LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

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-BP030723.M
Title : SVOA CALIBRATION

Signal : TIC: BP014002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	39	42	50	rVB	17696	26833	0.93%	0.087%
2	3.722	88	91	101	rBV	13092	24529	0.85%	0.080%
3	3.881	114	118	121	rVB3	4487	5710	0.20%	0.019%
4	3.975	130	134	140	rVB	18700	26224	0.91%	0.085%
5	4.099	150	155	162	rVB	21936	36732	1.27%	0.120%
6	4.205	169	173	180	rVB2	10481	16138	0.56%	0.053%
7	4.305	186	190	196	rVB6	10031	15223	0.53%	0.050%
8	4.428	207	211	215	rBV6	5267	7186	0.25%	0.023%
9	4.587	232	238	243	rVB9	4419	8010	0.28%	0.026%
10	4.769	266	269	276	rVB9	4615	7640	0.27%	0.025%
11	5.140	326	332	339	rBV	35573	59551	2.07%	0.194%
12	5.252	345	351	354	rBV7	3463	6697	0.23%	0.022%
13	6.058	482	488	493	rVB9	2949	6852	0.24%	0.022%
14	6.446	548	554	561	rVB2	9702	17768	0.62%	0.058%
15	6.746	598	605	611	rVB2	40332	64206	2.23%	0.209%
16	7.228	682	687	703	rVB	276152	479416	16.63%	1.563%
17	7.399	710	716	726	rBV	218530	349709	12.13%	1.140%
18	7.511	731	735	744	rVB	4072	9188	0.32%	0.030%
19	7.605	744	751	761	rBV	290237	474907	16.48%	1.548%
20	7.899	795	801	804	rBV7	3021	4133	0.14%	0.013%
21	8.081	822	832	841	rBV	472211	766025	26.58%	2.497%
22	8.293	865	868	874	rVB7	3424	5240	0.18%	0.017%
23	8.787	945	952	963	rBV	274615	465676	16.16%	1.518%
24	8.916	968	974	980	rVB	34699	58369	2.03%	0.190%
25	9.252	1023	1031	1044	rBV	278835	470579	16.33%	1.534%
26	9.640	1091	1097	1103	rVB2	10300	16247	0.56%	0.053%
27	9.981	1145	1155	1170	rBV	245679	424493	14.73%	1.384%
28	10.346	1211	1217	1221	rVB8	3289	6389	0.22%	0.021%
29	10.522	1240	1247	1263	rBV	344390	621152	21.55%	2.025%
30	10.904	1300	1312	1320	rBV	638084	1061682	36.84%	3.461%
31	11.046	1329	1336	1355	rBV	218847	447974	15.54%	1.460%
32	11.369	1386	1391	1399	rVB5	6608	14041	0.49%	0.046%
33	11.451	1399	1405	1411	rBV5	3885	11173	0.39%	0.036%
34	12.134	1517	1521	1526	rVB7	3155	5586	0.19%	0.018%
35	12.293	1545	1548	1557	rVB7	3986	7827	0.27%	0.026%
36	12.487	1574	1581	1588	rVB4	7566	12458	0.43%	0.041%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

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-BP030723.M
Title : SVOA CALIBRATION

37	13.087	1676	1683	1689	rVV10	5162	10424	0.36%	0.034%
38	13.457	1744	1746	1752	rVB5	3058	4661	0.16%	0.015%
39	13.528	1752	1758	1764	rVV5	9490	15379	0.53%	0.050%
40	13.593	1764	1769	1775	rVB5	9578	16988	0.59%	0.055%
41	13.687	1777	1785	1793	rVB5	3348	10737	0.37%	0.035%
42	13.916	1818	1824	1829	rBV9	3871	7624	0.26%	0.025%
43	14.040	1839	1845	1851	rBV2	116348	171211	5.94%	0.558%
44	14.122	1851	1859	1873	rVV	769592	1102109	38.24%	3.593%
45	14.263	1874	1883	1888	rVB6	23046	40837	1.42%	0.133%
46	14.351	1894	1898	1902	rBV6	3020	4583	0.16%	0.015%
47	14.416	1902	1909	1916	rVV	774903	1169604	40.58%	3.813%
48	14.475	1916	1919	1926	rVV8	10856	18441	0.64%	0.060%
49	14.551	1926	1932	1935	rVV7	5136	9097	0.32%	0.030%
50	14.592	1935	1939	1944	rVV7	6320	10995	0.38%	0.036%
51	14.669	1947	1952	1955	rVV2	20480	32010	1.11%	0.104%
52	14.716	1955	1960	1968	rVV	1063378	1615199	56.04%	5.265%
53	14.787	1968	1972	1979	rVB9	15058	31844	1.10%	0.104%
54	14.910	1987	1993	2004	rBV	198104	436908	15.16%	1.424%
55	15.087	2018	2023	2026	rBV7	6869	13416	0.47%	0.044%
56	15.128	2026	2030	2040	rVV9	14993	27877	0.97%	0.091%
57	15.204	2040	2043	2047	rVB6	3539	4439	0.15%	0.014%
58	15.387	2068	2074	2079	rVB9	3383	8610	0.30%	0.028%
59	15.539	2097	2100	2105	rVB6	3506	7125	0.25%	0.023%
60	15.598	2105	2110	2117	rBV6	6157	11795	0.41%	0.038%
61	15.710	2122	2129	2136	rBV	1108793	1587436	55.08%	5.175%
62	15.828	2143	2149	2162	rBV	317467	479849	16.65%	1.564%
63	15.951	2167	2170	2175	rVB6	6979	10303	0.36%	0.034%
64	16.039	2181	2185	2186	rBV4	7507	8419	0.29%	0.027%
65	16.075	2186	2191	2196	rVV	64412	96789	3.36%	0.316%
66	16.122	2197	2199	2204	rVB6	5372	6144	0.21%	0.020%
67	16.187	2204	2210	2216	rBV4	24415	37631	1.31%	0.123%
68	16.281	2223	2226	2231	rBV7	4466	6934	0.24%	0.023%
69	16.410	2244	2248	2249	rBV4	6440	7686	0.27%	0.025%
70	16.563	2270	2274	2280	rBV9	4251	6645	0.23%	0.022%
71	16.716	2296	2300	2304	rBV7	5621	7914	0.27%	0.026%
72	17.004	2344	2349	2355	rBV2	19554	27199	0.94%	0.089%
73	17.263	2390	2393	2401	rVB7	5707	11531	0.40%	0.038%
74	17.351	2403	2408	2414	rBV6	19350	36065	1.25%	0.118%
75	17.422	2418	2420	2423	rBV4	4035	6282	0.22%	0.020%
76	17.475	2423	2429	2434	rBV	1504474	2135406	74.09%	6.961%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

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-BP030723.M
Title : SVOA CALIBRATION

77	17.575	2439	2446	2455	rVV	1149263	1674265	58.09%	5.458%
78	17.651	2455	2459	2469	rVB7	18855	44478	1.54%	0.145%
79	17.739	2472	2474	2480	rVB6	4125	6399	0.22%	0.021%
80	17.822	2486	2488	2490	rBV3	4349	4743	0.16%	0.015%
81	18.216	2553	2555	2562	rVB7	10098	18470	0.64%	0.060%
82	18.275	2563	2565	2567	rBV3	5745	6633	0.23%	0.022%
83	18.328	2570	2574	2586	rBV	217126	357091	12.39%	1.164%
84	18.633	2620	2626	2631	rBV10	8633	24271	0.84%	0.079%
85	18.733	2639	2643	2647	rVB4	36301	43153	1.50%	0.141%
86	19.157	2712	2715	2716	rBV3	10565	8882	0.31%	0.029%
87	19.216	2722	2725	2732	rVB8	16097	23923	0.83%	0.078%
88	19.369	2749	2751	2757	rVB4	29911	41521	1.44%	0.135%
89	19.439	2757	2763	2765	rBV3	42544	79382	2.75%	0.259%
90	19.469	2765	2768	2775	rVB	67984	91099	3.16%	0.297%
91	19.557	2779	2783	2789	rBV3	65241	107901	3.74%	0.352%
92	19.792	2817	2823	2835	rBV	1870909	2569774	89.16%	8.377%
93	20.216	2892	2895	2899	rVB	42247	47591	1.65%	0.155%
94	20.580	2954	2957	2964	rBV	75737	96698	3.35%	0.315%
95	20.727	2980	2982	2986	rVB	50889	49652	1.72%	0.162%
96	21.080	3038	3042	3049	rBV	1196487	1272622	44.15%	4.149%
97	21.222	3062	3066	3078	rBV	359476	599260	20.79%	1.953%
98	21.551	3117	3122	3128	rBV	2124302	2882235	100.00%	9.396%
99	23.927	3519	3526	3540	rVB	1228932	2593510	89.98%	8.454%
100	24.092	3547	3554	3563	rVB2	1288468	2737280	94.97%	8.923%

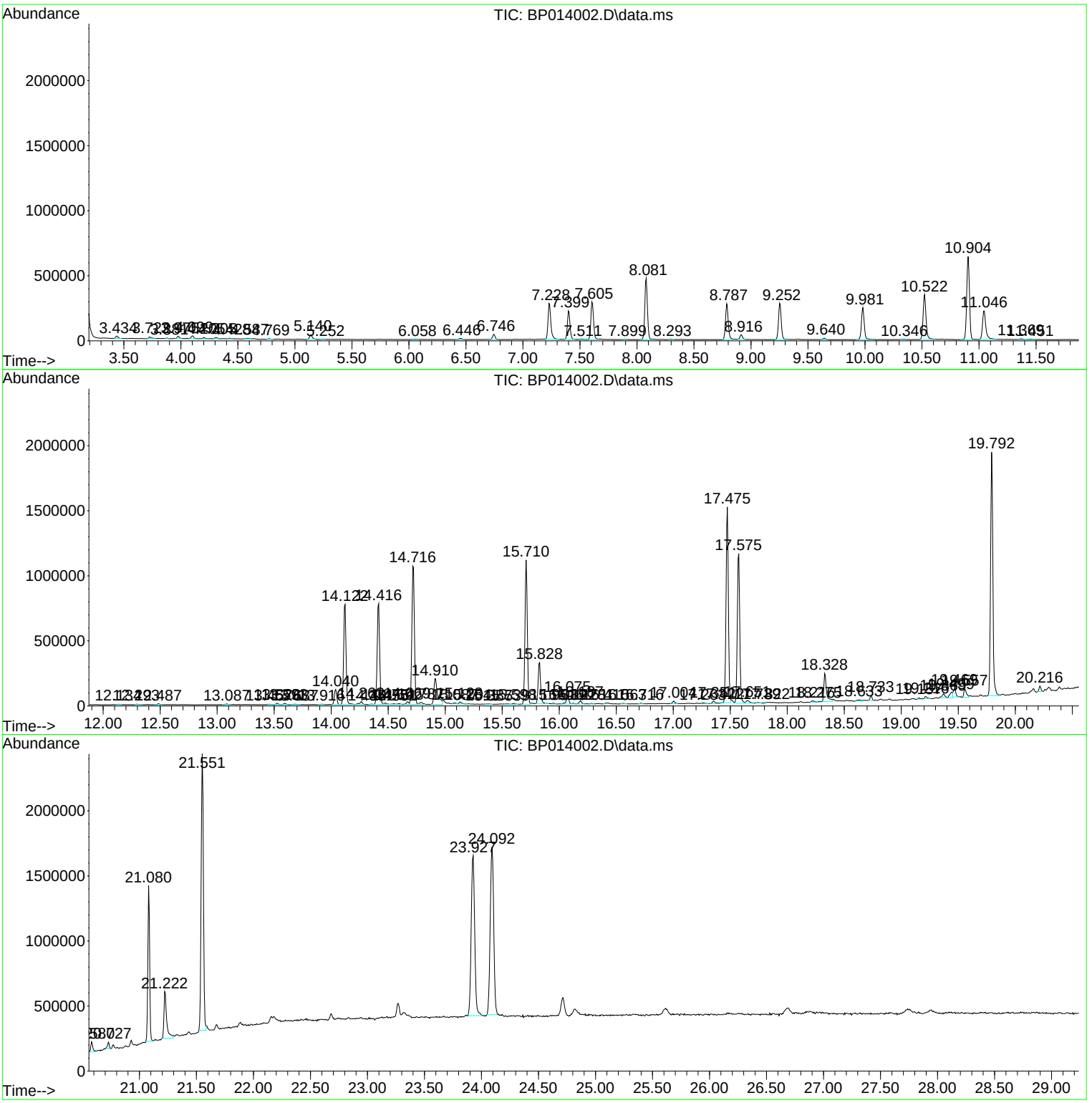
Sum of corrected areas: 30676542

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

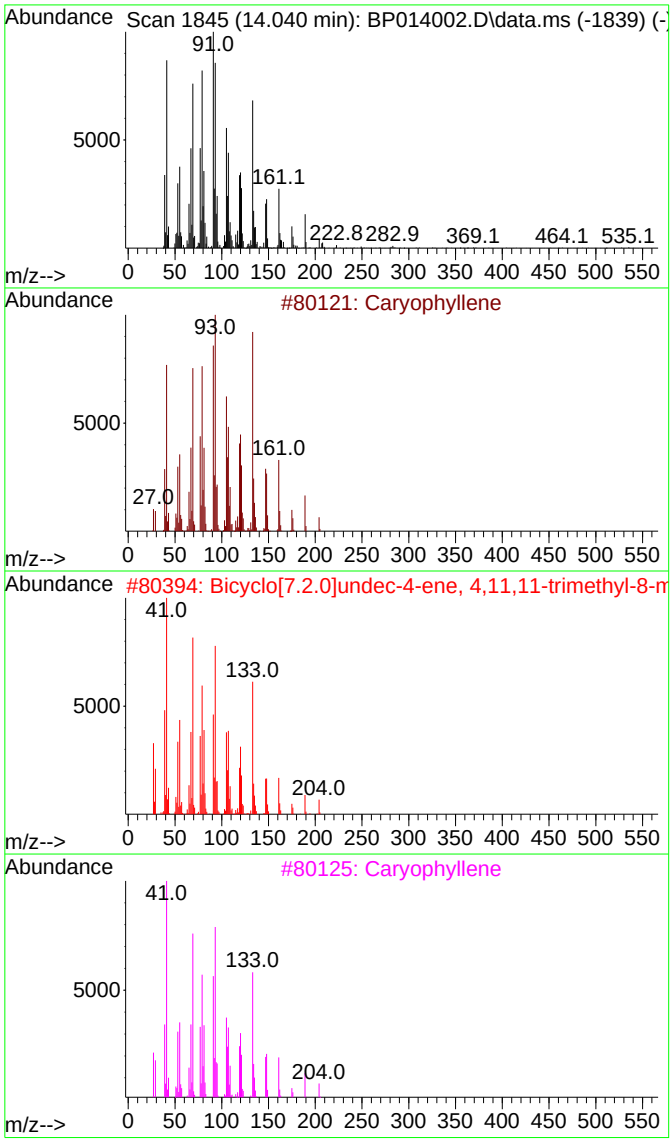
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

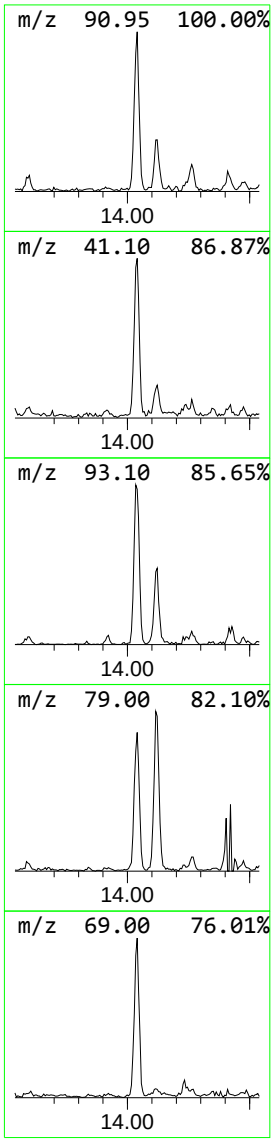
****

Peak Number 1 Caryophyllene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.040	2.12 ng/ul	171211	Acenaphthene-d10	14.716

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	91
3	Caryophyllene	204	C15H24	000087-44-5	90
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	90
5	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

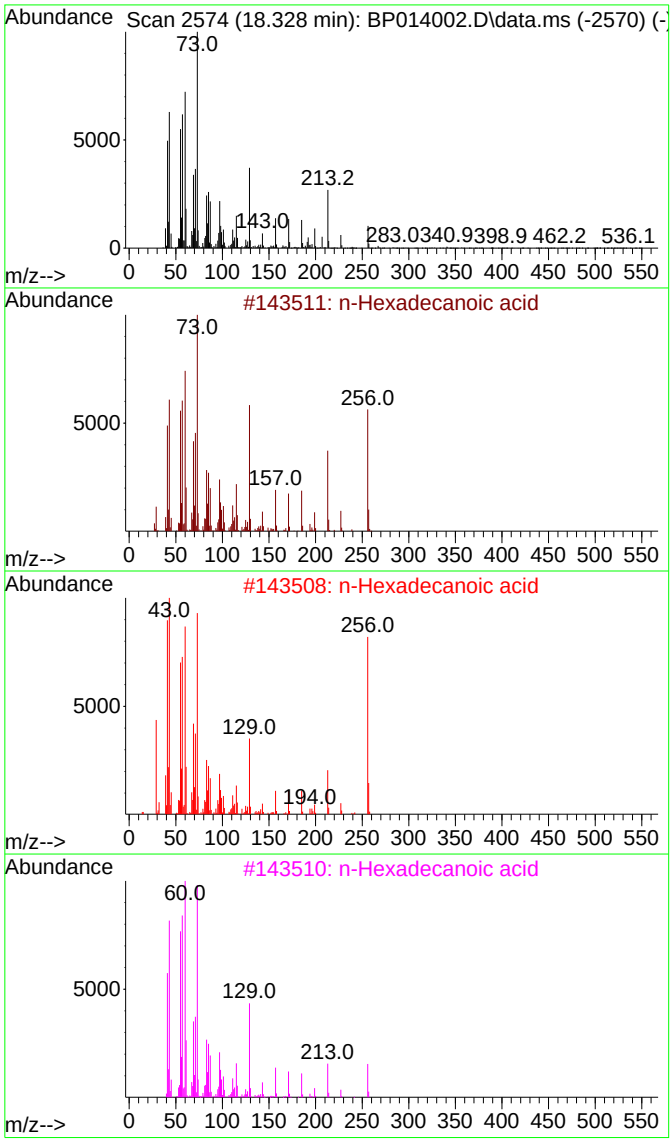
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

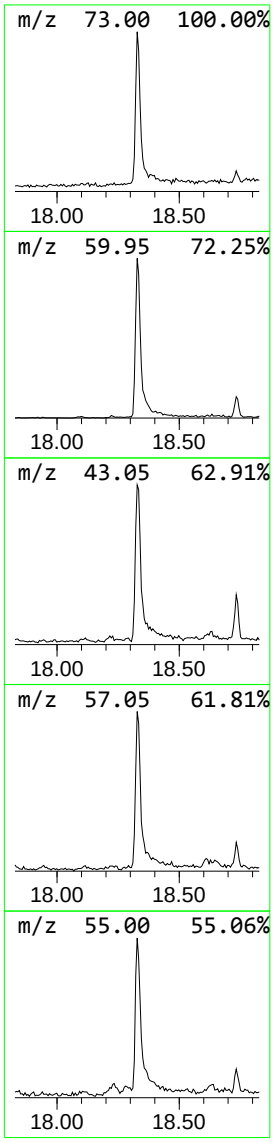
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.328	3.34 ng/ul	357091	Phenanthrene-d10	17.475

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

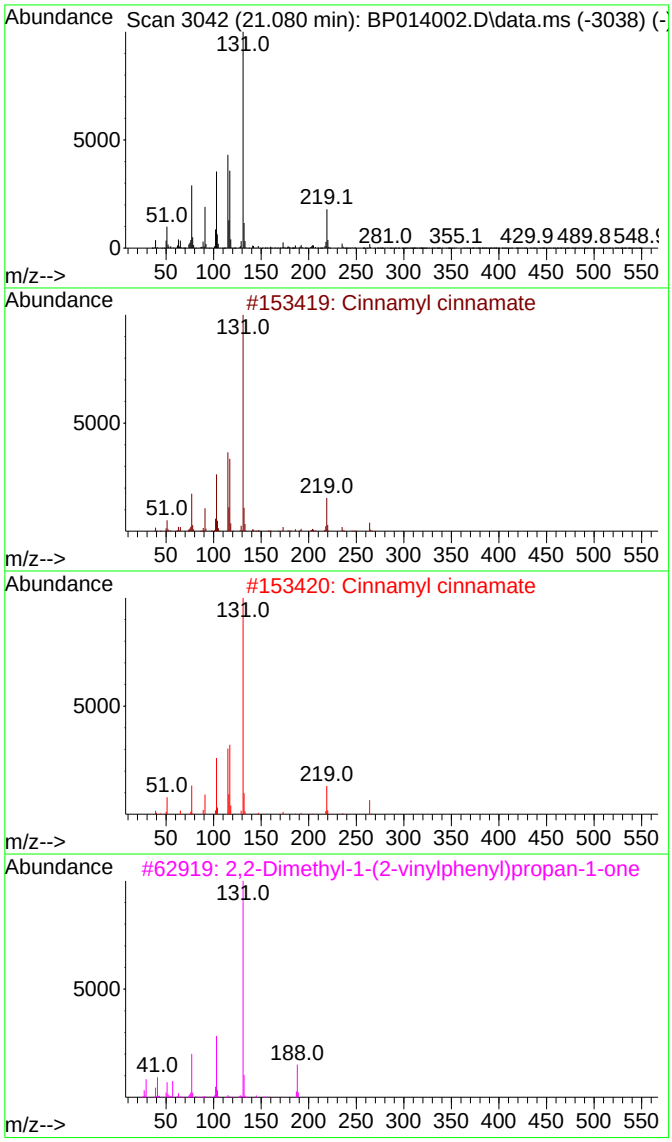
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

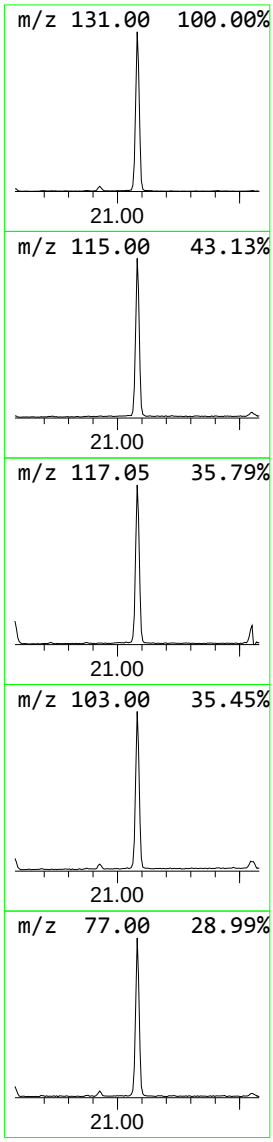
****

Peak Number 3 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	8.83 ng/ul	1272620	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	90
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
4	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47
5	1,3-Phenylene, bis(3-phenylprope...	370	C24H18O4	1000259-62-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

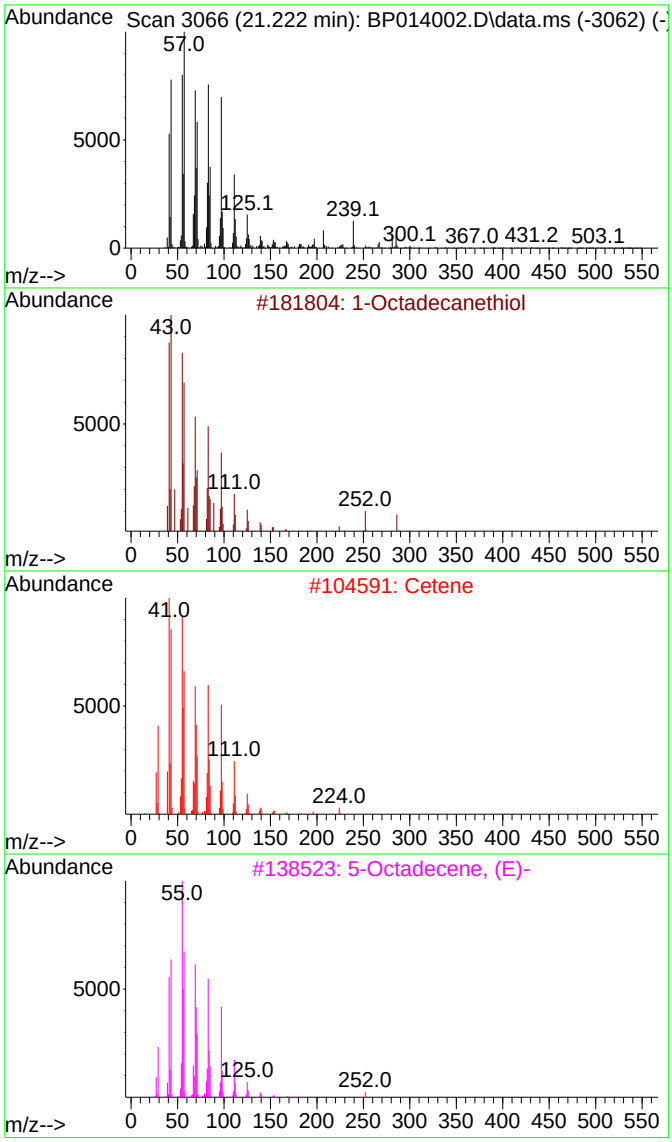
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

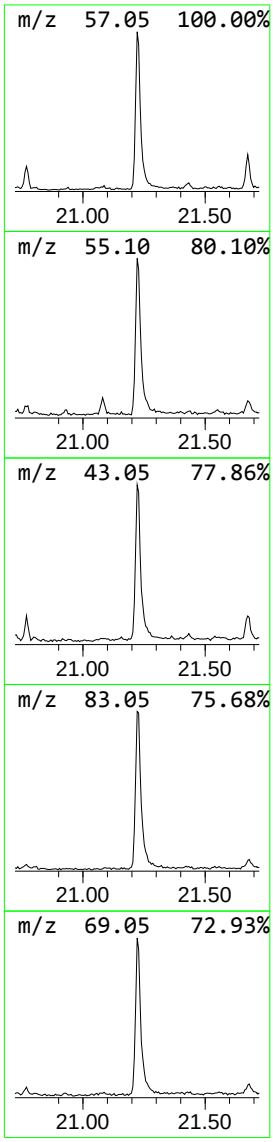
****

Peak Number 4 1-Octadecanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.222	4.16 ng/ul	599260	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9	97
2	Cetene	224	C16H32	000629-73-2	95
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP014002.D
Acq On : 09 Mar 2023 10:22
Operator : CG/JU
Sample : 01713-10
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBZZ0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.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
Caryophyllene	14.040	2.1	ng/ul	171211	3	14.716	1615200	20.0
n-Hexadecanoic ...	18.328	3.3	ng/ul	357091	4	17.475	2135410	20.0
Cinnamyl cinnamate	21.080	8.8	ng/ul	1272620	5	21.551	2882240	20.0
1-Octadecanethiol	21.222	4.2	ng/ul	599260	5	21.551	2882240	20.0