LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

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-BP102521.M
Title : SVOA CALIBRATION

Signal : TIC: BP007752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	10	13	18	rBV	34603	43662	0.61%	0.084%
2	3.793	84	86	100	rBV	55438	91150	1.27%	0.175%
3	4.022	121	125	129	rVB	27093	36812	0.51%	0.071%
4	4.116	137	141	146	rBV2	9662	11395	0.16%	0.022%
5	4.210	154	157	162	rVB5	12644	18097	0.25%	0.035%
6	5.040	294	298	304	rVB3	10375	16092	0.22%	0.031%
7	6.022	461	465	470	rVB7	5998	8017	0.11%	0.015%
8	6.316	510	515	521	rVB3	10982	19731	0.28%	0.038%
9	7.093	641	647	658	rVB	320869	504525	7.04%	0.969%
10	7.257	669	675	686	rBV	716757	1117825	15.59%	2.147%
11	7.463	702	710	720	rBV	779943	1240199	17.29%	2.382%
12	7.928	782	789	798	rBV	315936	503321	7.02%	0.967%
13	8.639	902	910	923	rBV	690915	1134302	15.82%	2.178%
14	9.087	978	986	994	rBV	876312	1434420	20.00%	2.755%
15	9.551	1059	1065	1071	rVB9	5808	11966	0.17%	0.023%
16	9.810	1101	1109	1123	rBV	714790	1183184	16.50%	2.272%
17	10.351	1192	1201	1214	rBV	1125975	1868503	26.06%	3.588%
18	10.516	1221	1229	1240	rBV	182337	297155	4.14%	0.571%
19	10.733	1259	1266	1273	rVB	448883	748505	10.44%	1.437%
20	10.869	1280	1289	1301	rBV	825390	1451119	20.24%	2.787%
21	12.045	1483	1489	1498	rVB7	7006	15844	0.22%	0.030%
22	12.322	1529	1536	1543	rVB	20424	33668	0.47%	0.065%
23	12.939	1636	1641	1645	rBV7	4861	9400	0.13%	0.018%
24	13.180	1676	1682	1689	rBV8	5825	10910	0.15%	0.021%
25	13.475	1727	1732	1739	rBV2	39358	63552	0.89%	0.122%
26	13.539	1739	1743	1748	rVB6	6337	10867	0.15%	0.021%
27	13.974	1810	1817	1829	rBV	2241767	3148090	43.90%	6.046%
28	14.257	1854	1865	1876	rBV	2393135	3728307	51.99%	7.160%
29	14.569	1911	1918	1924	rBV	708791	1065803	14.86%	2.047%
30	14.757	1943	1950	1966	rBV	308366	494168	6.89%	0.949%
31	14.927	1976	1979	1982	rVB5	5482	7552	0.11%	0.015%
32	14.986	1986	1989	1993	rBV5	10051	14583	0.20%	0.028%
33	15.310	2041	2044	2049	rVB4	5358	8433	0.12%	0.016%
34	15.392	2053	2058	2062	rVV3	9954	15817	0.22%	0.030%
35	15.563	2080	2087	2100	rBV	3346346	4821071	67.23%	9.259%
36	15.674	2100	2106	2119	rBV	890774	1263884	17.62%	2.427%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

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-BP102521.M
Title : SVOA CALIBRATION

37	15.804	2123	2128	2135	rVB2	40277	61980	0.86%	0.119%
38	15.933	2146	2150	2156	rVB9	6642	10474	0.15%	0.020%
39	16.016	2159	2164	2166	rBV5	7862	10667	0.15%	0.020%
40	16.127	2179	2183	2189	rBV9	5358	9722	0.14%	0.019%
41	16.257	2200	2205	2211	rVB9	8651	15737	0.22%	0.030%
42	16.357	2218	2222	2226	rVB7	7369	11698	0.16%	0.022%
43	16.463	2237	2240	2247	rVB8	9598	15359	0.21%	0.029%
44	16.568	2252	2258	2262	rBV9	5024	9320	0.13%	0.018%
45	16.733	2281	2286	2291	rVB9	5993	10531	0.15%	0.020%
46	17.004	2327	2332	2337	rBV7	4772	9873	0.14%	0.019%
47	17.263	2372	2376	2379	rBV6	4569	7961	0.11%	0.015%
48	17.321	2379	2386	2396	rBV	937256	1320294	18.41%	2.536%
49	17.421	2397	2403	2414	rVV2	3871154	5668482	79.05%	10.886%
50	17.568	2424	2428	2433	rBV8	6831	12091	0.17%	0.023%
51	17.715	2447	2453	2459	rBV5	9413	22709	0.32%	0.044%
52	18.004	2497	2502	2507	rBV	92056	108307	1.51%	0.208%
53	18.215	2534	2538	2545	rBV	121257	168060	2.34%	0.323%
54	19.110	2686	2690	2691	rBV3	28357	34241	0.48%	0.066%
55	19.139	2691	2695	2698	rVB	216691	258118	3.60%	0.496%
56	19.233	2707	2711	2714	rBV2	60941	84150	1.17%	0.162%
57	19.268	2714	2717	2719	rVV	52075	58397	0.81%	0.112%
58	19.304	2719	2723	2727	rVB	53164	67976	0.95%	0.131%
59	19.451	2744	2748	2756	rBV3	54878	90344	1.26%	0.174%
60	19.598	2771	2773	2777	rVB5	16287	15749	0.22%	0.030%
61	19.657	2777	2783	2789	rBV	5002041	6736623	93.94%	12.938%
62	21.127	3030	3033	3040	rBV2	151678	229665	3.20%	0.441%
63	21.415	3077	3082	3087	rBV	1142031	1614141	22.51%	3.100%
64	22.703	3298	3301	3309	rVB	133077	179724	2.51%	0.345%
65	23.698	3463	3470	3479	rVB2	3572511	7171073	100.00%	13.772%
66	23.856	3491	3497	3505	rVB2	795314	1604887	22.38%	3.082%

Sum of corrected areas: 52070282

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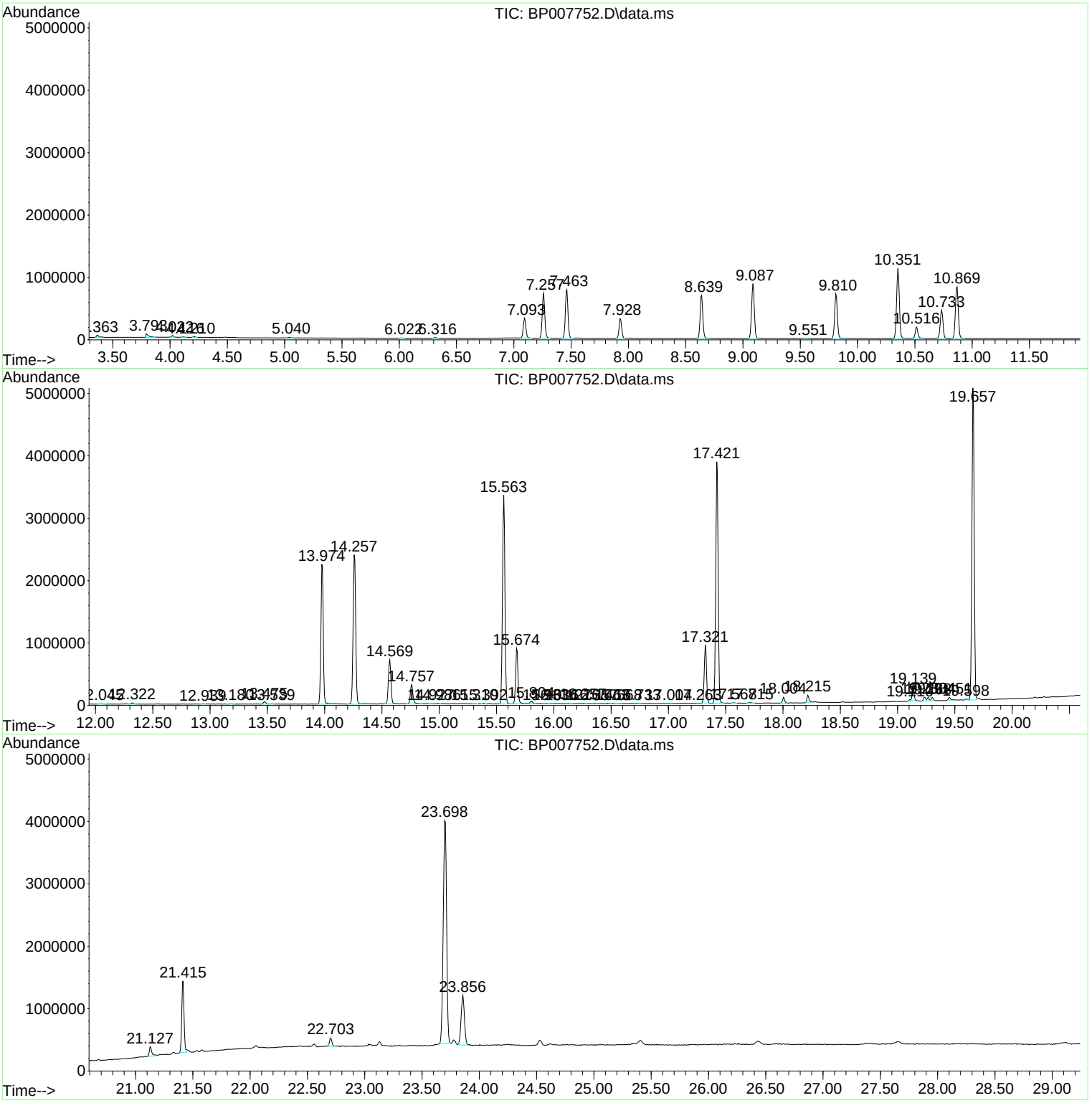
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BFFX4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
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Instrument : BNA_P
ClientSampleId : BFFX4

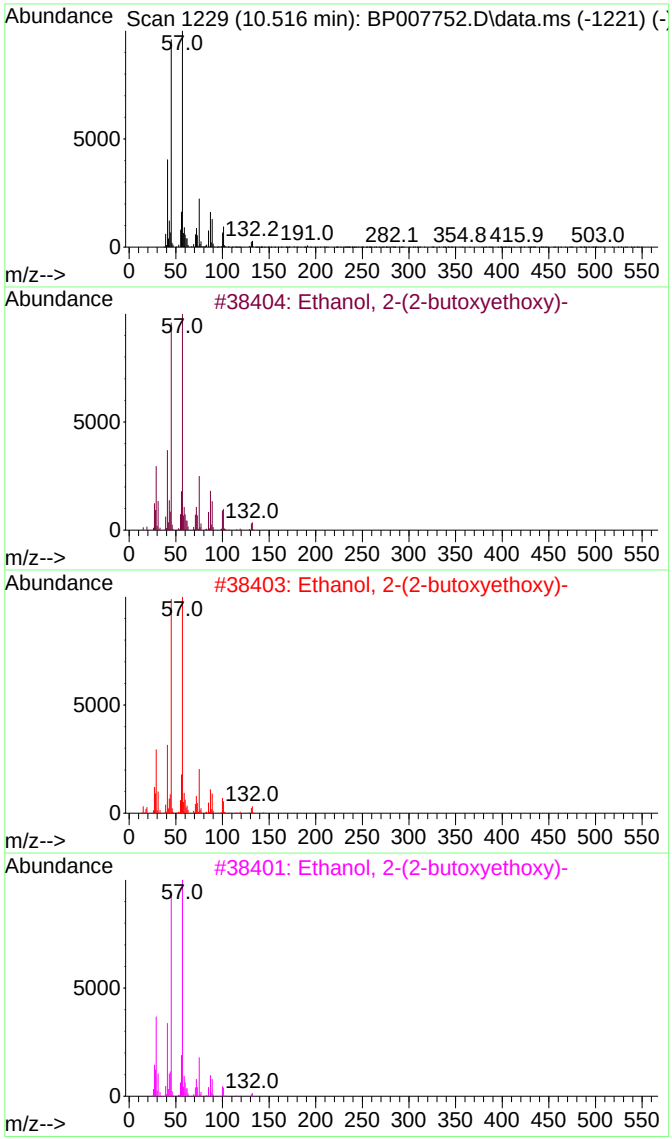
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

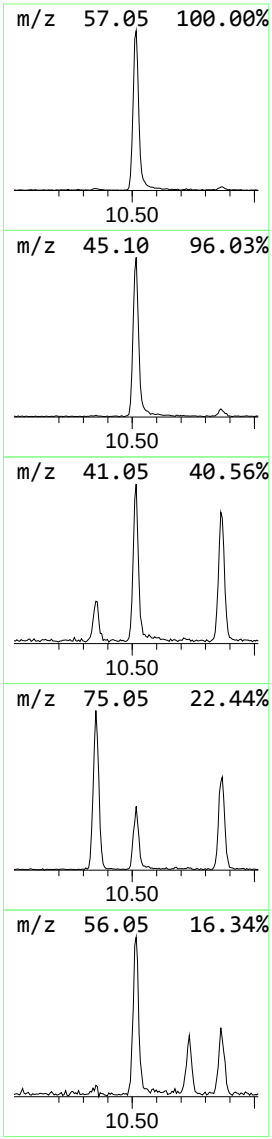
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.516	7.94 ng/ul	297155	Naphthalene-d8	10.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

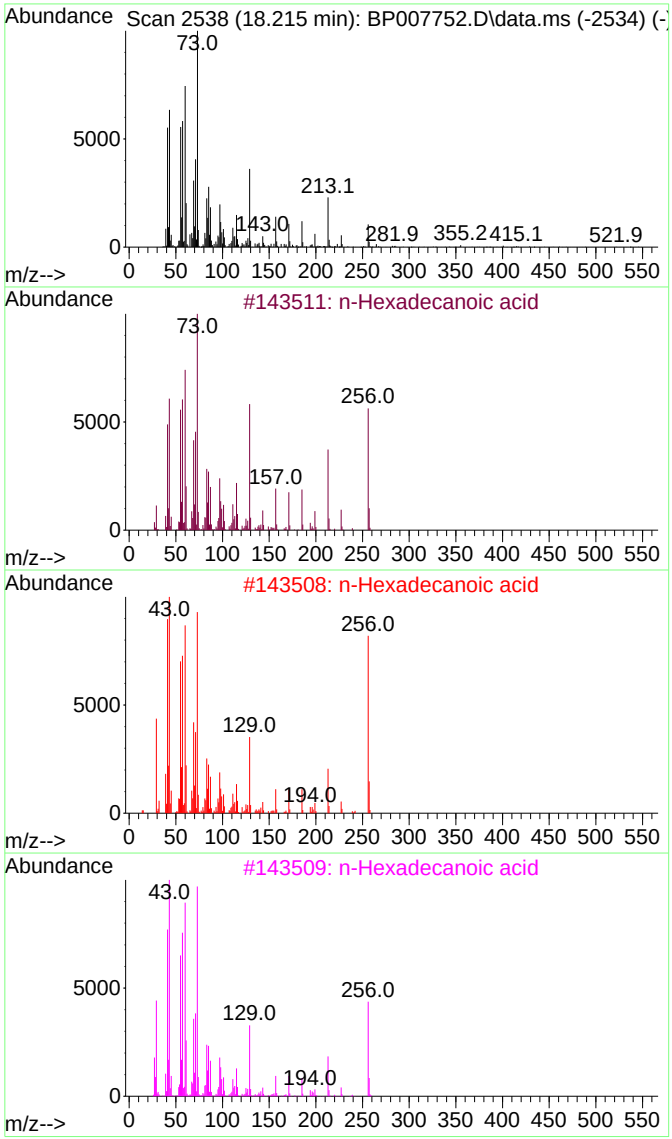
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

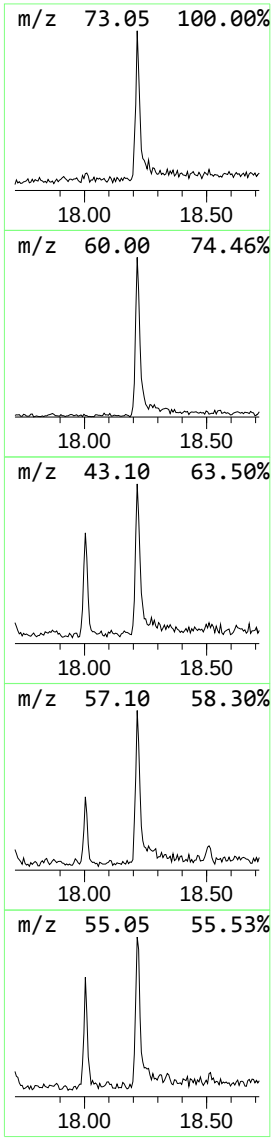
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	2.55 ng/ul	168060	Phenanthrene-d10	17.321

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	98
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

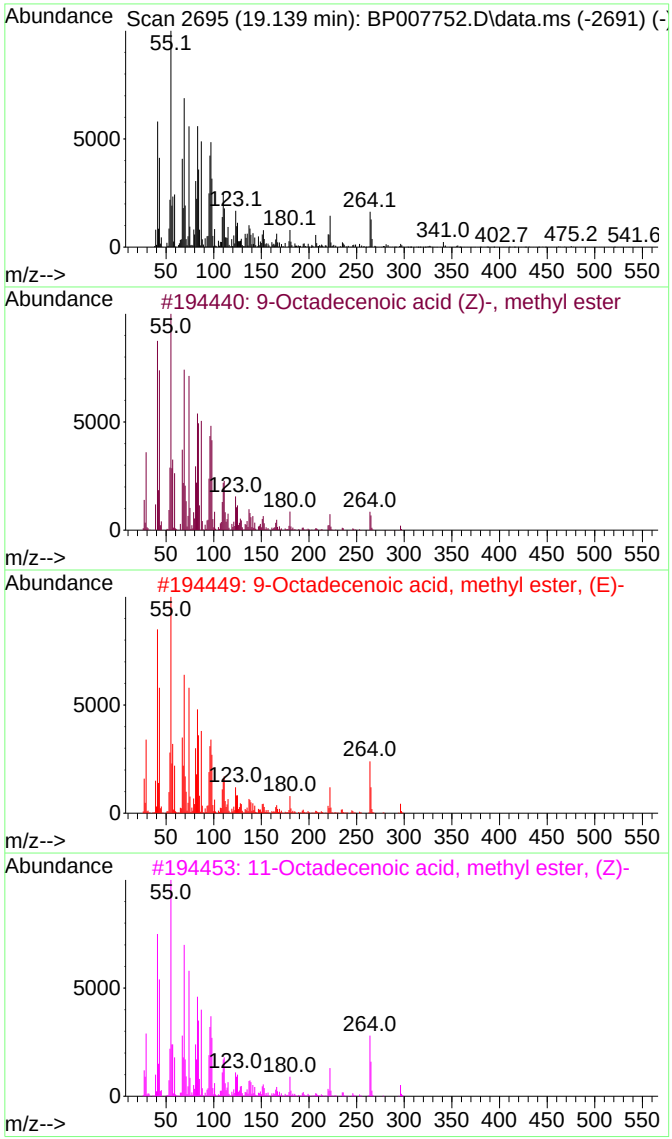
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

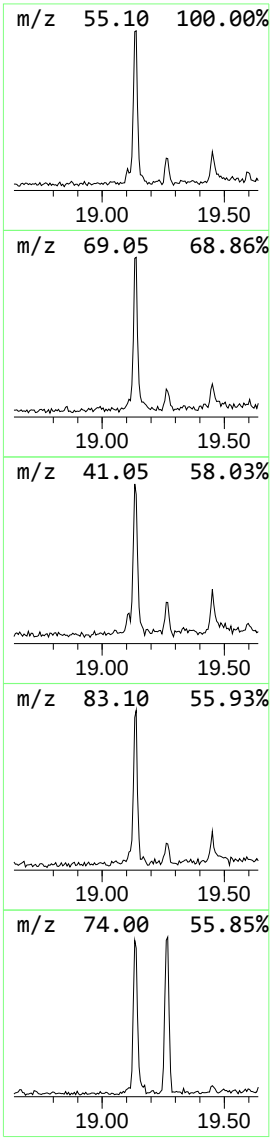
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.139	3.91 ng/ul	258118	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
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Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

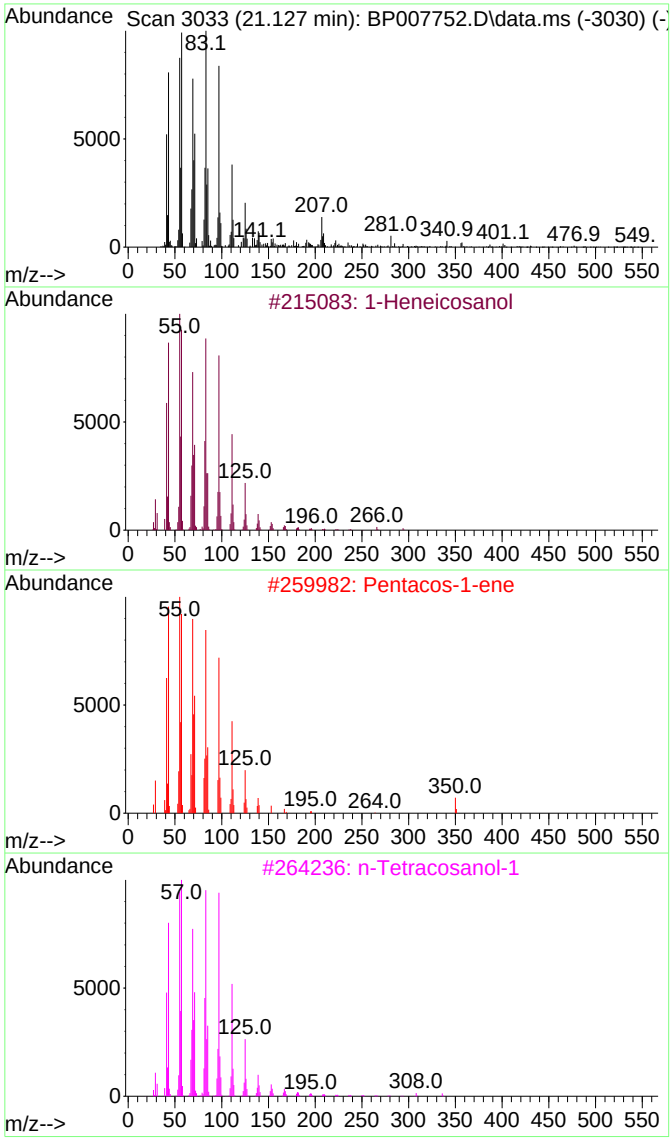
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

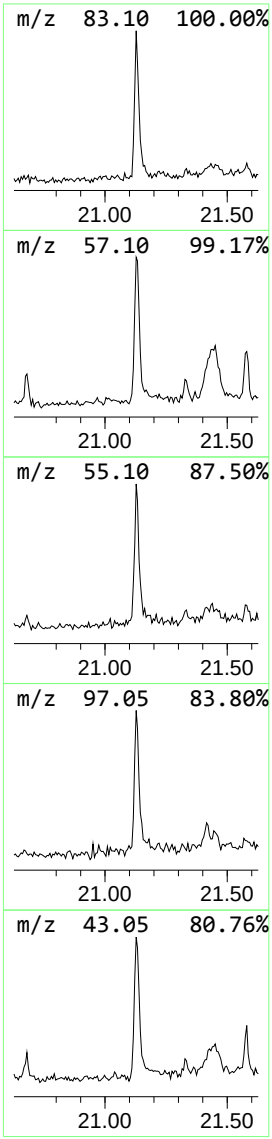
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	2.85 ng/ul	229665	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93





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Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
Sample : M4282-20
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BFFX4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.M
Quant Title : SVOA CALIBRATION

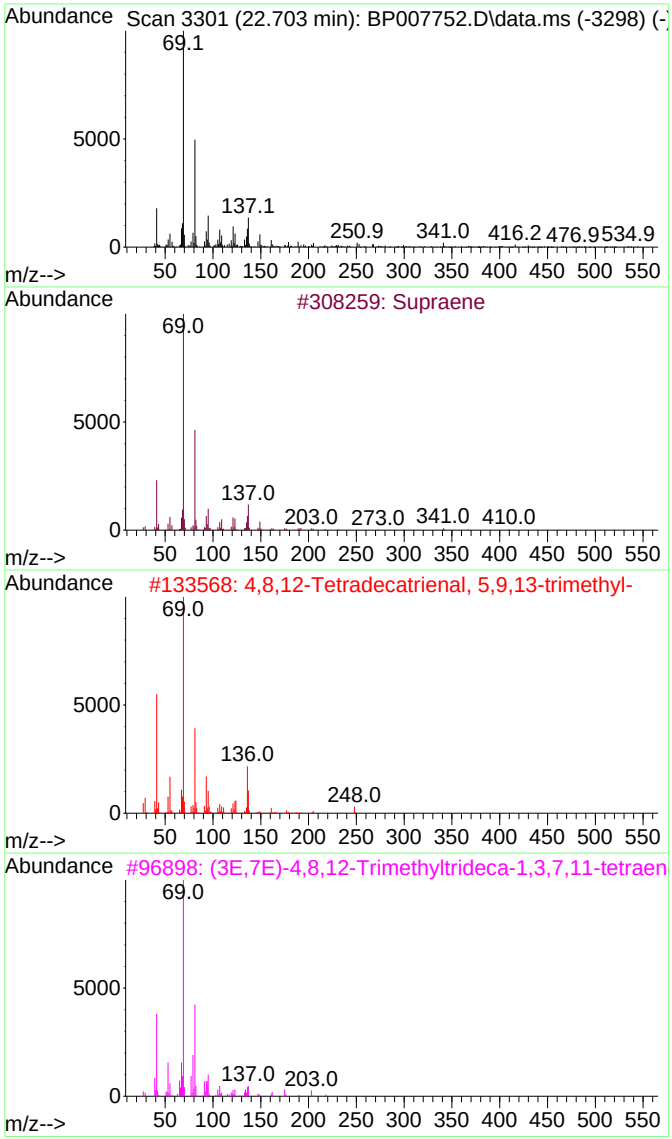
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

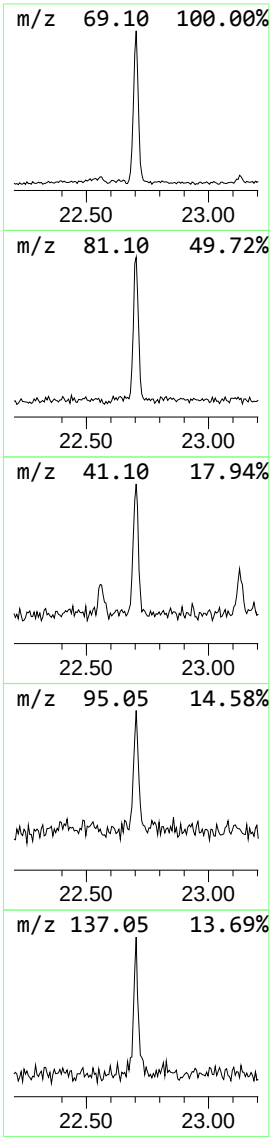
****

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.703	2.24 ng/ul	179724	Perylene-d12	23.856

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	64
4	(E)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	1010161-30-7	59
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102821\
Data File : BP007752.D
Acq On : 28 Oct 2021 14:29
Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\SFAM-EPA-BP102521.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
Ethanol, 2-(2-b...	10.516	7.9	ng/ul	297155	2	10.733	748505	20.0
n-Hexadecanoic ...	18.215	2.5	ng/ul	168060	4	17.321	1320290	20.0
9-Octadecenoic ...	19.139	3.9	ng/ul	258118	4	17.321	1320290	20.0
1-Heneicosanol	21.127	2.9	ng/ul	229665	5	21.415	1614140	20.0
Supraene	22.703	2.2	ng/ul	179724	6	23.856	1604890	20.0