LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBYC5

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: BP013139.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	32	rVB	140636	182458	1.25%	0.101%
2	3.628	73	75	82	rVB2	19619	30672	0.21%	0.017%
3	3.769	96	99	112	rBV	767702	1168738	7.98%	0.647%
4	3.875	112	117	121	rVB	110615	150767	1.03%	0.083%
5	3.999	133	138	146	rVB	87154	139021	0.95%	0.077%
6	4.093	151	154	159	rBV	41043	58335	0.40%	0.032%
7	4.475	216	219	224	rVB6	20740	30245	0.21%	0.017%
8	4.664	247	251	255	rVB3	30513	39436	0.27%	0.022%
9	5.040	308	315	325	rBV	751605	1090738	7.45%	0.604%
10	5.134	327	331	336	rVB4	21079	32589	0.22%	0.018%
11	6.934	632	637	642	rBV5	20914	36469	0.25%	0.020%
12	7.110	659	667	678	rBV	2246730	3602903	24.60%	1.995%
13	7.281	690	696	709	rBV	2091426	3157572	21.56%	1.748%
14	7.481	723	730	740	rVV	2386001	3761058	25.68%	2.082%
15	7.569	740	745	750	rVB4	22665	35937	0.25%	0.020%
16	7.957	803	811	818	rBV	2207918	3523812	24.06%	1.951%
17	8.016	818	821	827	rVV2	21771	33827	0.23%	0.019%
18	8.093	827	834	838	rVV	19690	34218	0.23%	0.019%
19	8.663	920	931	942	rBV	1927819	3056402	20.87%	1.692%
20	8.787	946	952	962	rVB	131767	212253	1.45%	0.118%
21	9.122	1001	1009	1021	rBV	2388365	3868471	26.42%	2.142%
22	9.222	1024	1026	1032	rVV6	16577	28194	0.19%	0.016%
23	9.281	1032	1036	1042	rVB6	19642	34785	0.24%	0.019%
24	9.528	1070	1078	1085	rBV	83979	129773	0.89%	0.072%
25	9.846	1125	1132	1148	rBV	1983479	3319103	22.67%	1.838%
26	9.987	1151	1156	1161	rBV3	26411	47460	0.32%	0.026%
27	10.069	1166	1170	1176	rVB6	16913	35755	0.24%	0.020%
28	10.387	1215	1224	1240	rBV	3052674	5048488	34.47%	2.795%
29	10.769	1281	1289	1300	rBV	3246951	5277212	36.04%	2.922%
30	10.904	1306	1312	1330	rBV	1857321	3278899	22.39%	1.815%
31	11.298	1373	1379	1388	rVB7	22564	43181	0.29%	0.024%
32	11.557	1416	1423	1428	rBV5	27683	62169	0.42%	0.034%
33	11.781	1456	1461	1467	rBV6	15786	28572	0.20%	0.016%
34	12.081	1507	1512	1516	rBV3	17489	30460	0.21%	0.017%
35	12.175	1523	1528	1536	rVB	63331	96700	0.66%	0.054%
36	12.287	1536	1547	1554	rBV2	47280	100237	0.68%	0.055%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

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	12.351	1554	1558	1567	rVB2	54443	93632	0.64%	0.052%
38	12.916	1650	1654	1659	rVV4	13112	28743	0.20%	0.016%
39	12.987	1662	1666	1670	rVV	22530	36587	0.25%	0.020%
40	13.128	1686	1690	1695	rVV2	23585	35455	0.24%	0.020%
41	13.410	1733	1738	1745	rVB	117873	158273	1.08%	0.088%
42	13.481	1745	1750	1754	rBV5	30386	57245	0.39%	0.032%
43	13.916	1820	1824	1831	rBV7	49968	72326	0.49%	0.040%
44	14.004	1831	1839	1845	rBV	5740088	7802385	53.28%	4.320%
45	14.116	1854	1858	1864	rVB5	53409	83501	0.57%	0.046%
46	14.181	1865	1869	1873	rBV	52473	67852	0.46%	0.038%
47	14.234	1873	1878	1881	rBV4	21277	35962	0.25%	0.020%
48	14.292	1881	1888	1899	rVB	6394342	9317657	63.63%	5.159%
49	14.434	1904	1912	1916	rVV10	18262	40920	0.28%	0.023%
50	14.481	1916	1920	1926	rVB	89236	117963	0.81%	0.065%
51	14.598	1933	1940	1947	rVB	4879479	7293680	49.81%	4.038%
52	14.657	1947	1950	1962	rVB9	44469	95195	0.65%	0.053%
53	14.792	1966	1973	1989	rBV	2061768	3360519	22.95%	1.861%
54	14.945	1995	1999	2004	rBV3	71387	102031	0.70%	0.056%
55	15.010	2004	2010	2015	rVB5	79121	128313	0.88%	0.071%
56	15.381	2068	2073	2076	rVV4	20213	38722	0.26%	0.021%
57	15.434	2079	2082	2086	rVB	34009	39901	0.27%	0.022%
58	15.592	2102	2109	2115	rBV	8398455	12044387	82.25%	6.669%
59	15.645	2115	2118	2122	rVV2	56007	80073	0.55%	0.044%
60	15.704	2122	2128	2144	rVV	2488285	3472279	23.71%	1.923%
61	15.834	2144	2150	2155	rVB3	58641	103394	0.71%	0.057%
62	15.957	2165	2171	2181	rVB	4360407	5976177	40.81%	3.309%
63	16.163	2202	2206	2212	rVB9	13308	25759	0.18%	0.014%
64	16.298	2225	2229	2237	rVB10	31622	65599	0.45%	0.036%
65	16.439	2249	2253	2257	rBV5	21782	31093	0.21%	0.017%
66	16.522	2262	2267	2273	rVB	169579	237519	1.62%	0.132%
67	16.733	2299	2303	2308	rBV4	45017	58346	0.40%	0.032%
68	16.886	2324	2329	2337	rBV	78903	117892	0.81%	0.065%
69	17.098	2361	2365	2368	rBV3	24819	28394	0.19%	0.016%
70	17.139	2368	2372	2376	rBV4	20467	39829	0.27%	0.022%
71	17.233	2384	2388	2395	rBV2	83831	134750	0.92%	0.075%
72	17.298	2395	2399	2402	rBV4	53921	64731	0.44%	0.036%
73	17.351	2402	2408	2414	rBV	6270160	8882015	60.65%	4.918%
74	17.451	2419	2425	2433	rVV	8519580	11834726	80.82%	6.553%
75	17.539	2436	2440	2450	rVB4	156081	262489	1.79%	0.145%
76	17.633	2453	2456	2459	rBV	21142	25637	0.18%	0.014%

LSC Area Percent Report

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Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

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

77	17.728	2469	2472	2485	rVB5	34423	69599	0.48%	0.039%
78	18.010	2516	2520	2523	rBV4	33803	41454	0.28%	0.023%
79	18.104	2531	2536	2541	rBV3	87945	153994	1.05%	0.085%
80	18.169	2542	2547	2551	rBV	359618	489435	3.34%	0.271%
81	18.228	2551	2557	2567	rBV	2660915	3624085	24.75%	2.007%
82	18.510	2601	2605	2609	rBV4	67166	104876	0.72%	0.058%
83	18.557	2610	2613	2619	rVB6	41715	69891	0.48%	0.039%
84	18.704	2634	2638	2641	rVB5	63568	84507	0.58%	0.047%
85	18.780	2649	2651	2658	rVB2	41386	55994	0.38%	0.031%
86	18.863	2662	2665	2668	rBV4	29399	36303	0.25%	0.020%
87	18.927	2673	2676	2680	rVB3	59281	71467	0.49%	0.040%
88	19.104	2701	2706	2715	rBV5	154662	351666	2.40%	0.195%
89	19.257	2729	2732	2738	rVB	155305	221560	1.51%	0.123%
90	19.333	2738	2745	2747	rBV4	335200	703624	4.80%	0.390%
91	19.357	2747	2749	2759	rVV	376616	554631	3.79%	0.307%
92	19.451	2761	2765	2780	rVV	577179	910159	6.22%	0.504%
93	19.680	2799	2804	2818	rVB	10641442	14644046	100.00%	8.108%
94	21.127	3046	3050	3055	rBV	2146233	3066778	20.94%	1.698%
95	21.439	3097	3103	3108	rBV	5621717	7958137	54.34%	4.406%
96	23.133	3387	3391	3397	rBV2	642826	1087967	7.43%	0.602%
97	23.757	3490	3497	3513	rVB2	4564409	9913872	67.70%	5.489%
98	23.915	3518	3524	3542	rVB2	3146498	6625617	45.24%	3.668%
99	24.539	3626	3630	3638	rVB	592047	1184313	8.09%	0.656%
100	28.509	4295	4305	4321	rVB2	3736930	14286675	97.56%	7.910%

Sum of corrected areas: 180609510

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
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Operator : CG/JU
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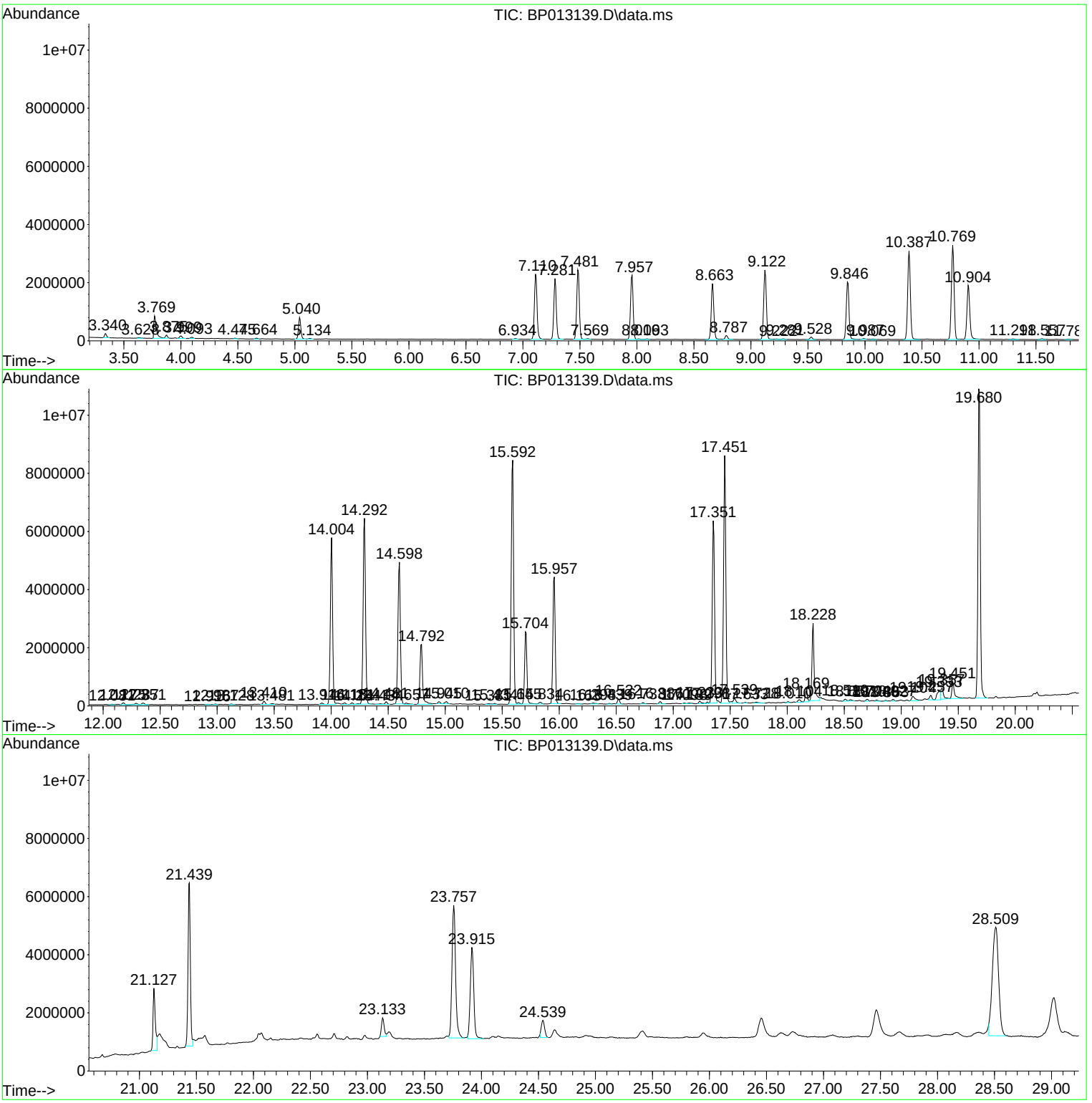
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

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 : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

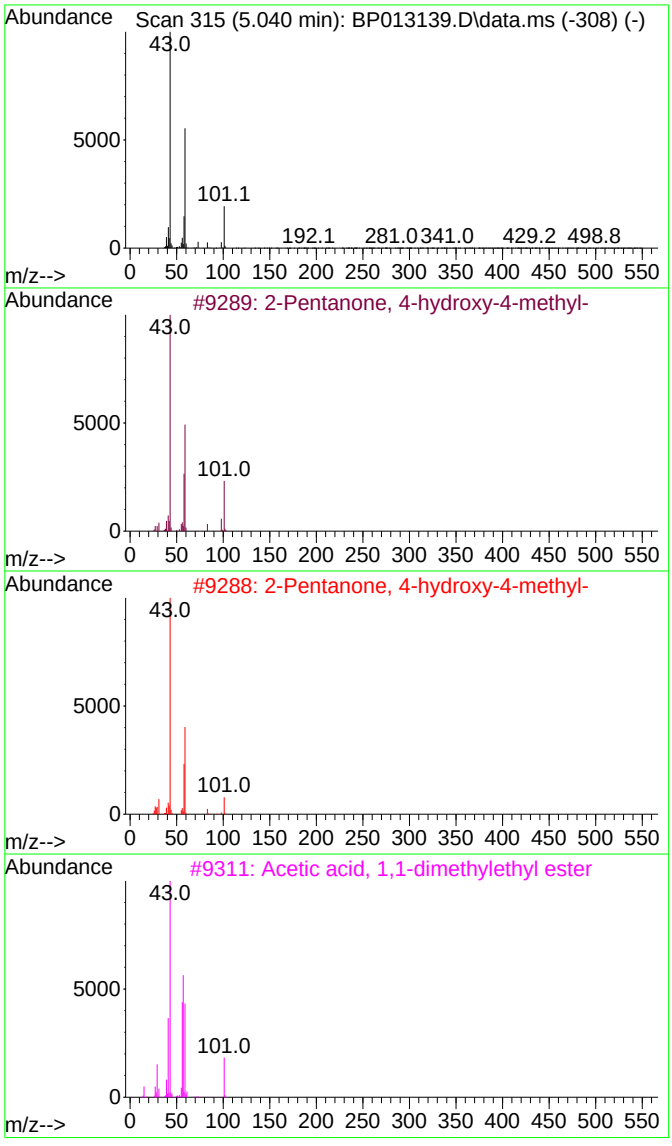
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

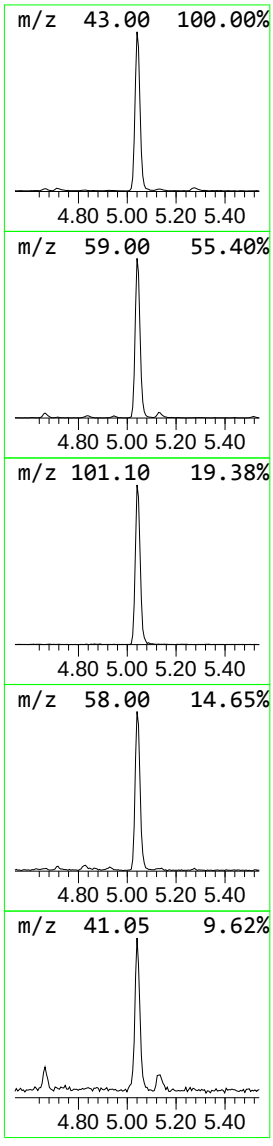
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	6.19 ng/ul	1090740	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

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

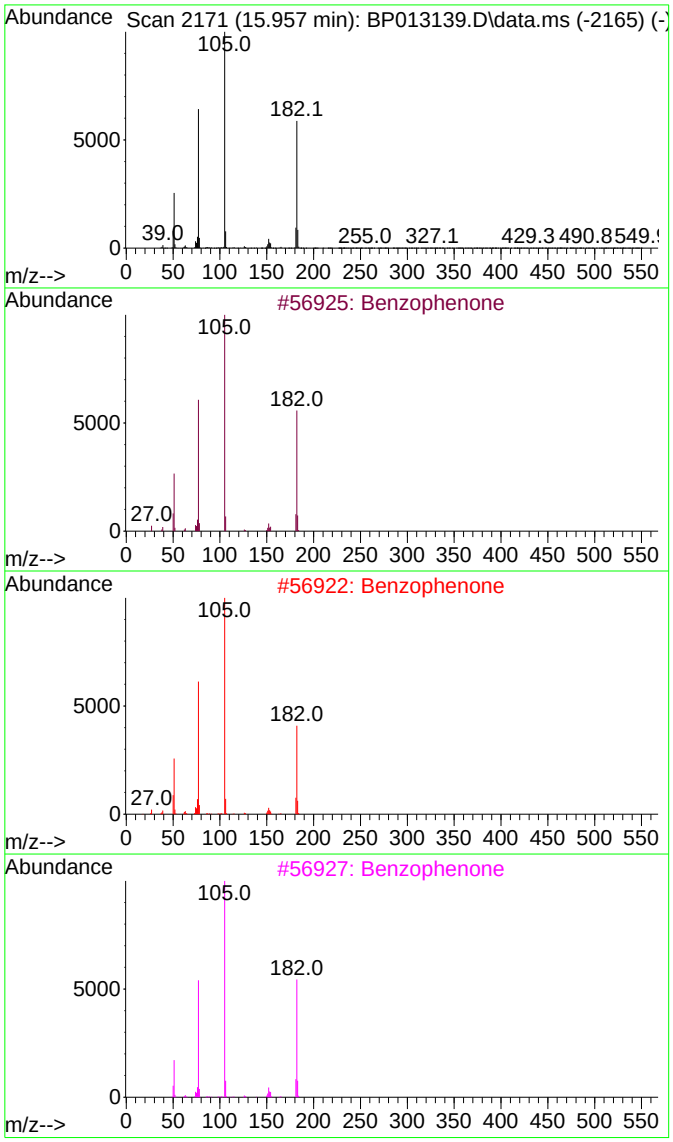
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

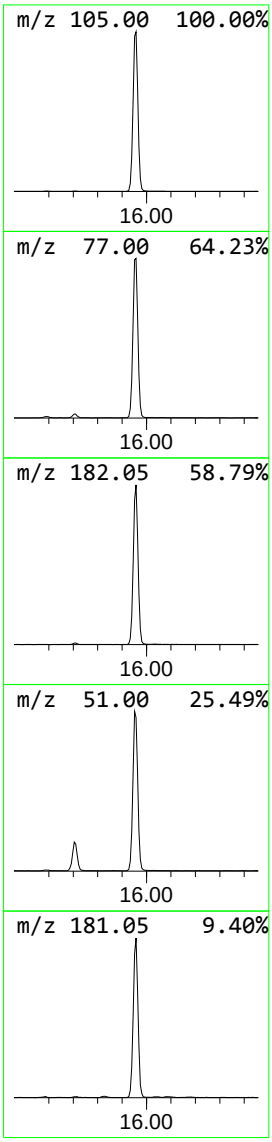
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	16.39 ng/ul	5976180	Acenaphthene-d10	14.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	93
5	Azobenzene	182	C12H10N2	000103-33-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
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Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

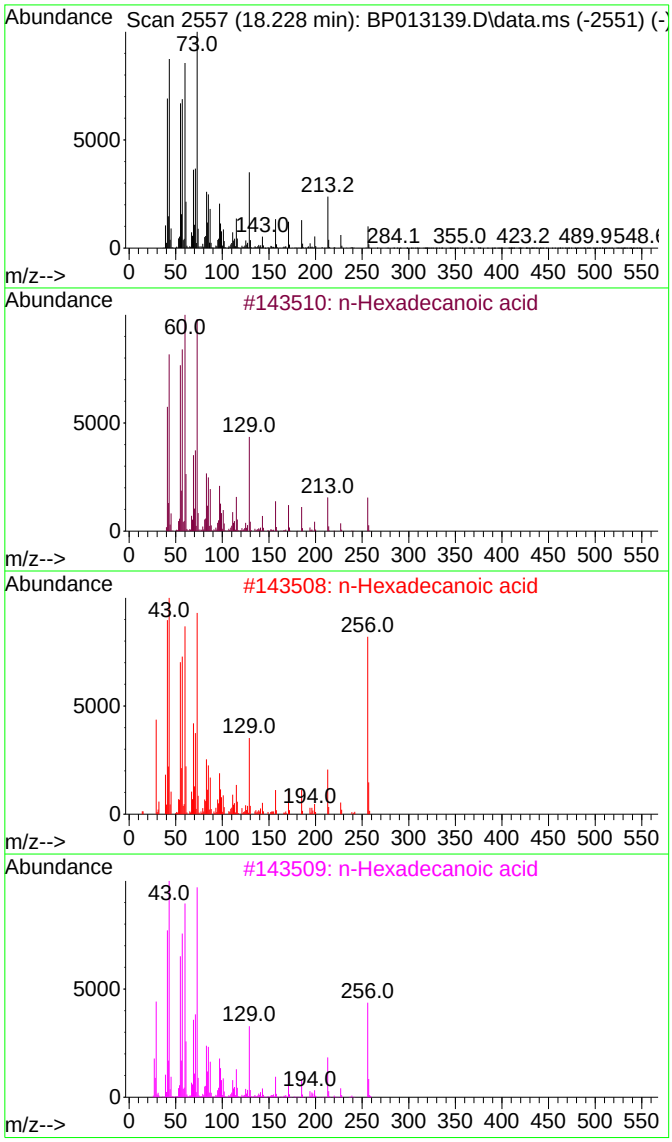
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

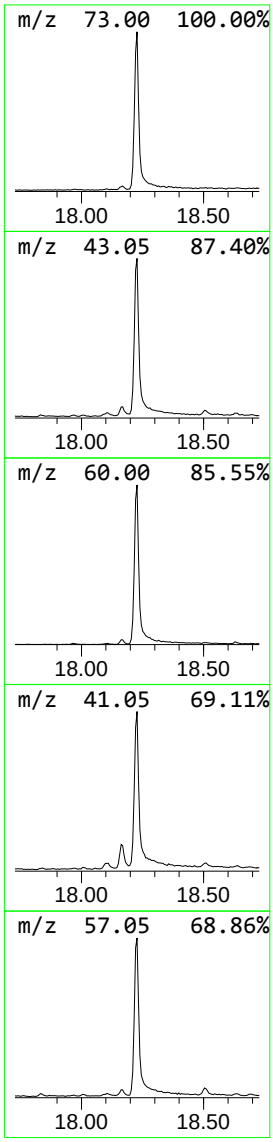
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	8.16 ng/ul	3624090	Phenanthrene-d10	17.351

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

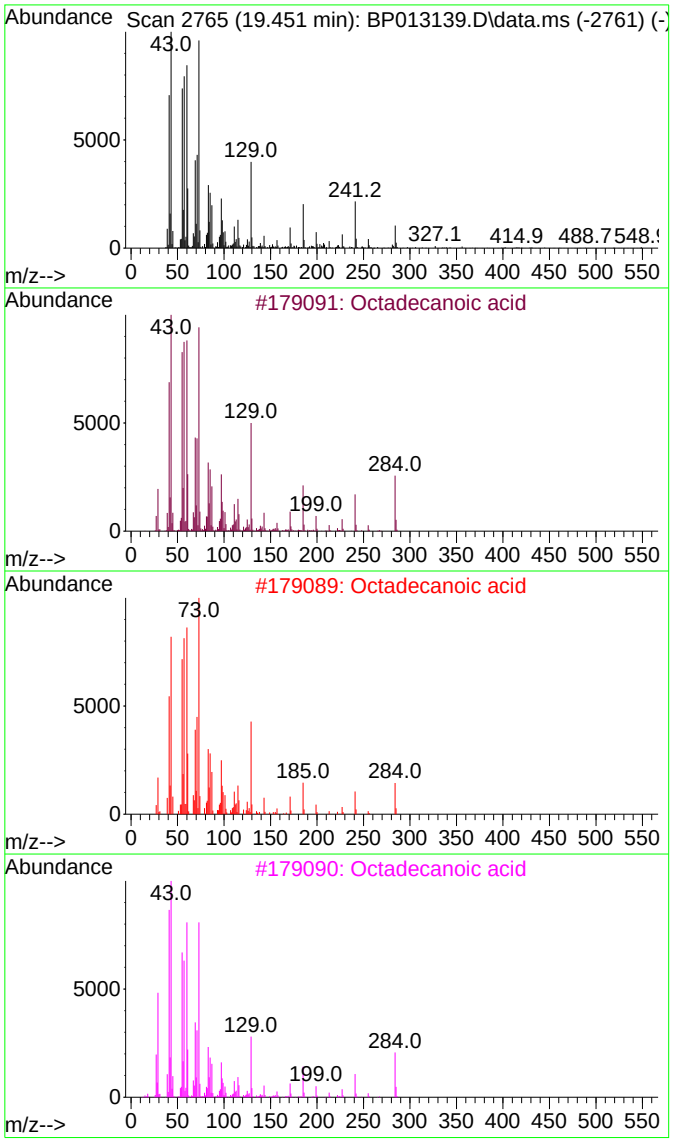
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

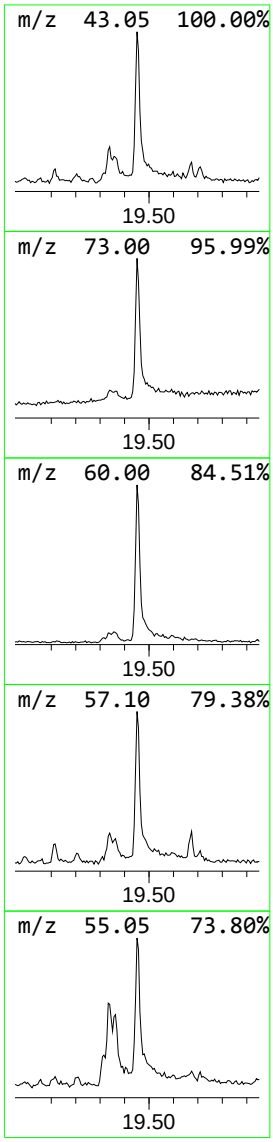
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.29 ng/ul	910159	Chrysene-d12	21.439

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	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

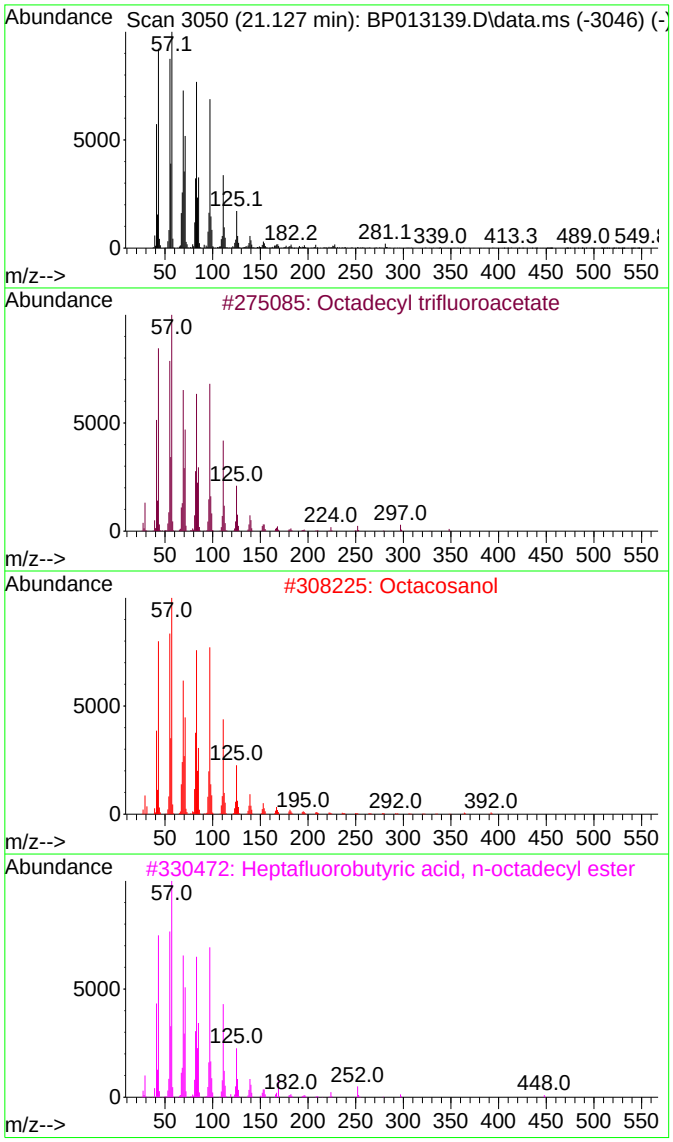
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

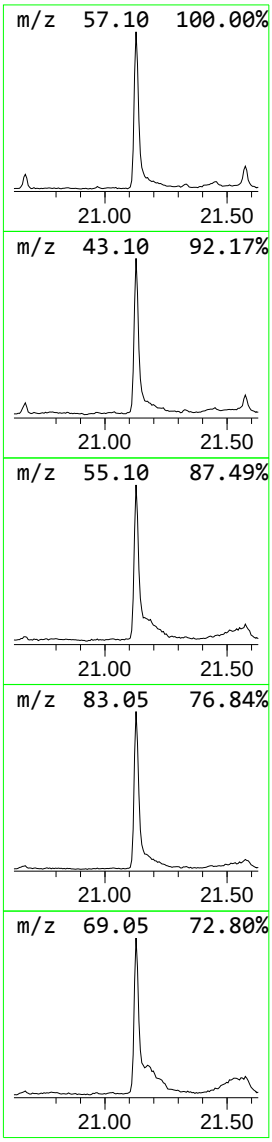
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	7.71 ng/ul	3066780	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2	Octacosanol	410	C28H58O	000557-61-9	94
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

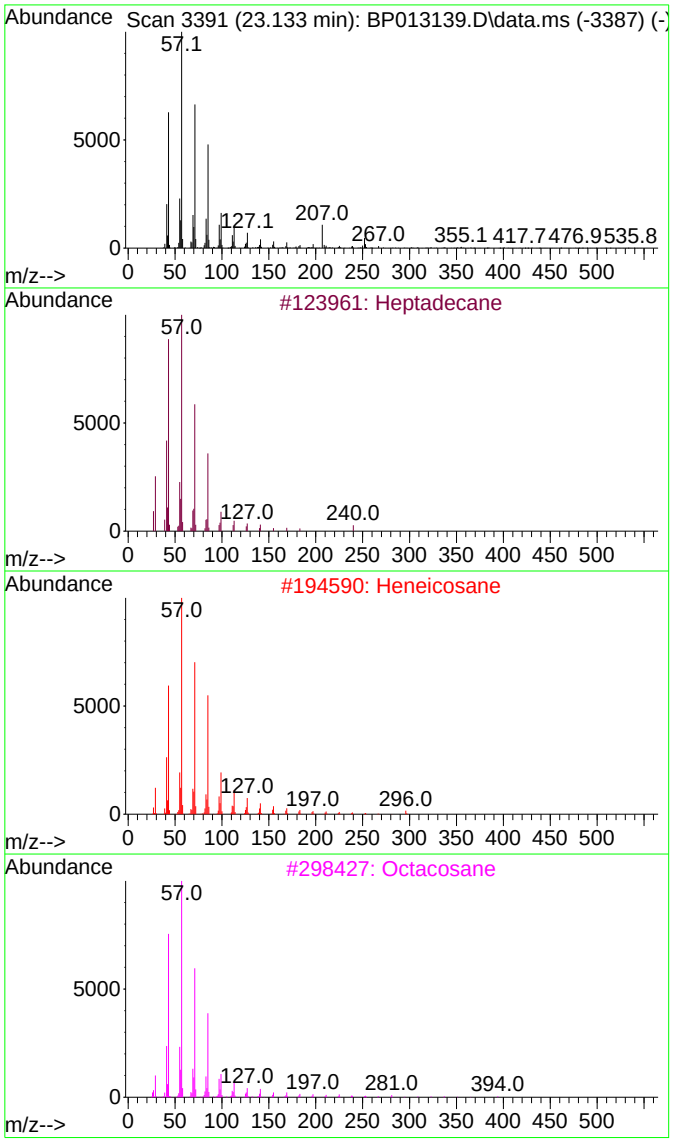
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

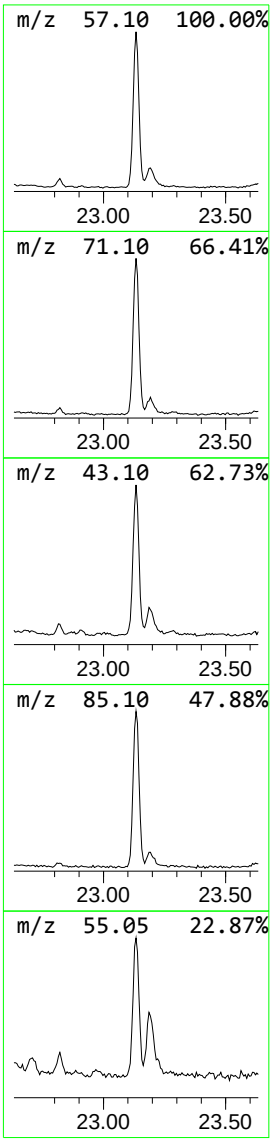
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.133	3.28 ng/ul	1087970	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	4-Methylheneicosane	310	C22H46	025117-29-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

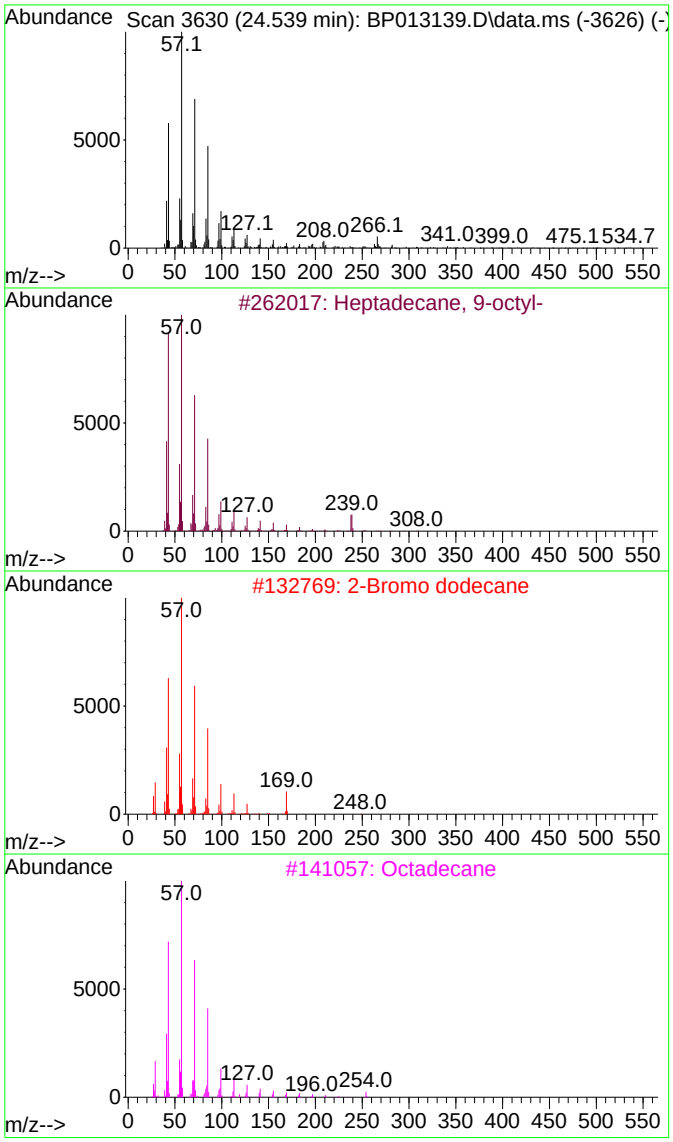
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

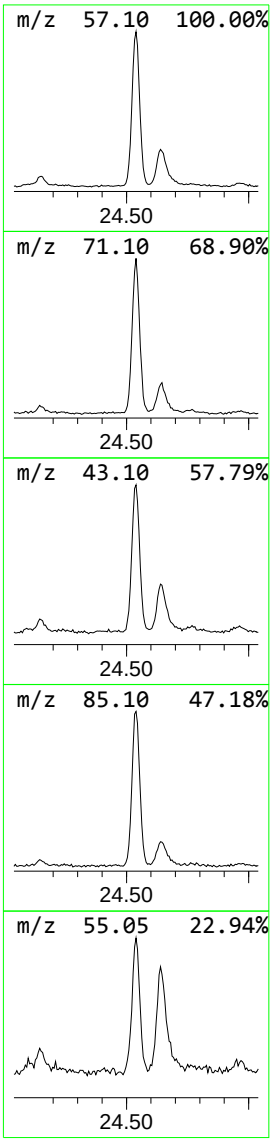
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	3.57 ng/ul	1184310	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	98
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	94
3	Octadecane	254	C18H38	000593-45-3	94
4	Eicosane	282	C20H42	000112-95-8	93
5	11-Methyltricosane	338	C24H50	027538-41-6	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

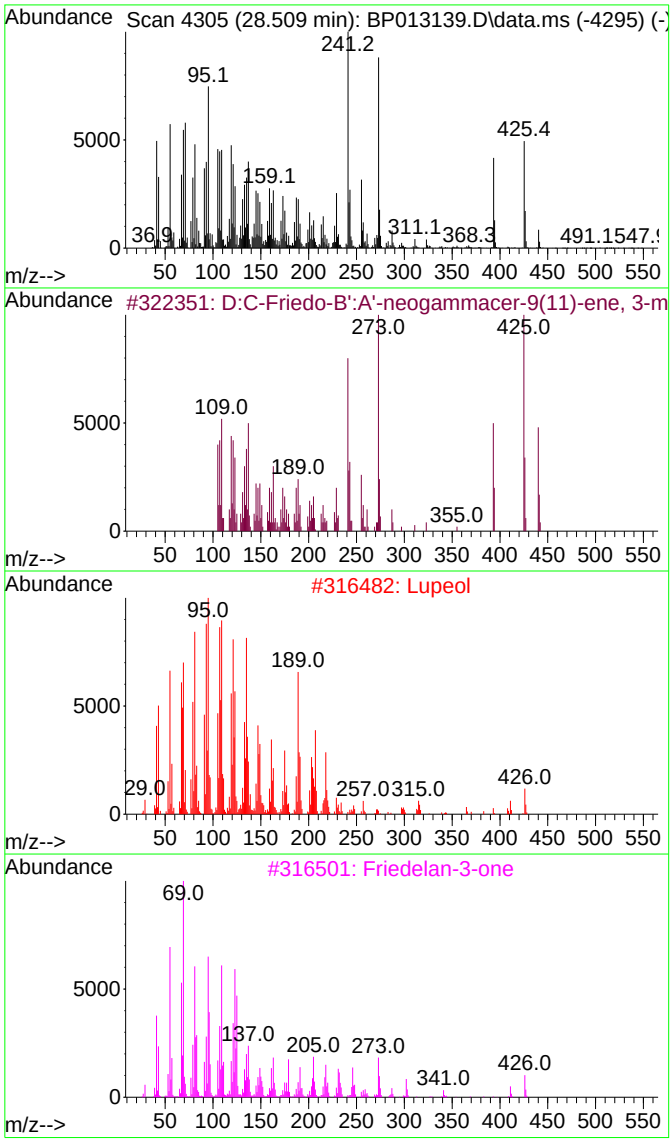
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

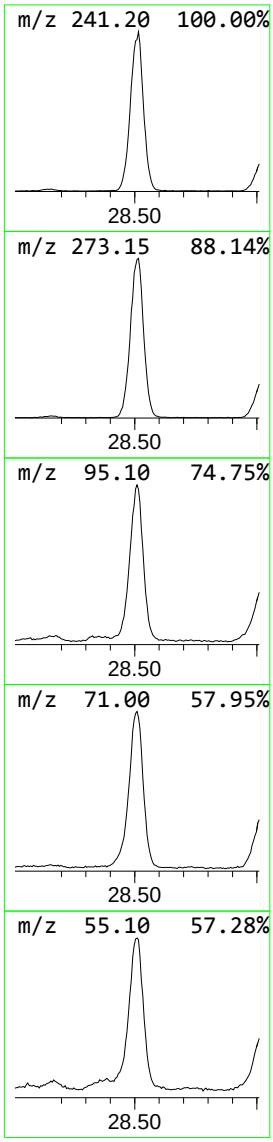
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	43.13 ng/ul	14286700	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	64
2	Lupeol	426	C30H50O	000545-47-1	38
3	Friedelan-3-one	426	C30H50O	000559-74-0	25
4	Coprost-25-en-16,22-epoxy-3.alph...	400	C27H44O2	122337-93-3	22
5	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013139.D
Acq On : 19 Dec 2022 22:20
Operator : CG/JU
Sample : N6006-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYC5

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	6.2	ng/ul	1090740	1	7.957	3523810	20.0
Benzophenone	15.957	16.4	ng/ul	5976180	3	14.598	7293680	20.0
n-Hexadecanoic ...	18.227	8.2	ng/ul	3624090	4	17.351	8882020	20.0
Octadecanoic acid	19.451	2.3	ng/ul	910159	5	21.439	7958140	20.0
Octadecyl trifl...	21.127	7.7	ng/ul	3066780	5	21.439	7958140	20.0
(DEL) Alkane: S...	23.133	3.3	ng/ul	1087970	6	23.916	6625620	20.0
(DEL) Alkane: S...	24.539	3.6	ng/ul	1184310	6	23.916	6625620	20.0
D:C-Friedo-B':A...	28.509	43.1	ng/ul	14286700	6	23.916	6625620	20.0