LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

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-BP100724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP022429.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.599	99	104	106	rBV	19886	27135	0.84%	0.083%
2	3.628	106	109	113	rVV2	27048	48438	1.49%	0.148%
3	3.675	113	117	120	rVV	28233	46019	1.42%	0.141%
4	3.717	120	124	128	rVV	47242	66438	2.05%	0.204%
5	3.764	128	132	139	rVV4	15726	32131	0.99%	0.098%
6	3.922	152	159	168	rBV3	77197	138893	4.29%	0.426%
7	4.087	182	187	191	rBV	19778	29518	0.91%	0.090%
8	4.181	195	203	209	rVB3	24969	45245	1.40%	0.139%
9	4.299	213	223	232	rBV	41002	64145	1.98%	0.197%
10	4.452	238	249	258	rBV2	640701	1272513	39.26%	3.899%
11	4.522	258	261	272	rVB	78763	118279	3.65%	0.362%
12	4.834	309	314	322	rVB	18474	27124	0.84%	0.083%
13	4.928	322	330	339	rVB7	11044	25901	0.80%	0.079%
14	5.605	439	445	449	rBV3	39550	70855	2.19%	0.217%
15	5.652	449	453	460	rVB	78722	126542	3.90%	0.388%
16	5.758	468	471	482	rVB6	14381	31868	0.98%	0.098%
17	5.981	497	509	511	rBV6	17578	47195	1.46%	0.145%
18	6.328	561	568	576	rBV	687642	1099478	33.92%	3.369%
19	6.528	593	602	616	rBV5	49428	104227	3.22%	0.319%
20	6.863	653	659	667	rVV	123620	212897	6.57%	0.652%
21	7.010	679	684	690	rBV	110237	160190	4.94%	0.491%
22	7.210	712	718	726	rBV	143216	233634	7.21%	0.716%
23	7.363	739	744	752	rBV3	31994	69699	2.15%	0.214%
24	7.669	789	796	804	rVV	420850	697616	21.52%	2.138%
25	7.846	820	826	833	rBV	65848	116177	3.58%	0.356%
26	7.916	833	838	843	rBV2	60050	111845	3.45%	0.343%
27	7.981	843	849	855	rVB	364449	578823	17.86%	1.774%
28	8.369	905	915	921	rVV	108562	194627	6.00%	0.596%
29	8.428	921	925	929	rVV3	20511	42923	1.32%	0.132%
30	8.475	929	933	944	rVB	40341	67510	2.08%	0.207%
31	8.804	983	989	998	rBV	136380	233646	7.21%	0.716%
32	8.899	998	1005	1009	rVV2	54942	93750	2.89%	0.287%
33	8.940	1009	1012	1020	rVB5	25121	44443	1.37%	0.136%
34	9.222	1051	1060	1075	rVV10	14730	50231	1.55%	0.154%
35	9.516	1104	1110	1120	rVB2	123581	213214	6.58%	0.653%
36	9.693	1132	1140	1146	rBV5	15494	33690	1.04%	0.103%

LSC Area Percent Report

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Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

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-BP100724.MA.M
Title : SVOA CALIBRATION

37	10.057	1190	1202	1218	rBV3	202953	498808	15.39%	1.529%
38	10.287	1235	1241	1247	rBV	17730	30936	0.95%	0.095%
39	10.422	1256	1264	1270	rBV	555627	973191	30.03%	2.982%
40	10.798	1321	1328	1333	rBV6	11939	30234	0.93%	0.093%
41	10.875	1333	1341	1348	rVV3	83178	157639	4.86%	0.483%
42	10.951	1348	1354	1360	rVB9	10986	26391	0.81%	0.081%
43	11.146	1381	1387	1394	rVB3	14600	34183	1.05%	0.105%
44	11.228	1394	1401	1410	rVB5	24500	54791	1.69%	0.168%
45	12.375	1590	1596	1601	rVB	32504	53877	1.66%	0.165%
46	12.475	1607	1613	1616	rBV2	22192	36117	1.11%	0.111%
47	13.028	1700	1707	1712	rBV6	13425	23965	0.74%	0.073%
48	13.151	1722	1728	1732	rVV3	27876	44833	1.38%	0.137%
49	13.592	1797	1803	1808	rVB2	106300	154144	4.76%	0.472%
50	13.681	1810	1818	1823	rBV	366356	592196	18.27%	1.815%
51	13.716	1823	1824	1830	rVV	83698	69500	2.14%	0.213%
52	13.969	1855	1867	1877	rBV	359968	737328	22.75%	2.259%
53	14.122	1886	1893	1899	rBV6	21702	42687	1.32%	0.131%
54	14.234	1906	1912	1914	rBV	61072	93707	2.89%	0.287%
55	14.275	1914	1919	1926	rVV	960146	1454762	44.88%	4.458%
56	14.345	1926	1931	1935	rVV4	24892	45161	1.39%	0.138%
57	14.510	1951	1959	1971	rBV2	107615	294507	9.09%	0.902%
58	15.098	2054	2059	2065	rBV5	10607	24928	0.77%	0.076%
59	15.198	2070	2076	2083	rVB10	14511	31451	0.97%	0.096%
60	15.275	2083	2089	2096	rBV	604098	860863	26.56%	2.638%
61	15.428	2106	2115	2121	rBV	120385	208057	6.42%	0.638%
62	15.545	2131	2135	2141	rVB5	21341	40500	1.25%	0.124%
63	15.657	2148	2154	2161	rVB	83693	133496	4.12%	0.409%
64	15.875	2188	2191	2197	rVB8	16714	23602	0.73%	0.072%
65	15.957	2200	2205	2211	rVB	144674	186654	5.76%	0.572%
66	16.034	2213	2218	2222	rBV7	14838	28013	0.86%	0.086%
67	16.175	2235	2242	2246	rBV10	12242	30306	0.94%	0.093%
68	16.481	2291	2294	2300	rBV7	15466	26215	0.81%	0.080%
69	16.728	2332	2336	2340	rBV2	24657	39204	1.21%	0.120%
70	16.769	2340	2343	2347	rVB5	18579	25589	0.79%	0.078%
71	16.898	2362	2365	2370	rVB2	22756	31549	0.97%	0.097%
72	16.986	2376	2380	2389	rVB5	40789	58677	1.81%	0.180%
73	17.081	2389	2396	2401	rBV	1280106	1939466	59.84%	5.943%
74	17.128	2401	2404	2409	rVB	306979	455126	14.04%	1.395%
75	17.186	2409	2414	2419	rBV2	638342	901346	27.81%	2.762%
76	17.504	2460	2468	2472	rBV2	41208	89745	2.77%	0.275%

LSC Area Percent Report

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Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

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-BP100724.MA.M
Title : SVOA CALIBRATION

77	17.686	2494	2499	2507	rVB5	34697	85796	2.65%	0.263%
78	17.898	2530	2535	2540	rBV6	33105	58050	1.79%	0.178%
79	18.022	2547	2556	2566	rBV2	358505	751040	23.17%	2.301%
80	18.192	2580	2585	2589	rBV3	131939	218655	6.75%	0.670%
81	18.292	2599	2602	2605	rBV3	37719	52160	1.61%	0.160%
82	18.510	2631	2639	2643	rBV2	66769	152037	4.69%	0.466%
83	18.557	2643	2647	2651	rVB	77005	117792	3.63%	0.361%
84	18.945	2711	2713	2717	rVB2	38589	44134	1.36%	0.135%
85	18.986	2717	2720	2725	rBV6	43625	53829	1.66%	0.165%
86	19.222	2754	2760	2765	rBV	1054272	1525520	47.07%	4.675%
87	19.357	2779	2783	2789	rVB4	154924	237031	7.31%	0.726%
88	19.563	2813	2818	2821	rBV	700069	1092075	33.69%	3.347%
89	19.598	2821	2824	2828	rVB	565738	737678	22.76%	2.261%
90	20.110	2909	2911	2915	rVB	120586	140765	4.34%	0.431%
91	20.151	2915	2918	2921	rBV	92580	89833	2.77%	0.275%
92	21.186	3090	3094	3100	rVB2	451939	656221	20.25%	2.011%
93	21.433	3132	3136	3140	rVB	238602	327241	10.10%	1.003%
94	21.516	3142	3150	3154	rVV2	1657028	3241232	100.00%	9.932%
95	21.563	3155	3158	3171	rVB	562908	910251	28.08%	2.789%
96	22.374	3293	3296	3299	rBV2	155894	221606	6.84%	0.679%
97	23.751	3523	3530	3536	rBV	450560	1213659	37.44%	3.719%
98	23.927	3556	3560	3566	rVB2	291339	544743	16.81%	1.669%
99	23.992	3568	3571	3581	rVB4	370128	824387	25.43%	2.526%
100	24.774	3697	3704	3716	rVB	896276	2176643	67.15%	6.670%

Sum of corrected areas: 32632981

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
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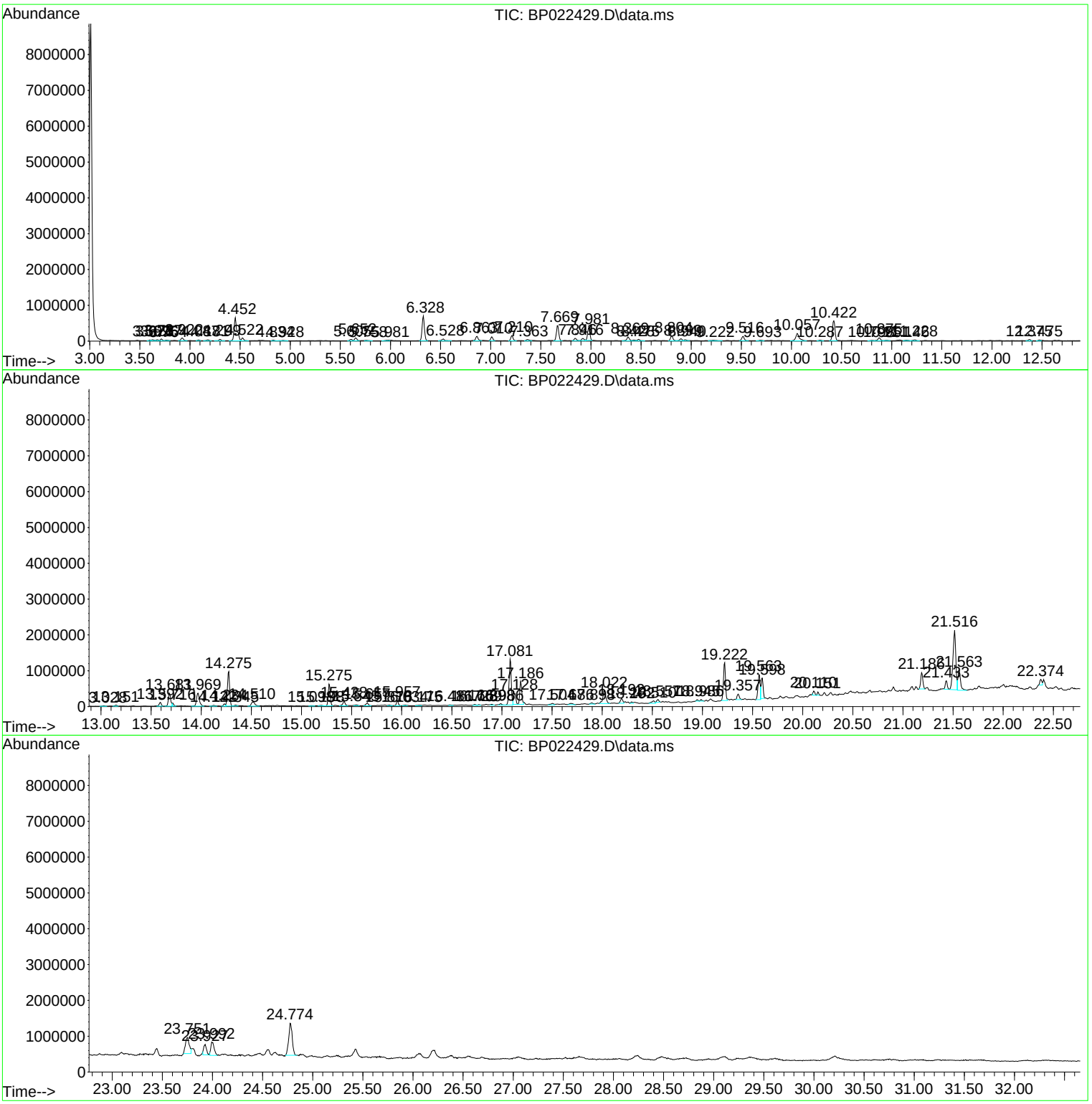
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

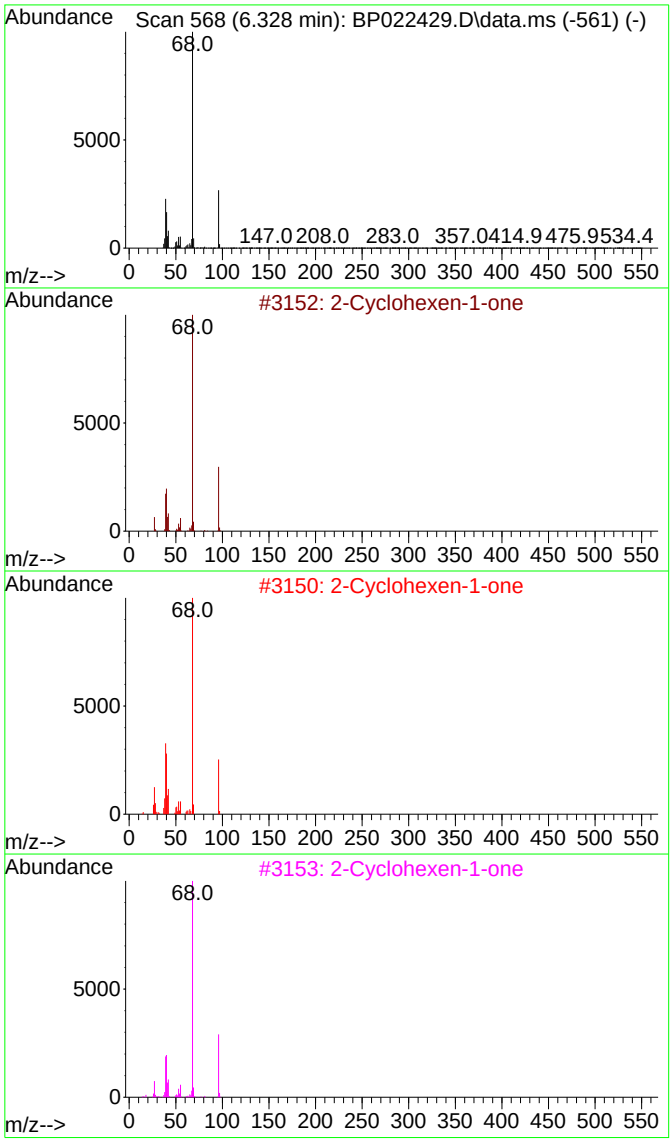
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

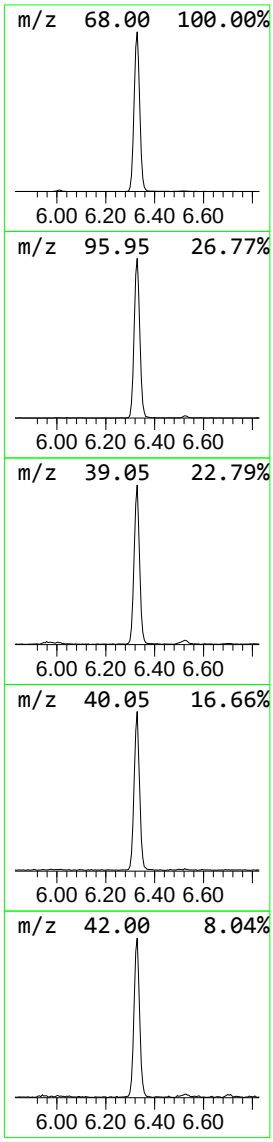
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Cyclohexen-1-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.328	31.52 ng/ul	1099480	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	58
5	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

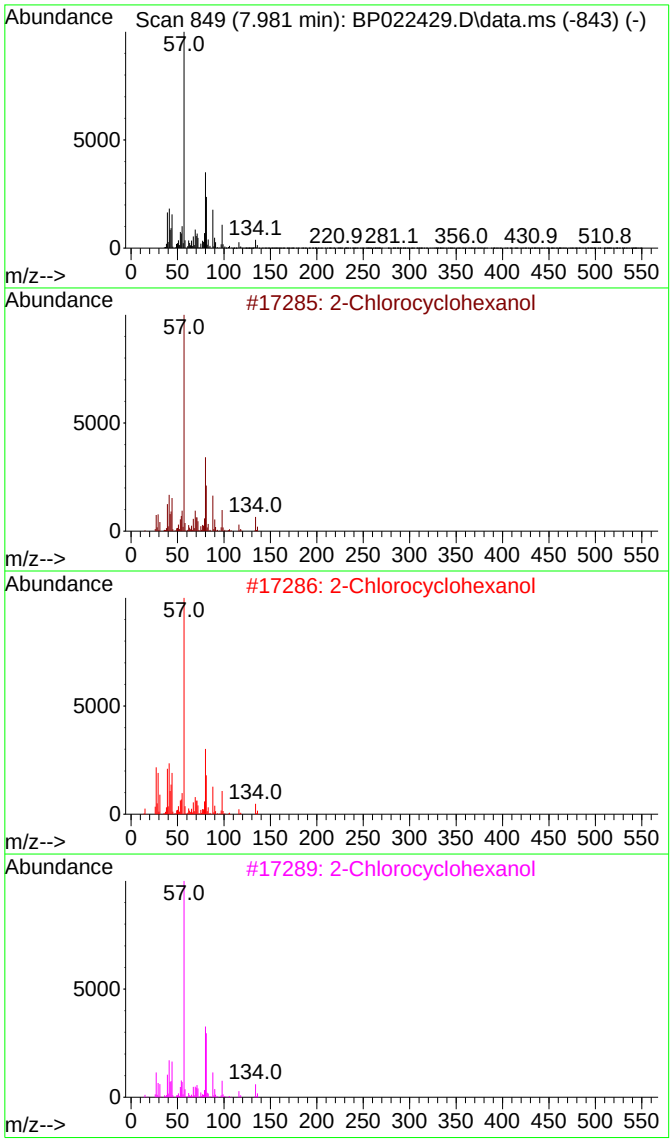
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

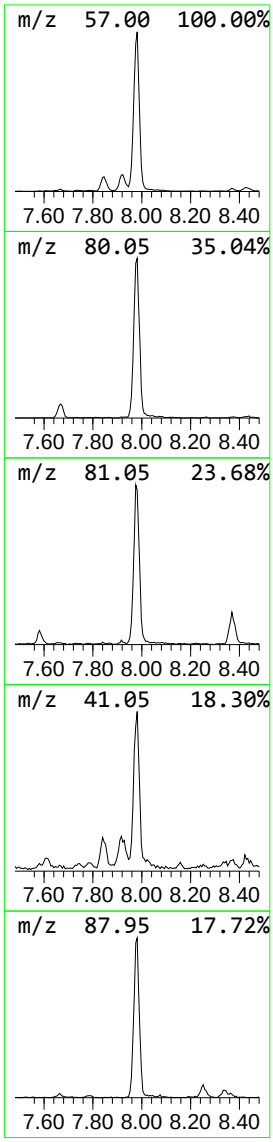
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.981	16.59 ng/ul	578823	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	93
2	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	91
3	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	83
4	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	83
5	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
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Sample : P4284-18
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

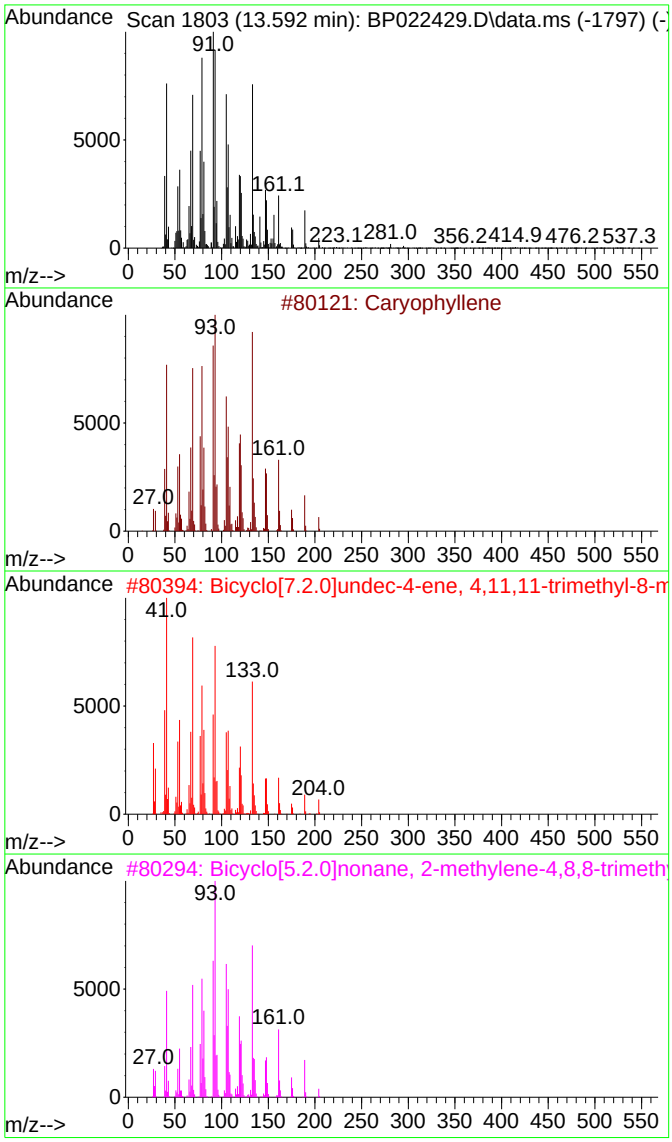
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

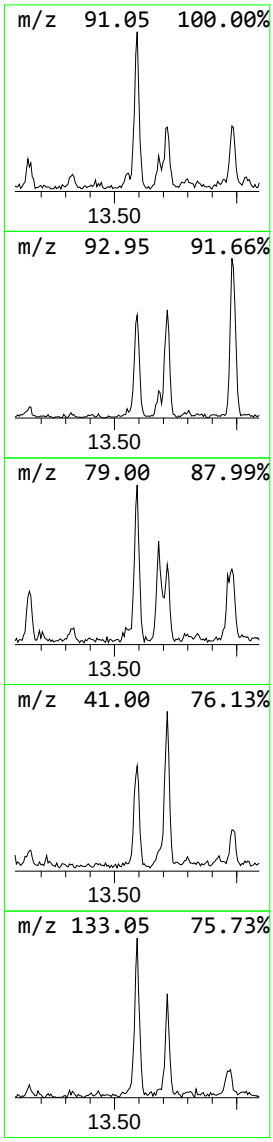
****

Peak Number 13 Caryophyllene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	2.12 ng/ul	154144	Acenaphthene-d10	14.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	97
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	97
3	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	90
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	81
5	Caryophyllene	204	C15H24	000087-44-5	74





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Sample : P4284-18
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

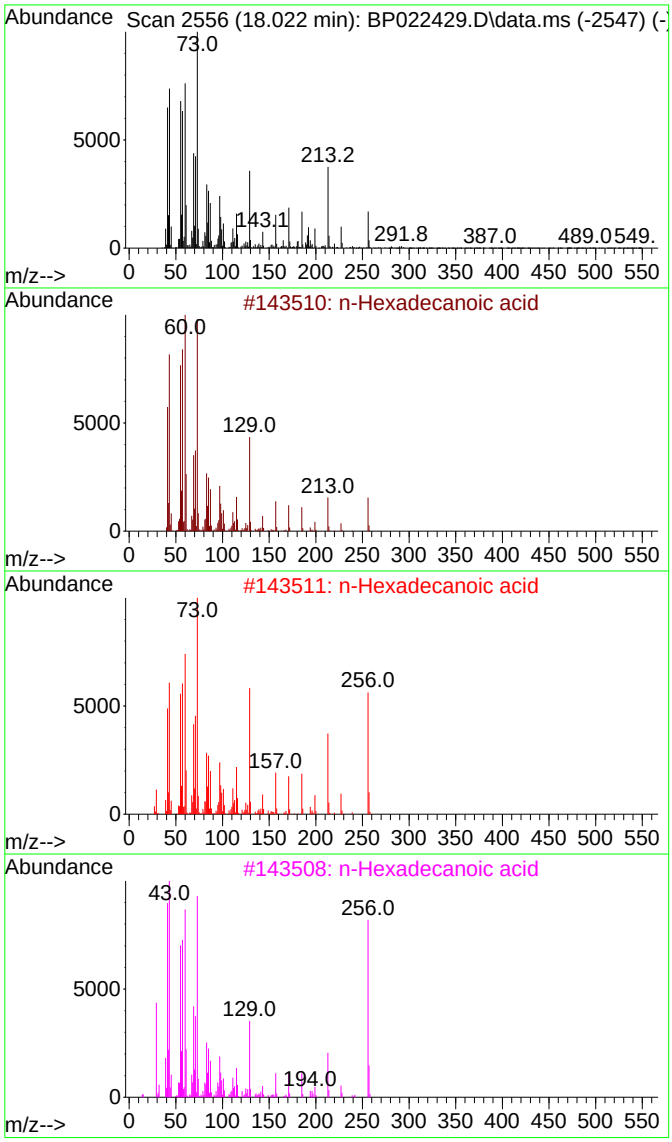
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

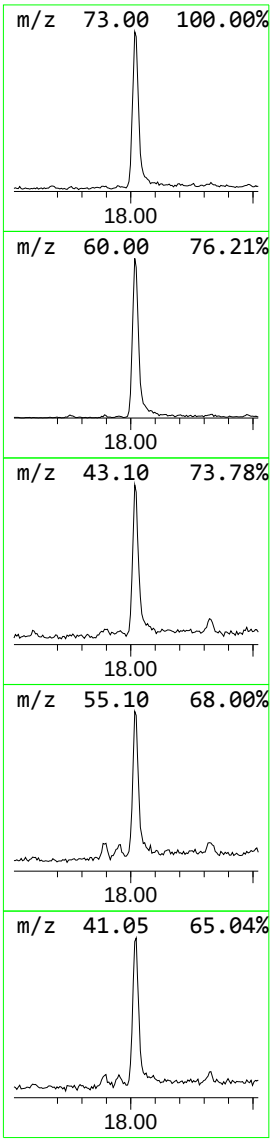
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	7.74 ng/ul	751040	Phenanthrene-d10	17.081

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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

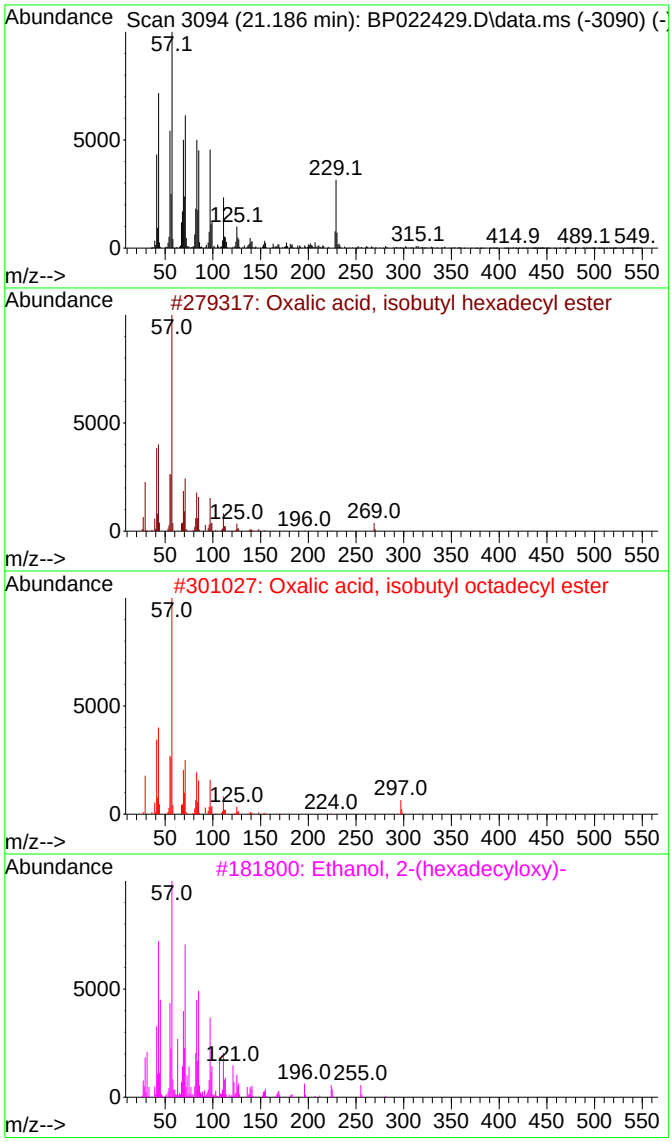
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

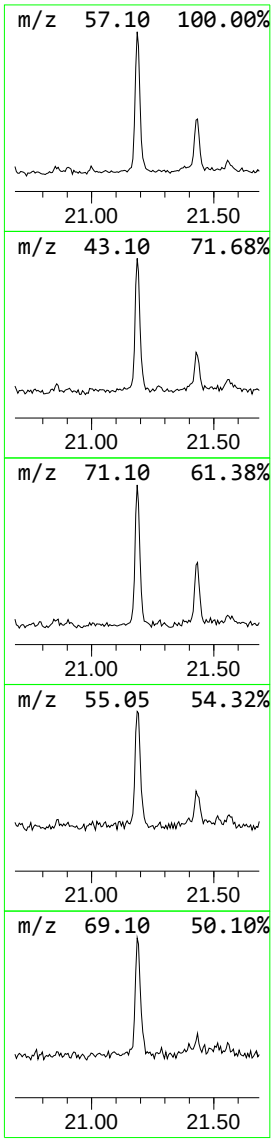
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Oxalic acid, isobutyl hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	4.05 ng/ul	656221	Chrysene-d12	21.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	90
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
3	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	76





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Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

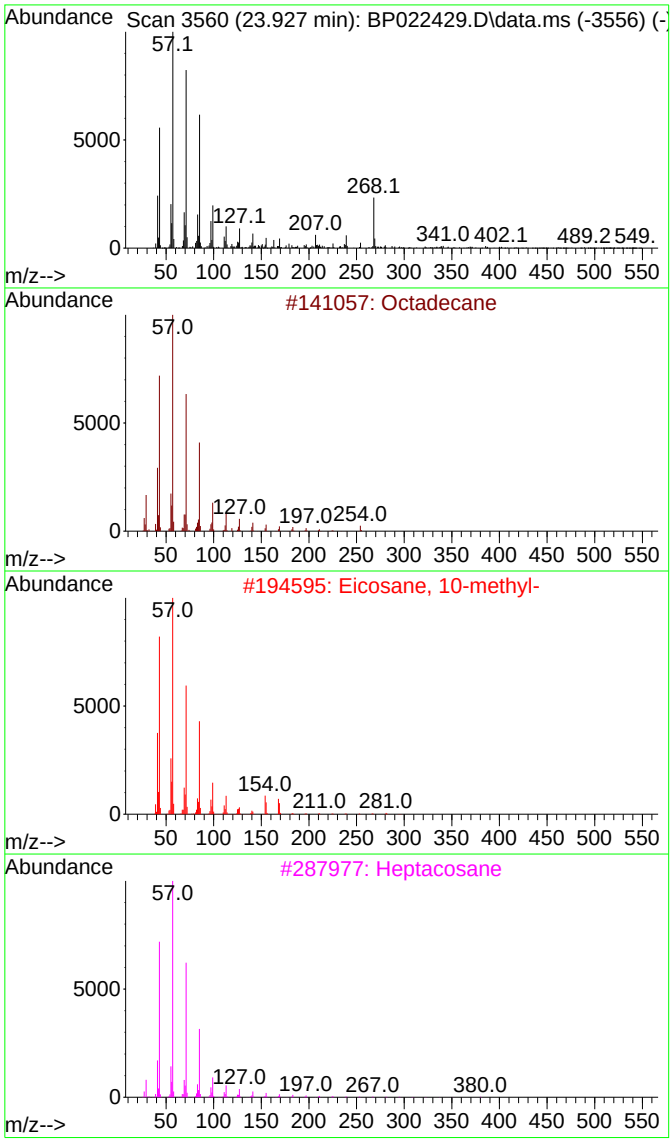
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

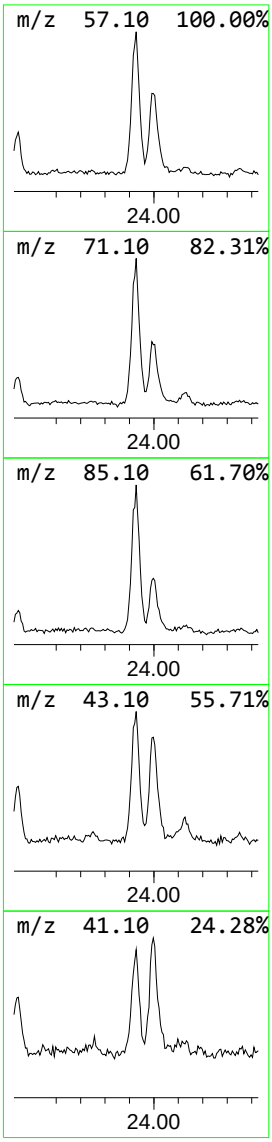
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.927	5.01 ng/ul	544743	Perylene-d12	24.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Octadecane	254	C18H38	000593-45-3	83
5	Docosane	310	C22H46	000629-97-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

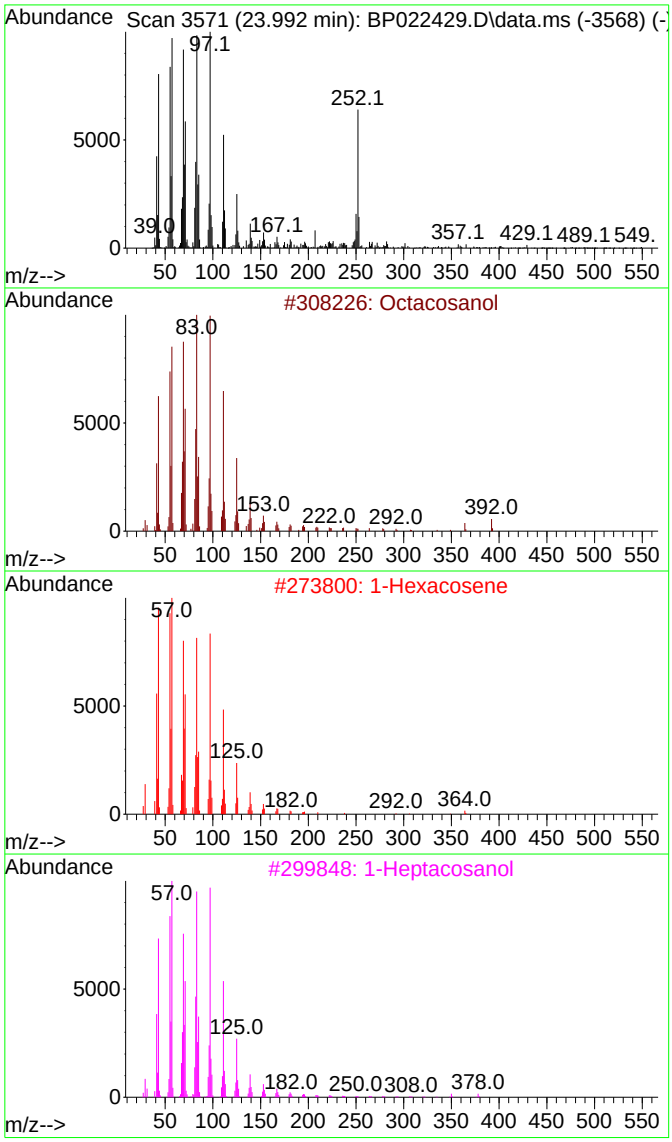
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

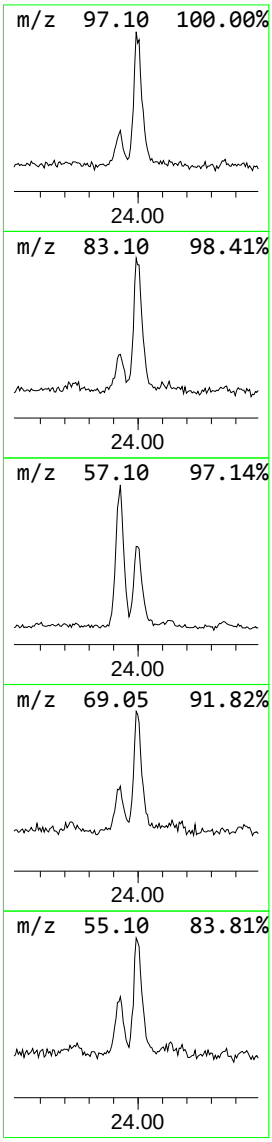
****

Peak Number 18 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.992	7.57 ng/ul	824387	Perylene-d12	24.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	93
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022429.D
Acq On : 17 Oct 2024 01:15
Operator : RC/JU
Sample : P4284-18
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EZ3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.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
2-Cyclohexen-1-one	6.328	31.5	ng/ul	1099480	1	7.669	697616	20.0
2-Chlorocyclohe...	7.981	16.6	ng/ul	578823	1	7.669	697616	20.0
Caryophyllene	13.592	2.1	ng/ul	154144	3	14.275	1454760	20.0
n-Hexadecanoic ...	18.022	7.7	ng/ul	751040	4	17.081	1939470	20.0
Oxalic acid, is...	21.186	4.0	ng/ul	656221	5	21.516	3241230	20.0
(DEL) Alkane: S...	23.927	5.0	ng/ul	544743	6	24.774	2176640	20.0
Octacosanol	23.992	7.6	ng/ul	824387	6	24.774	2176640	20.0