LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : E1ZS3

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: BP021357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	26	30	37	rVB	24271	30341	0.88%	0.072%
2	3.464	77	81	96	rBV	42784	92278	2.67%	0.220%
3	3.587	100	102	116	rBV	200412	376514	10.89%	0.896%
4	3.876	148	151	156	rVB2	10444	16961	0.49%	0.040%
5	6.852	650	657	673	rBV	213259	649627	18.79%	1.546%
6	6.981	673	679	702	rVB	292142	545429	15.77%	1.298%
7	7.175	706	712	731	rBV	353729	688856	19.92%	1.639%
8	7.334	735	739	742	rBV6	3759	6497	0.19%	0.015%
9	7.622	781	788	807	rBV	532781	1033325	29.88%	2.459%
10	8.369	908	915	940	rBV2	307718	890973	25.77%	2.120%
11	8.793	979	987	1009	rBV	310246	679120	19.64%	1.616%
12	8.934	1009	1011	1015	rVB4	3137	3890	0.11%	0.009%
13	9.111	1036	1041	1047	rBV9	4562	8979	0.26%	0.021%
14	9.358	1075	1083	1091	rBV3	16326	41622	1.20%	0.099%
15	9.422	1093	1094	1102	rVB7	3077	4216	0.12%	0.010%
16	9.505	1102	1108	1125	rBV	256413	563085	16.28%	1.340%
17	10.069	1194	1204	1229	rBV	250005	873570	25.26%	2.079%
18	10.381	1250	1257	1271	rBV	746778	1434338	41.48%	3.413%
19	10.569	1282	1289	1322	rBV	270604	834122	24.12%	1.985%
20	10.981	1353	1359	1360	rBV5	5348	7300	0.21%	0.017%
21	11.187	1385	1394	1408	rBV4	33918	133394	3.86%	0.317%
22	11.940	1518	1522	1525	rBV6	2863	5290	0.15%	0.013%
23	12.004	1528	1533	1539	rVV3	4814	11407	0.33%	0.027%
24	12.599	1628	1634	1638	rBV9	2094	4491	0.13%	0.011%
25	13.228	1736	1741	1747	rVB10	3048	4658	0.13%	0.011%
26	13.681	1809	1818	1838	rBV	895932	1480959	42.83%	3.524%
27	13.957	1856	1865	1875	rBV	1004162	1761471	50.94%	4.191%
28	14.146	1895	1897	1903	rVB7	4665	6913	0.20%	0.016%
29	14.263	1903	1917	1932	rBV	1261545	2020967	58.45%	4.809%
30	14.463	1945	1951	1952	rBV	35522	44302	1.28%	0.105%
31	14.481	1952	1954	1963	rVB4	42051	79451	2.30%	0.189%
32	14.634	1974	1980	1988	rBV2	126646	362109	10.47%	0.862%
33	15.051	2049	2051	2057	rVB5	9530	16172	0.47%	0.038%
34	15.122	2060	2063	2068	rVB7	6482	9564	0.28%	0.023%
35	15.287	2083	2091	2106	rBV	1320527	2322941	67.18%	5.527%
36	15.475	2116	2123	2131	rBV	186355	530457	15.34%	1.262%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

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	15.698	2159	2161	2165	rVB5	3888	3744	0.11%	0.009%
38	15.857	2183	2188	2196	rVB5	5880	14983	0.43%	0.036%
39	16.010	2210	2214	2216	rBV5	7728	11226	0.32%	0.027%
40	16.093	2225	2228	2229	rBV3	4661	4884	0.14%	0.012%
41	16.487	2292	2295	2308	rVB3	10598	24990	0.72%	0.059%
42	16.828	2349	2353	2355	rBV5	7834	10500	0.30%	0.025%
43	16.875	2358	2361	2368	rVB6	8609	15539	0.45%	0.037%
44	16.987	2376	2380	2387	rVB8	15281	24878	0.72%	0.059%
45	17.087	2390	2397	2407	rBV	1576438	2509366	72.57%	5.971%
46	17.192	2409	2415	2428	rBV	1722772	2519148	72.85%	5.994%
47	17.510	2465	2469	2472	rBV6	6412	9262	0.27%	0.022%
48	17.587	2479	2482	2485	rBV5	5648	7183	0.21%	0.017%
49	17.775	2510	2514	2522	rVB4	22698	37500	1.08%	0.089%
50	17.892	2531	2534	2540	rBV8	11840	22799	0.66%	0.054%
51	18.016	2550	2555	2566	rBV	283998	485875	14.05%	1.156%
52	19.128	2741	2744	2752	rVB6	27816	43236	1.25%	0.103%
53	19.198	2754	2756	2758	rBV2	22609	21655	0.63%	0.052%
54	19.357	2779	2783	2790	rBV	83613	153518	4.44%	0.365%
55	19.575	2815	2820	2832	rBV2	2289651	3282061	94.92%	7.809%
56	20.104	2899	2910	2917	rBV5	350086	1174420	33.96%	2.794%
57	20.192	2918	2925	2937	rVV	1153808	3278993	94.83%	7.802%
58	20.292	2940	2942	2951	rVB2	270484	474424	13.72%	1.129%
59	21.180	3089	3093	3103	rVB2	309720	571893	16.54%	1.361%
60	21.533	3148	3153	3165	rVB2	1785135	2922952	84.53%	6.955%
61	24.598	3665	3674	3686	rVB	1308614	3457828	100.00%	8.228%
62	24.827	3704	3713	3728	rVB2	1188689	3369178	97.44%	8.017%

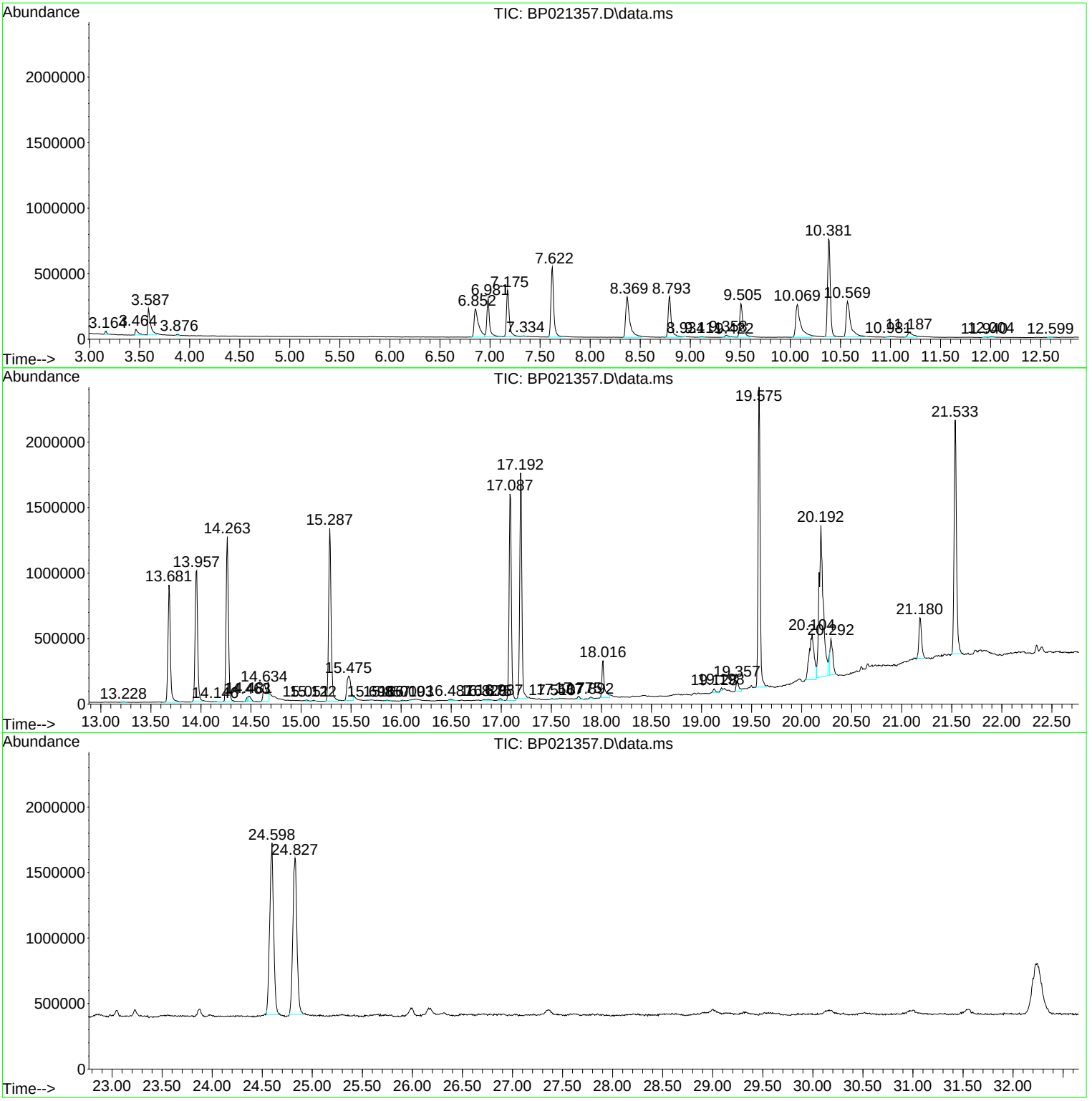
Sum of corrected areas: 42027624

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

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\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

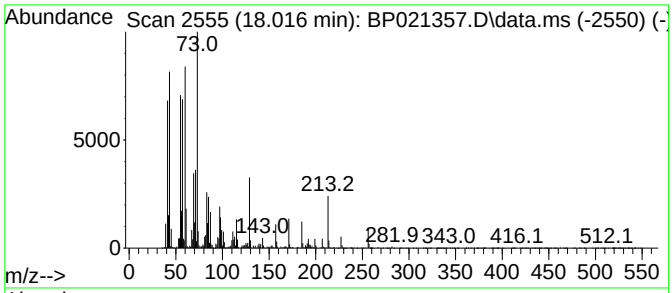
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

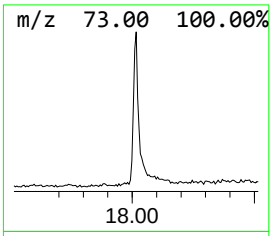
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

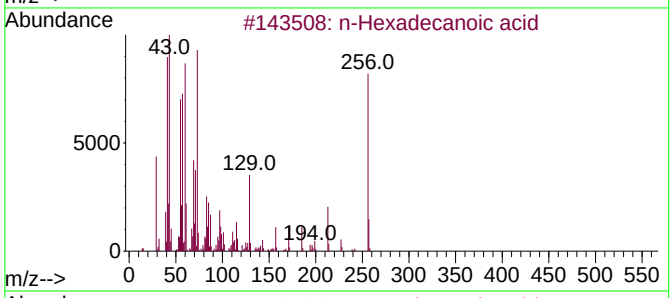
****
Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

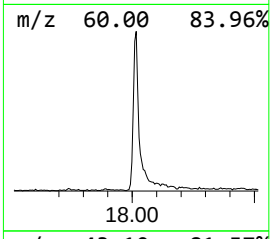
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	3.87 ng/ul	485875	Phenanthrene-d10	17.087

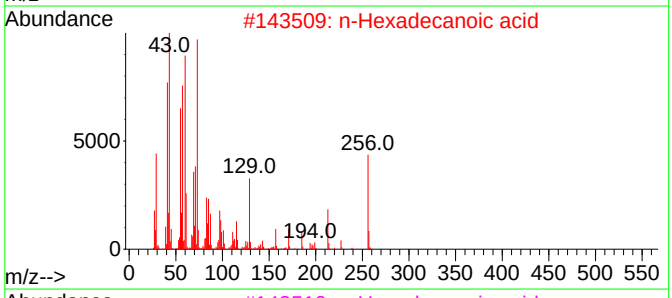
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93

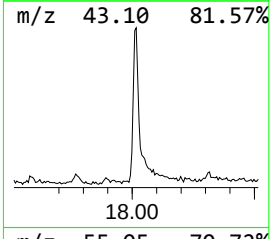


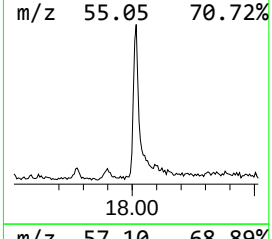


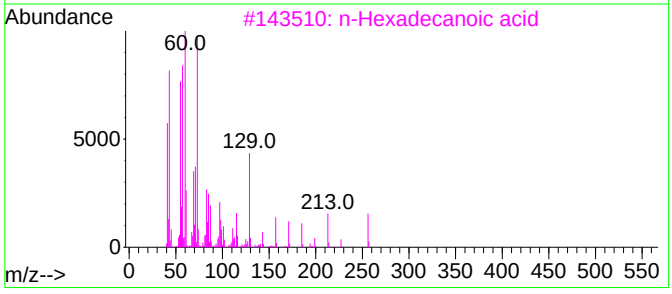


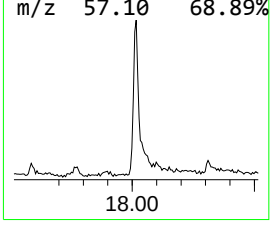












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

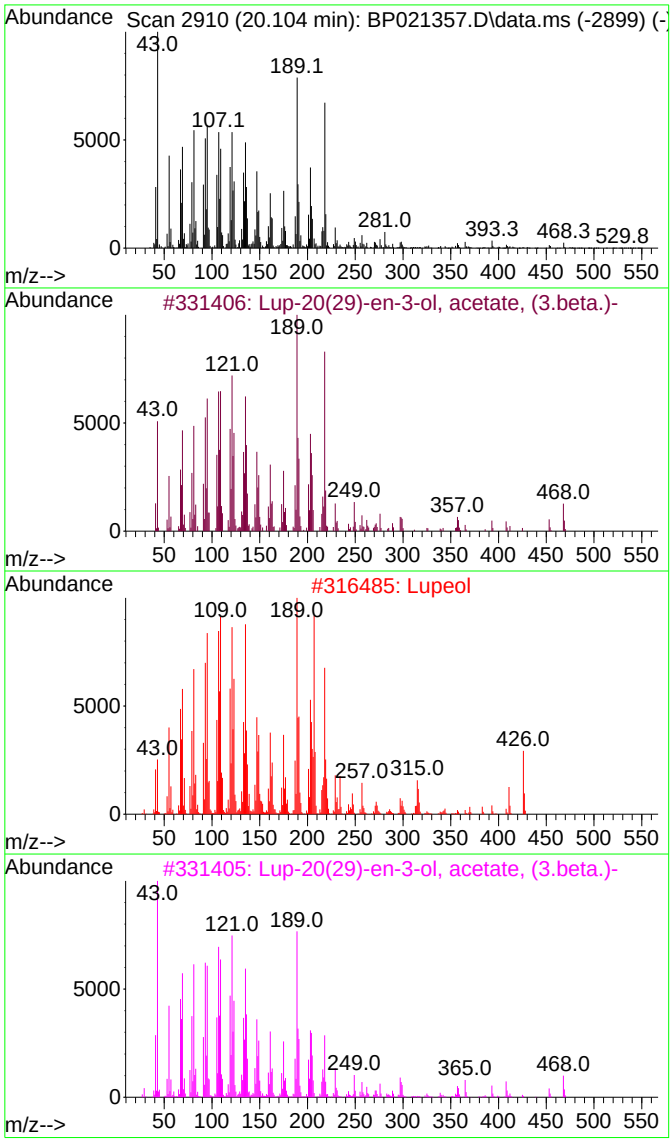
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

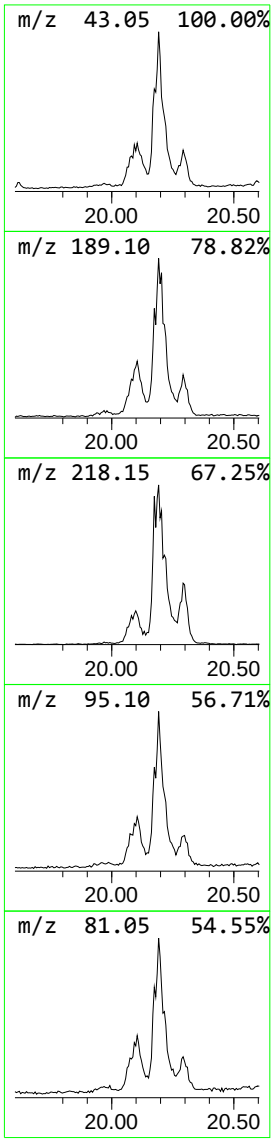
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Lup-20(29)-en-3-ol, acetate... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.104	8.04 ng/ul	1174420	Chrysene-d12	21.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-ol, acetate, (3....	468	C32H52O2	001617-68-1	94
2	Lupeol	426	C30H50O	000545-47-1	74
3	Lup-20(29)-en-3-ol, acetate, (3....	468	C32H52O2	001617-68-1	74
4	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	72
5	Lup-20(29)-en-3-ol, acetate, (3....	468	C32H52O2	001617-68-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

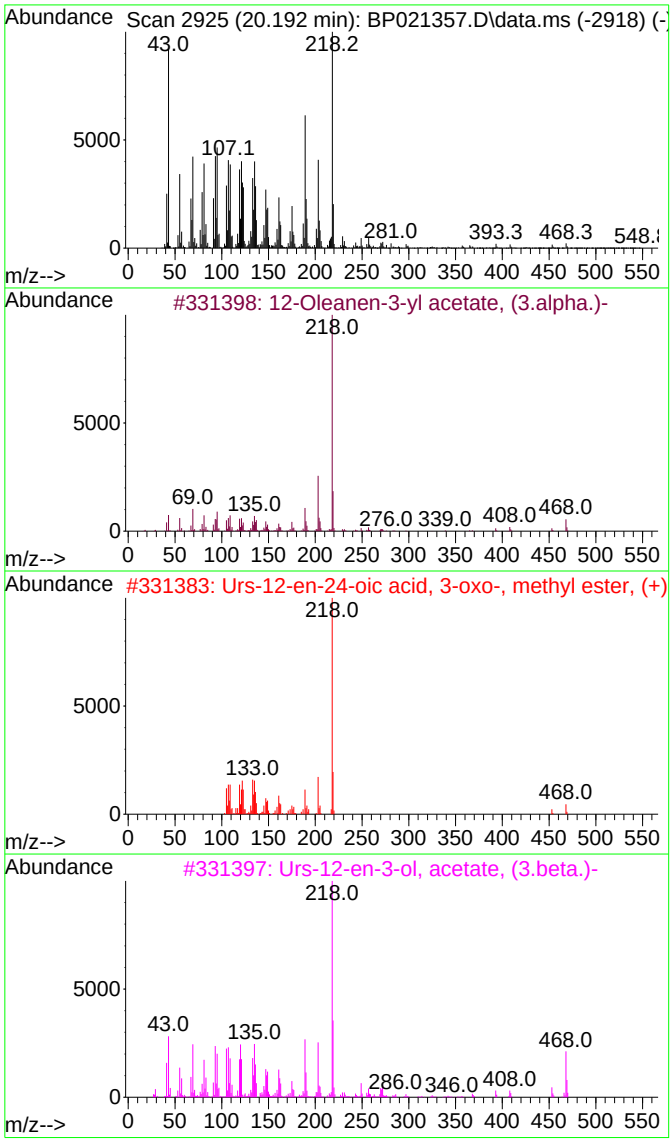
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

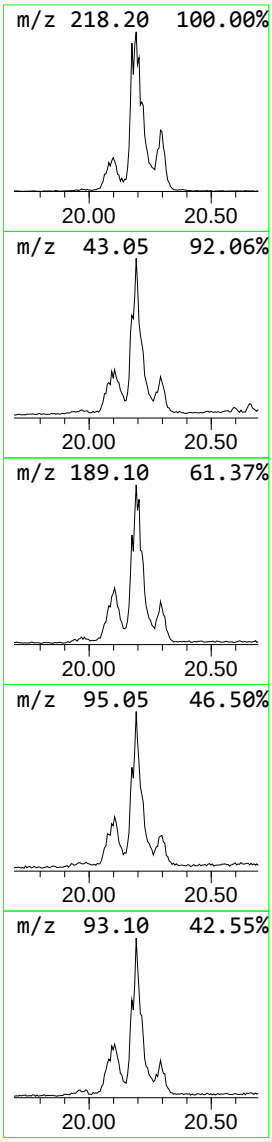
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 12-Oleanen-3-yl acetate, (3... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.192	22.44 ng/ul	3278990	Chrysene-d12	21.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Oleanen-3-yl acetate, (3.alph...	468	C32H52O2	033055-28-6	89
2	Urs-12-en-24-oic acid, 3-oxo-, m...	468	C31H48O3	020475-86-9	89
3	Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	86
4	.alpha.-Boswellic acid, O,O-bis-...	484	C32H52O3	1010507-05-0	86
5	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1000513-01-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

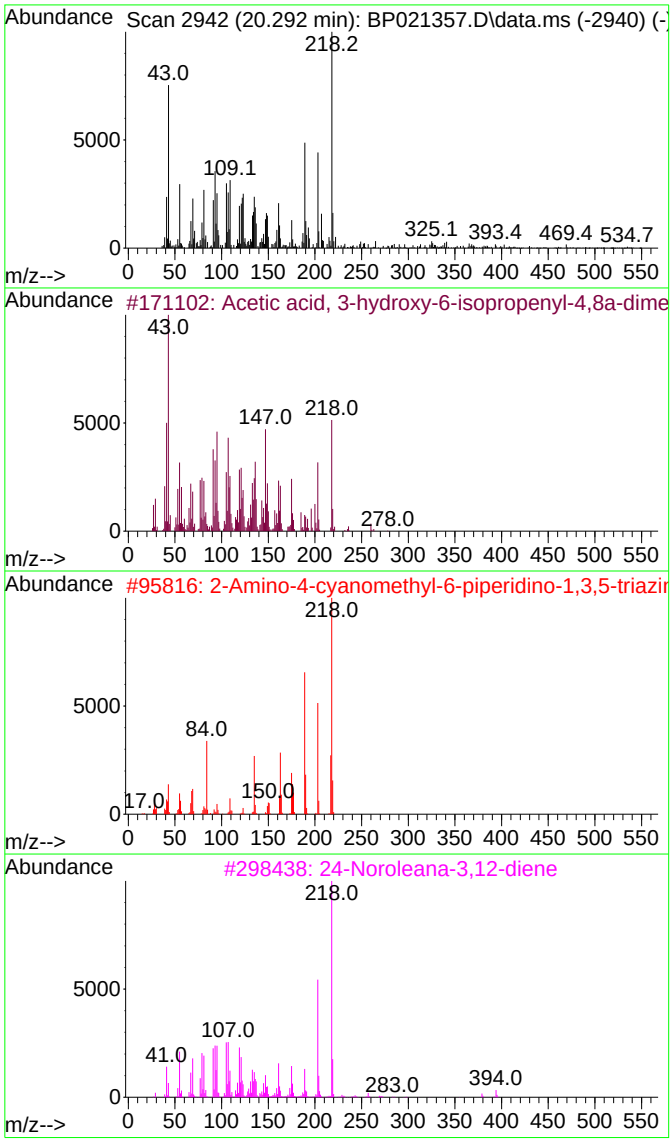
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

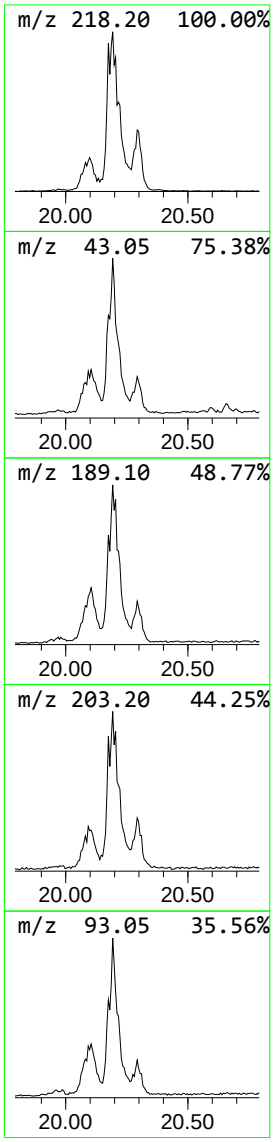
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetic acid, 3-hydroxy-6-is... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.292	3.25 ng/ul	474424	Chrysene-d12	21.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 3-hydroxy-6-isoprop...	278	C17H26O3	1000185-44-8	78
2	2-Amino-4-cyanomethyl-6-piperidi...	218	C10H14N6	1000241-05-9	60
3	24-Noroleana-3,12-diene	394	C29H46	201358-24-9	60
4	Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	52
5	.alpha.-Amyrin	426	C30H50O	000638-95-9	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

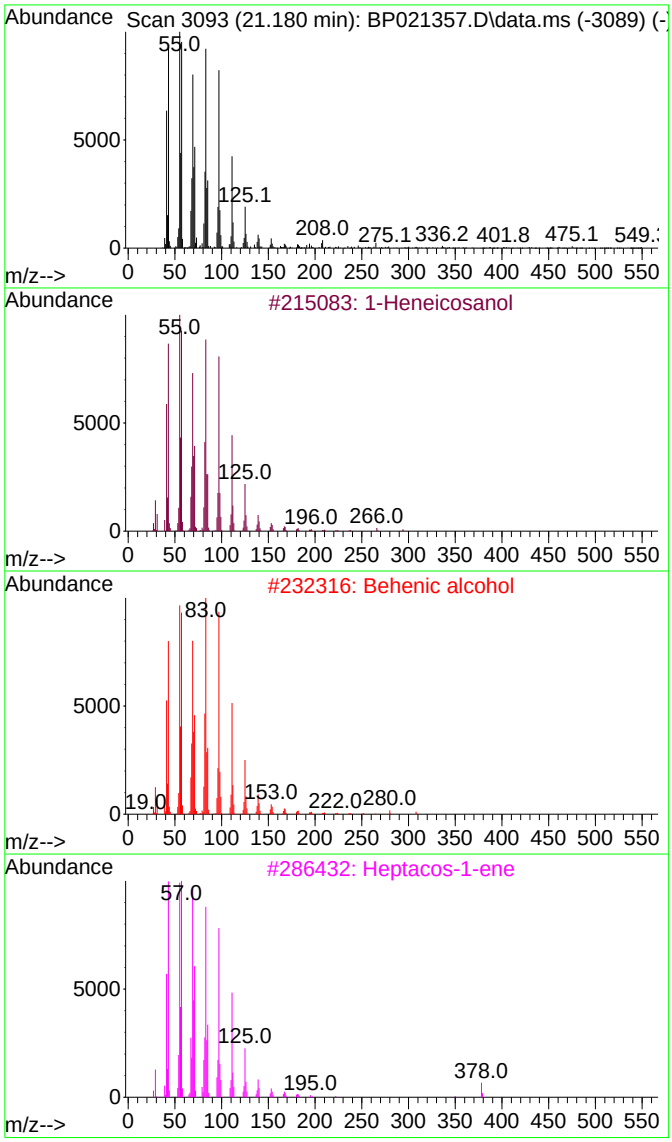
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

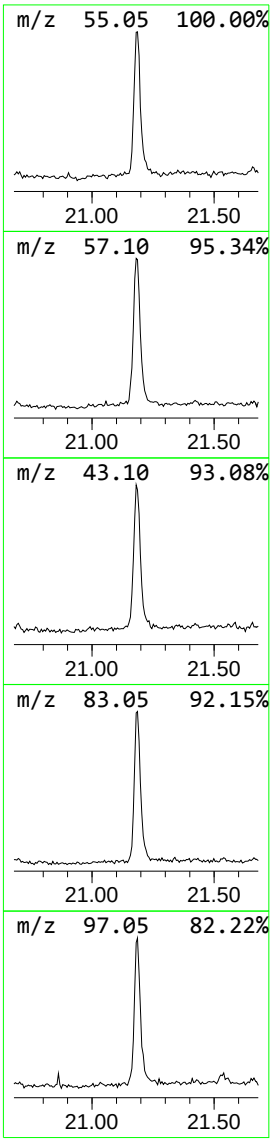
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	3.91 ng/ul	571893	Chrysene-d12	21.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptacos-1-ene	378	C27H54	015306-27-1	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080324\
Data File : BP021357.D
Acq On : 04 Aug 2024 01:13
Operator : CG/JU
Sample : P3278-23
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1ZS3

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
n-Hexadecanoic ...	18.016	3.9	ng/ul	485875	4	17.087	2509370	20.0
Lup-20(29)-en-3...	20.104	8.0	ng/ul	1174420	5	21.533	2922950	20.0
12-Oleanen-3-yl...	20.192	22.4	ng/ul	3278990	5	21.533	2922950	20.0
Acetic acid, 3-...	20.292	3.3	ng/ul	474424	5	21.533	2922950	20.0
1-Heneicosanol	21.180	3.9	ng/ul	571893	5	21.533	2922950	20.0