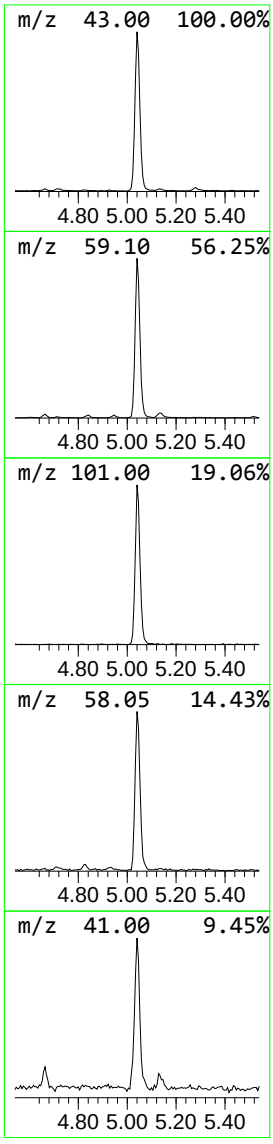
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	4.46 ng/ul	745336	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

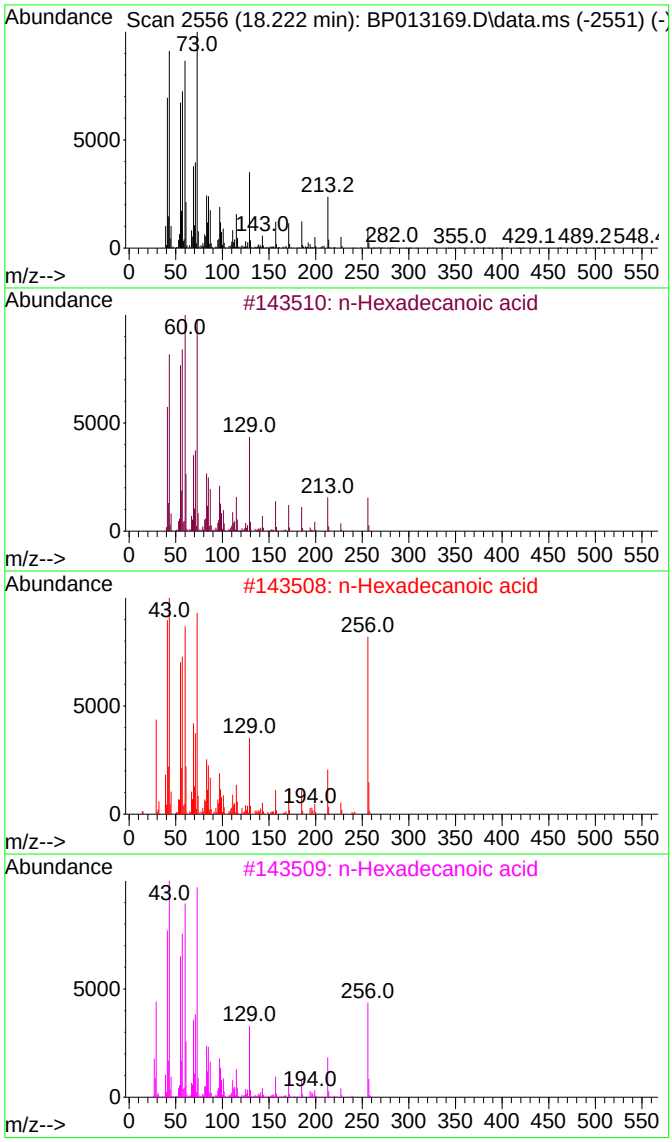
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

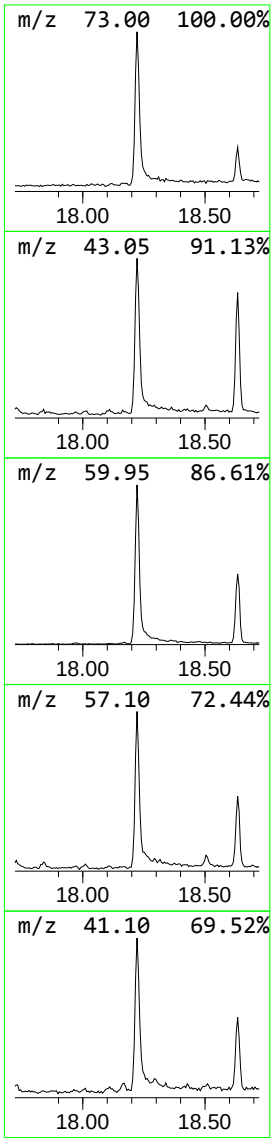
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	3.07 ng/ul	976875	Phenanthrene-d10	17.351

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	Tridecanoic acid	214	C13H26O2	000638-53-9	96
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

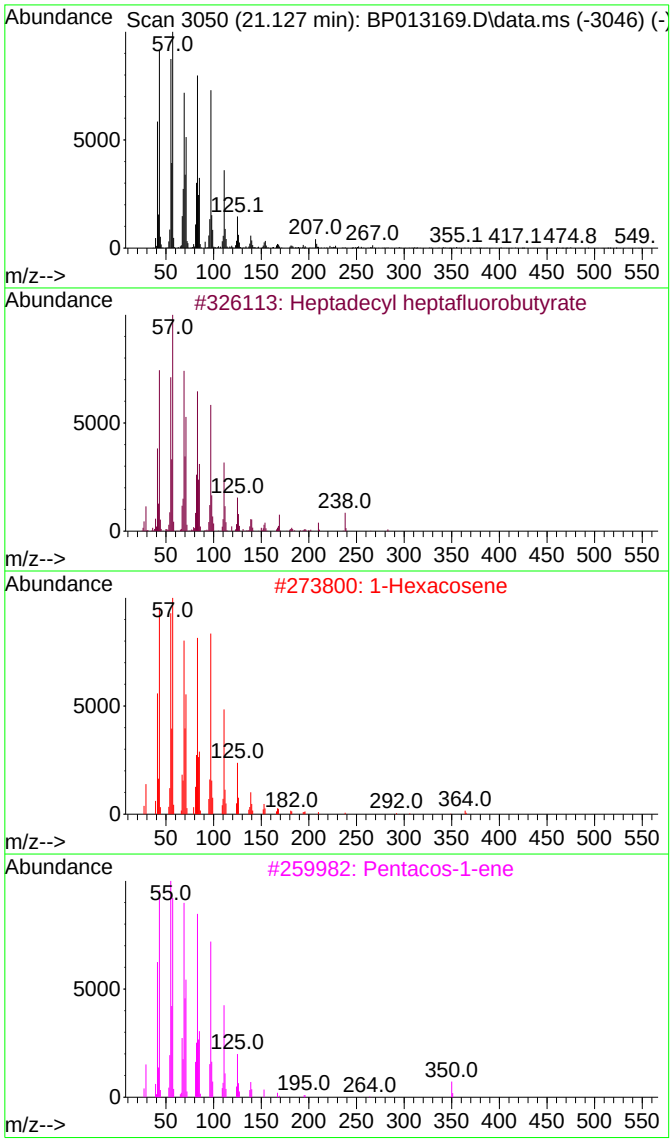
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

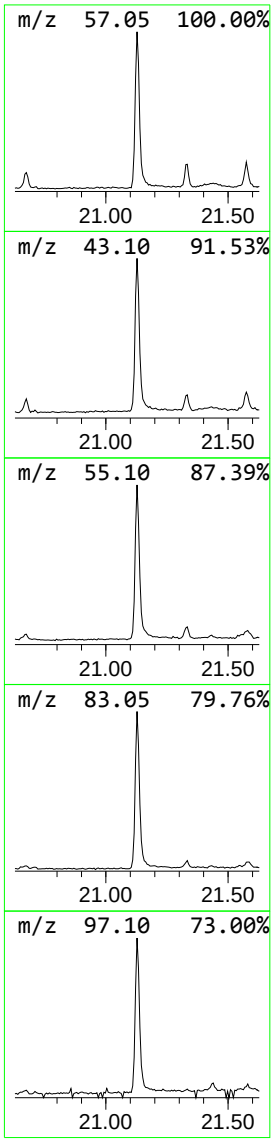
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	5.74 ng/ul	1674120	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91





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Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

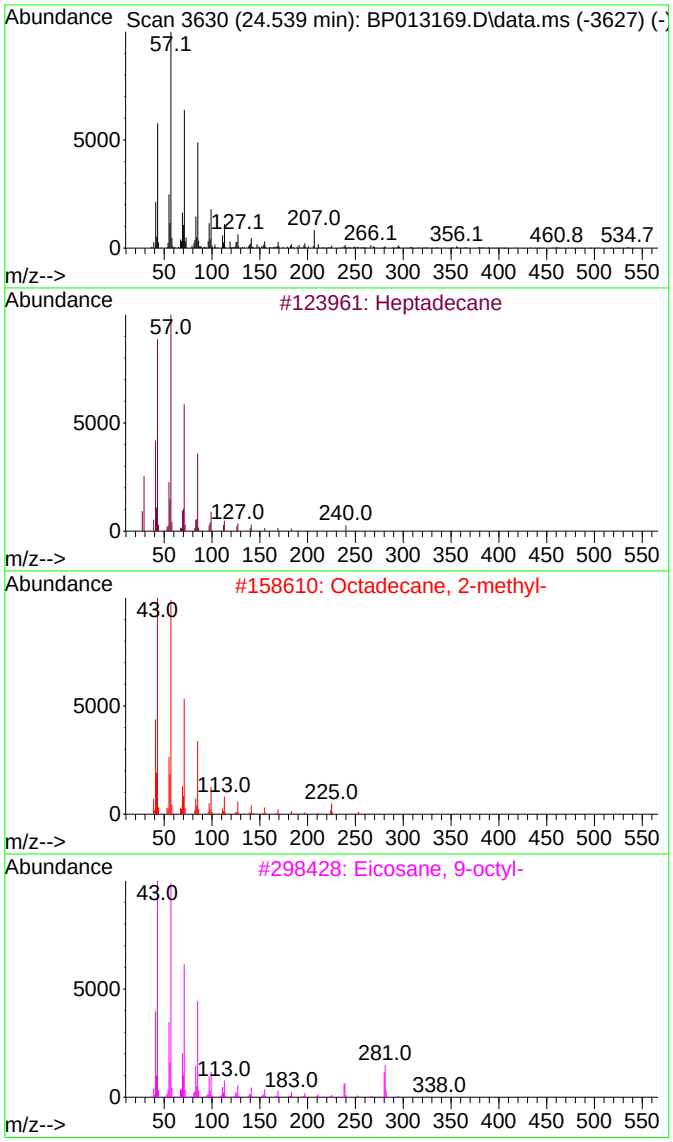
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

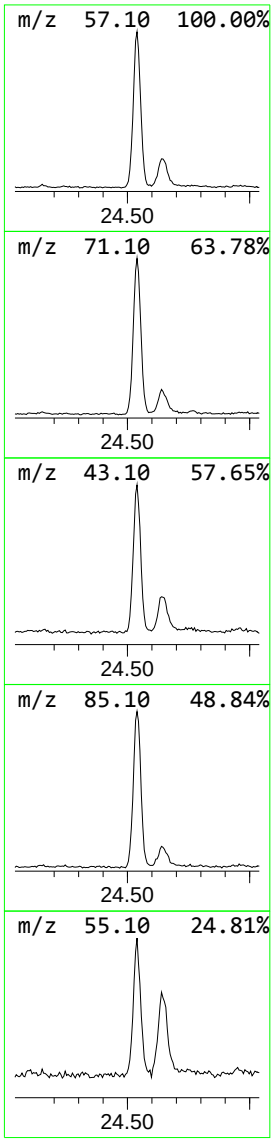
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	3.63 ng/ul	1198970	Perylene-d12	23.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
5	Heneicosane	296	C21H44	000629-94-7	90





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Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

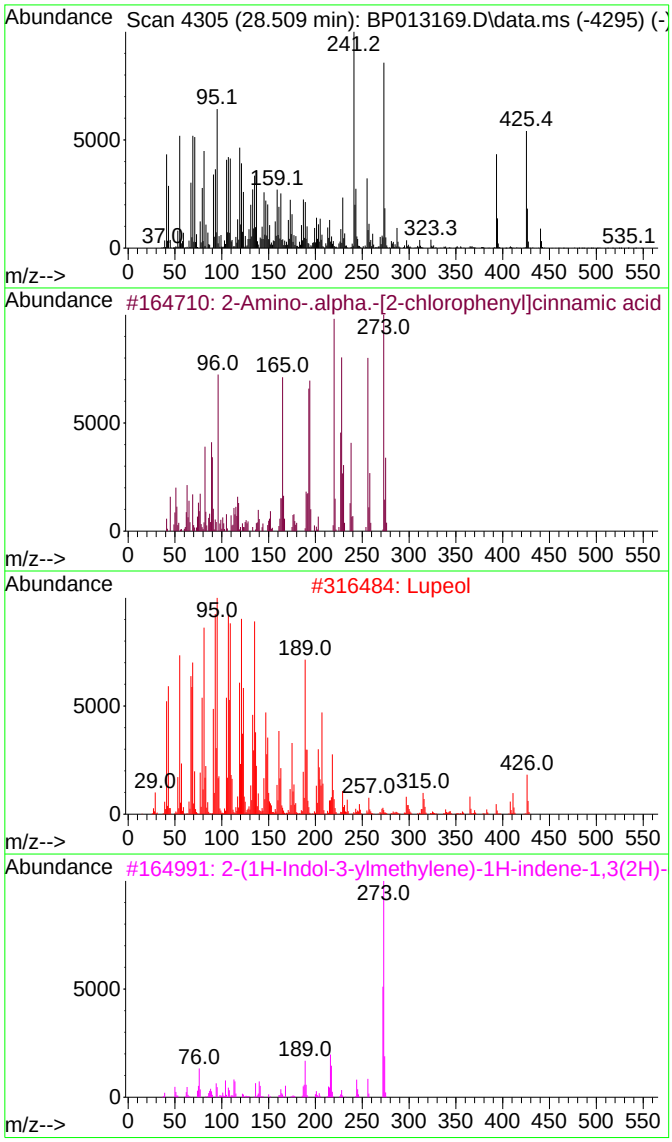
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

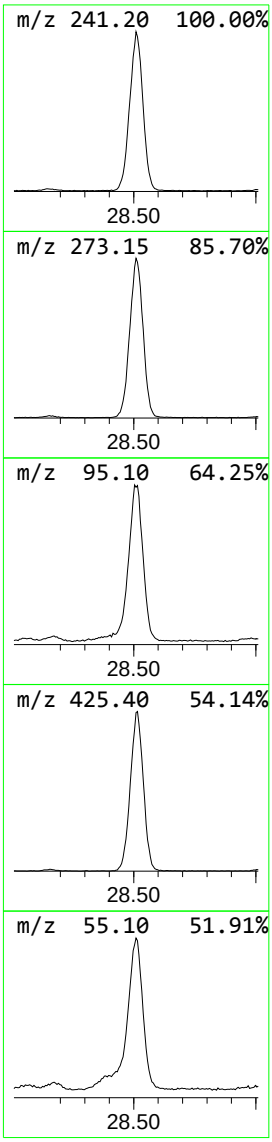
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	48.79 ng/ul	16117700	Perylene-d12	23.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2	Lupeol	426	C30H50O	000545-47-1	30
3	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25
4	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	20
5	2-{[(4-Methyl-2-pyridinyl)amino]...	256	C13H16N4Si	1010494-07-4	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013169.D
Acq On : 20 Dec 2022 16:29
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
2-Pentanone, 4-...	5.040	4.5	ng/ul	745336	1	7.958	3339360	20.0
n-Hexadecanoic ...	18.222	3.1	ng/ul	976875	4	17.351	6374350	20.0
Heptadecyl hept...	21.128	5.7	ng/ul	1674120	5	21.439	5832670	20.0
(DEL) Alkane: S...	24.539	3.6	ng/ul	1198970	6	23.921	6606690	20.0
2-Amino-.alpha....	28.509	48.8	ng/ul	16117700	6	23.921	6606690	20.0