LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXR9

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: BP013212.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	22	25	31	rVB	78857	101704	1.19%	0.110%
2	3.764	96	98	118	rBV	974835	1513280	17.72%	1.643%
3	4.093	150	154	160	rVB	46292	65765	0.77%	0.071%
4	5.046	311	316	322	rVB2	37130	56192	0.66%	0.061%
5	5.252	348	351	354	rBV5	15140	16672	0.20%	0.018%
6	5.422	377	380	386	rVB7	11738	14835	0.17%	0.016%
7	7.110	660	667	680	rVB	1245041	1935059	22.66%	2.101%
8	7.275	689	695	704	rVB	1039968	1570423	18.39%	1.705%
9	7.481	722	730	740	rVV	1276722	2003819	23.46%	2.175%
10	7.557	741	743	749	rVB7	7297	10974	0.13%	0.012%
11	7.952	803	810	817	rBV	1741169	2694065	31.54%	2.925%
12	8.016	817	821	827	rVB8	9214	18015	0.21%	0.020%
13	8.193	847	851	858	rBV3	21408	41255	0.48%	0.045%
14	8.657	923	930	942	rBV	1395461	2233490	26.15%	2.425%
15	9.116	1001	1008	1016	rBV	1128193	1839663	21.54%	1.997%
16	9.275	1032	1035	1041	rVB8	11787	19645	0.23%	0.021%
17	9.516	1072	1076	1082	rVB2	31024	49466	0.58%	0.054%
18	9.840	1122	1131	1145	rBV	912135	1564952	18.32%	1.699%
19	10.381	1215	1223	1237	rBV	1475019	2461214	28.82%	2.672%
20	10.540	1244	1250	1258	rVB	87902	151434	1.77%	0.164%
21	10.763	1280	1288	1295	rBV	2262616	3708543	43.42%	4.026%
22	10.816	1295	1297	1301	rVB5	10237	9826	0.12%	0.011%
23	10.904	1304	1312	1325	rBV	1138830	2100615	24.60%	2.280%
24	11.151	1350	1354	1358	rVB5	7912	12937	0.15%	0.014%
25	11.298	1373	1379	1381	rBV7	6381	9709	0.11%	0.011%
26	12.175	1523	1528	1534	rBV9	8998	22447	0.26%	0.024%
27	12.351	1552	1558	1566	rVB	22494	40866	0.48%	0.044%
28	13.116	1681	1688	1691	rBV9	9032	15007	0.18%	0.016%
29	13.304	1713	1720	1721	rBV7	7493	8836	0.10%	0.010%
30	13.404	1730	1737	1741	rBV3	24211	38599	0.45%	0.042%
31	13.581	1760	1767	1771	rBV2	26617	40087	0.47%	0.044%
32	13.628	1771	1775	1782	rVB5	18074	36745	0.43%	0.040%
33	13.998	1831	1838	1847	rBV	2444530	3332823	39.02%	3.618%
34	14.063	1847	1849	1853	rVV5	11154	14476	0.17%	0.016%
35	14.287	1879	1887	1897	rBV	2826257	4103090	48.04%	4.454%
36	14.475	1917	1919	1924	rVB4	14141	16522	0.19%	0.018%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR9

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	14.592	1932	1939	1947	rBV	3237159	4621788	54.12%	5.017%
38	14.786	1966	1972	1993	rBV	737483	1350866	15.82%	1.466%
39	14.992	2004	2007	2014	rVB9	15541	25938	0.30%	0.028%
40	15.422	2076	2080	2087	rVB9	8558	16451	0.19%	0.018%
41	15.586	2101	2108	2122	rBV	3603443	5229081	61.23%	5.677%
42	15.704	2122	2128	2139	rBV	824277	1126554	13.19%	1.223%
43	15.828	2145	2149	2153	rVB2	19334	29799	0.35%	0.032%
44	15.951	2165	2170	2177	rVB	141301	190835	2.23%	0.207%
45	16.216	2213	2215	2219	rVB5	9520	11145	0.13%	0.012%
46	16.298	2225	2229	2235	rBV9	9704	14574	0.17%	0.016%
47	16.375	2239	2242	2245	rBV5	7159	10273	0.12%	0.011%
48	16.522	2264	2267	2269	rBV4	7742	9446	0.11%	0.010%
49	16.728	2300	2302	2308	rBV7	13041	17823	0.21%	0.019%
50	17.228	2384	2387	2390	rBV5	16305	24508	0.29%	0.027%
51	17.298	2396	2399	2401	rBV4	8844	11659	0.14%	0.013%
52	17.351	2401	2408	2417	rBV	3809627	5766765	67.52%	6.260%
53	17.445	2418	2424	2437	rVB2	3886911	5456837	63.89%	5.924%
54	17.704	2464	2468	2477	rVB6	60446	82814	0.97%	0.090%
55	18.010	2517	2520	2522	rVB4	19355	20957	0.25%	0.023%
56	18.216	2551	2555	2565	rBV	427254	614313	7.19%	0.667%
57	19.257	2729	2732	2736	rVB3	53940	65659	0.77%	0.071%
58	19.322	2741	2743	2746	rVV2	39239	48223	0.56%	0.052%
59	19.451	2761	2765	2770	rBV3	84042	117824	1.38%	0.128%
60	19.680	2798	2804	2812	rBV	5534082	7268911	85.11%	7.891%
61	21.127	3046	3050	3060	rBV	943123	1614384	18.90%	1.753%
62	21.433	3097	3102	3108	rBV	5139787	6891233	80.69%	7.481%
63	23.751	3489	3496	3512	rVB2	3972911	8540602	100.00%	9.272%
64	23.915	3517	3524	3534	rVB2	3754529	7645067	89.51%	8.299%
65	24.145	3559	3563	3574	rVB2	557802	1028860	12.05%	1.117%
66	24.639	3641	3647	3663	rVB2	921465	2389479	27.98%	2.594%

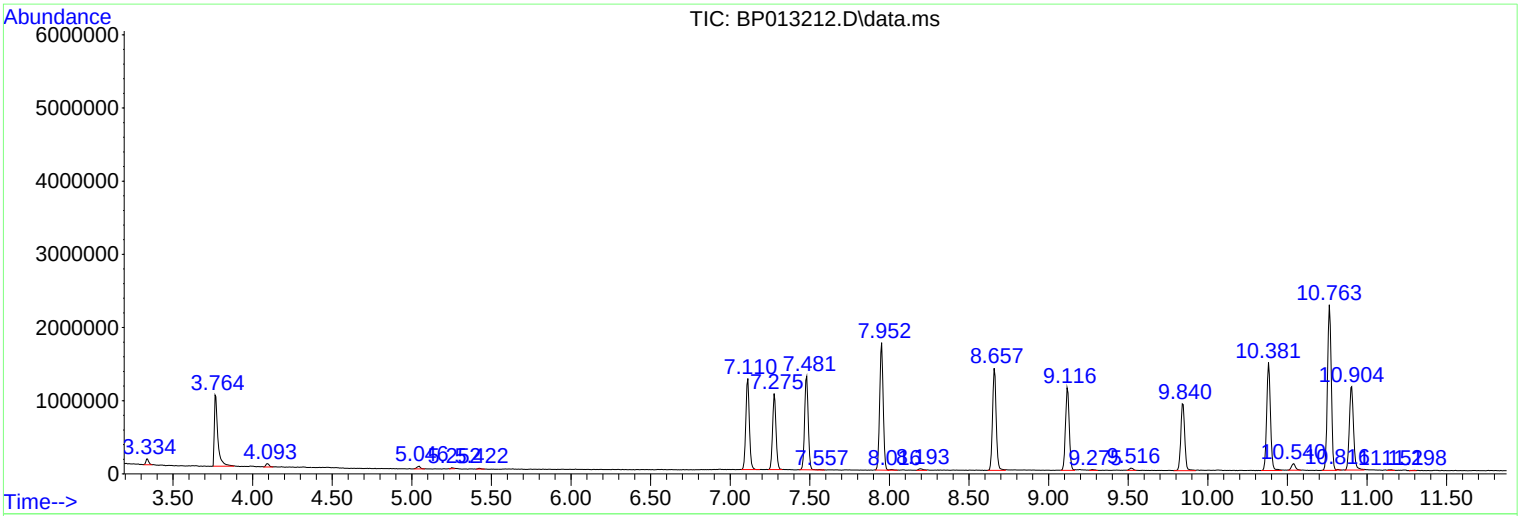
Sum of corrected areas: 92115718

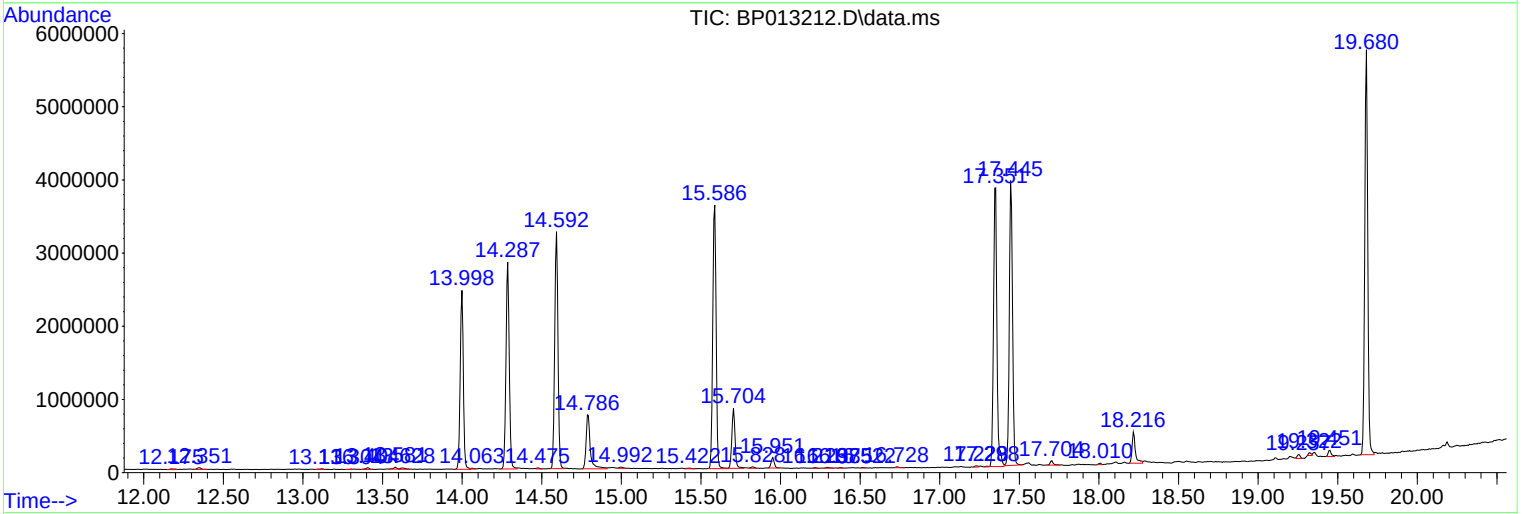
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

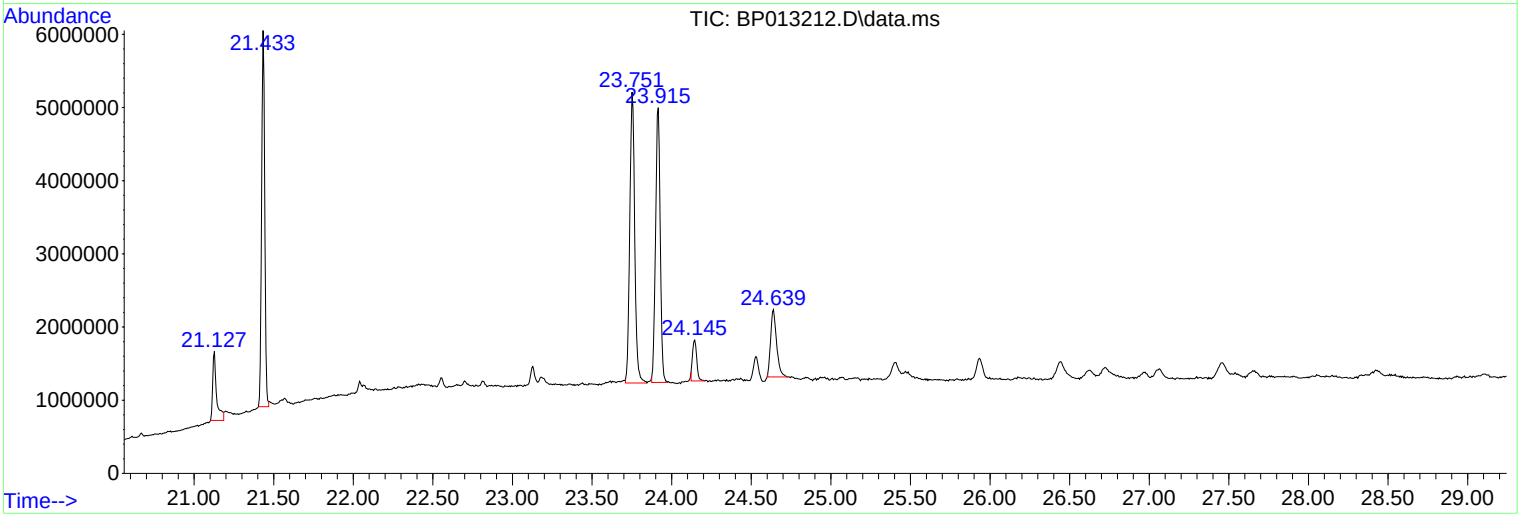
Instrument :
BNA_P
ClientSampleId :
DBXR9

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 : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
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ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
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DBXR9

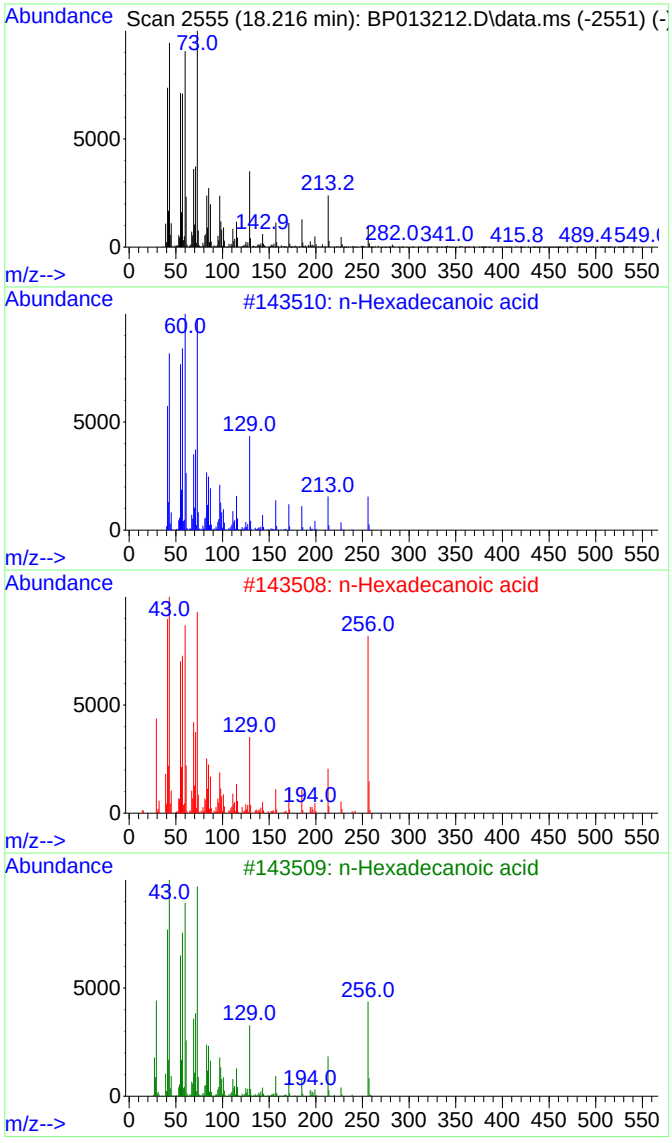
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

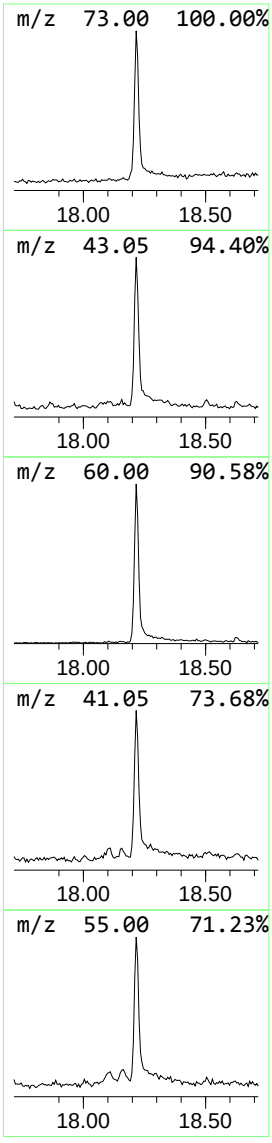
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	2.13 ng/ul	614313	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	97
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	Octadecanoic acid	284	C18H36O2	000057-11-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR9

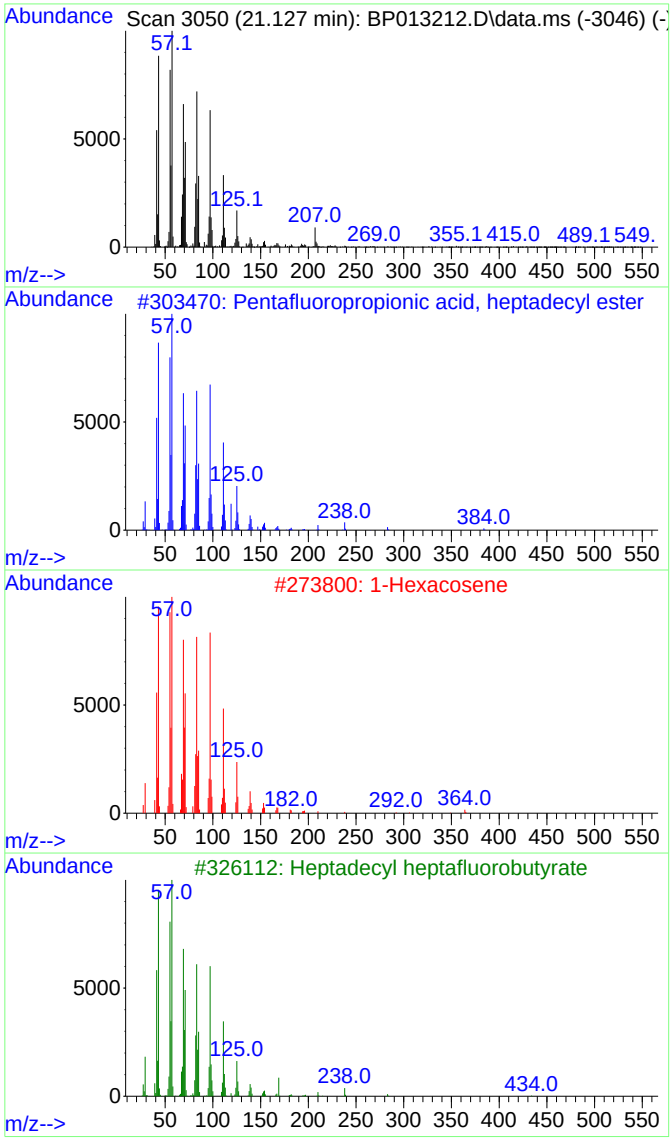
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

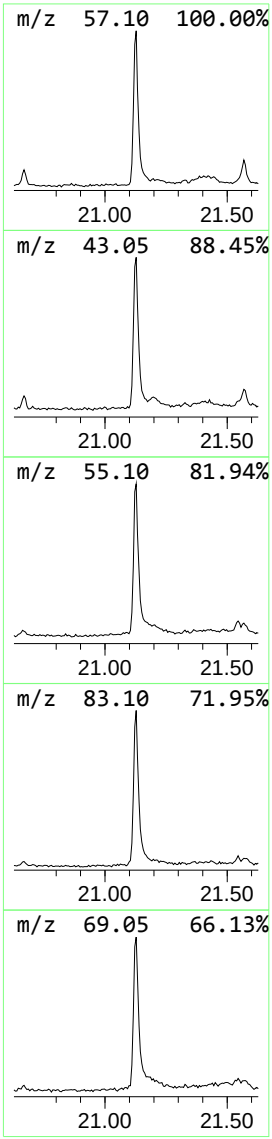
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.69 ng/ul	1614380	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR9

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

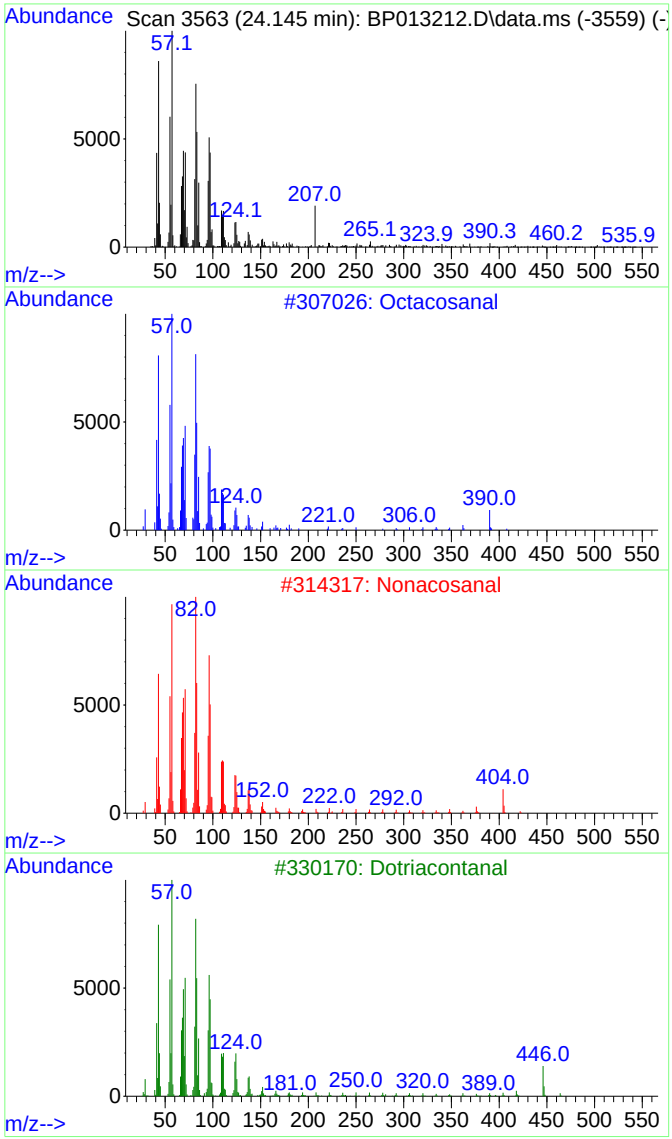
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

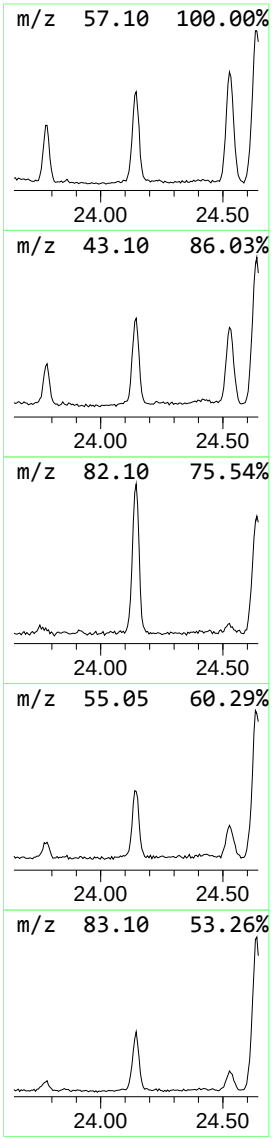
****

Peak Number 3 Octacosanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.145	2.69 ng/ul	1028860	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanal	408	C28H56O	022725-64-0	95
2	Nonacosanal	422	C29H58O	072934-04-4	91
3	Dotriacontanal	464	C32H64O	057878-00-9	90
4	Tetradecanal	212	C14H28O	000124-25-4	87
5	Hexacosanal	380	C26H52O	026627-85-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR9

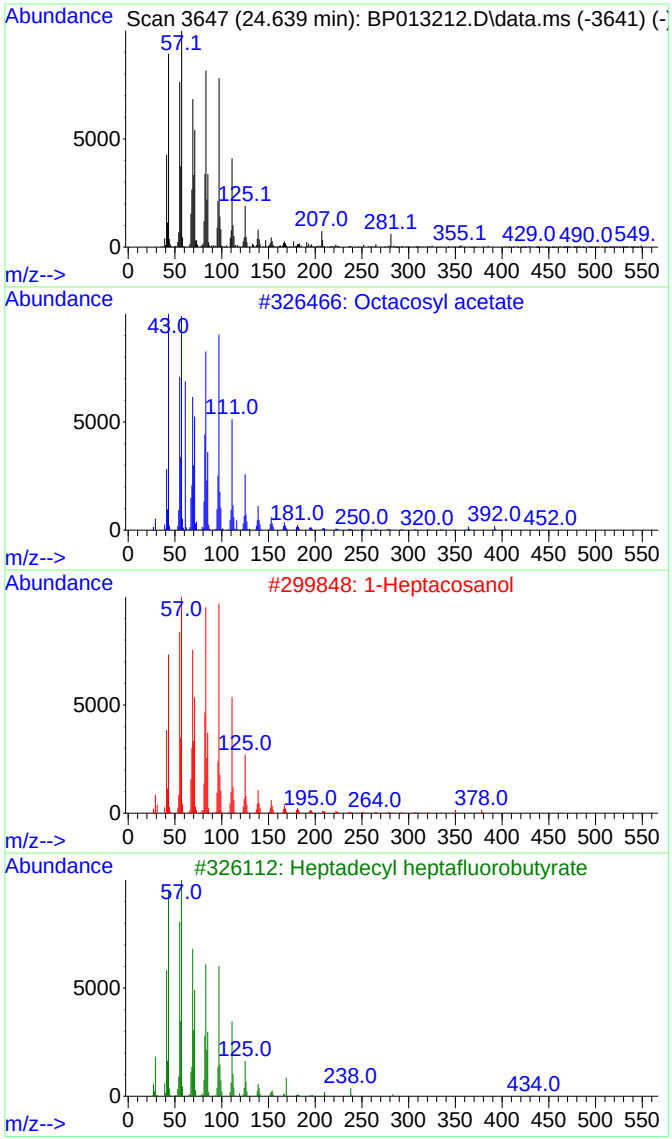
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

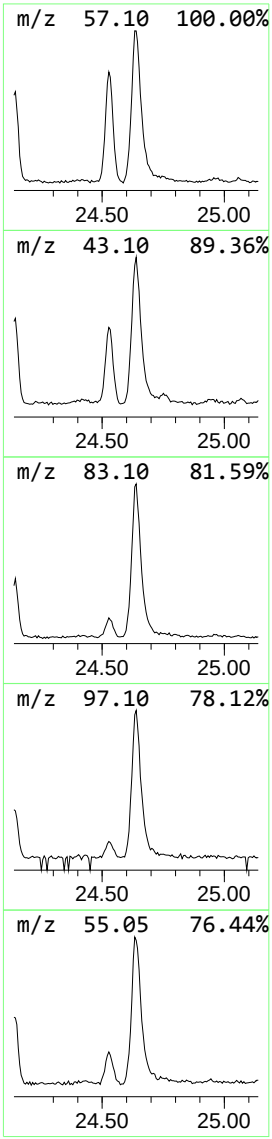
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octacosyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.639	6.25 ng/ul	2389480	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl acetate	452	C30H60O2	018206-97-8	97
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Octacosanol	410	C28H58O	000557-61-9	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013212.D
Acq On : 21 Dec 2022 17:29
Operator : CG/JU
Sample : N6014-08
Misc :
ALS Vial : 94 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR9

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
n-Hexadecanoic ...	18.216	2.1	ng/ul	614313	4	17.351	5766770	20.0
Pentafluoroprop...	21.127	4.7	ng/ul	1614380	5	21.433	6891230	20.0
Octacosanal	24.145	2.7	ng/ul	1028860	6	23.915	7645070	20.0
Octacosyl acetate	24.639	6.3	ng/ul	2389480	6	23.915	7645070	20.0