LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A4EW3

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: BP022423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.475	78	83	90	rVB2	11894	20477	0.81%	0.099%
2	3.599	100	104	106	rBV2	16937	22602	0.90%	0.109%
3	3.622	106	108	114	rVV2	21591	33625	1.34%	0.162%
4	3.675	114	117	121	rVV3	17405	20158	0.80%	0.097%
5	3.711	121	123	128	rVB	18774	23512	0.94%	0.114%
6	3.764	128	132	139	rBV3	13095	21637	0.86%	0.104%
7	3.846	142	146	151	rVB6	8187	14405	0.57%	0.070%
8	3.916	151	158	168	rBV2	69921	126893	5.05%	0.613%
9	3.999	168	172	182	rVB8	6976	12880	0.51%	0.062%
10	4.087	182	187	194	rBV	19866	31984	1.27%	0.154%
11	4.158	194	199	201	rBV	27426	45407	1.81%	0.219%
12	4.299	218	223	230	rBV	35280	51598	2.05%	0.249%
13	4.452	240	249	258	rBV2	600476	1173096	46.66%	5.666%
14	4.522	258	261	265	rVV	68973	99659	3.96%	0.481%
15	4.552	265	266	271	rVB	20329	22263	0.89%	0.108%
16	4.693	284	290	292	rBV3	9781	15168	0.60%	0.073%
17	4.828	308	313	320	rVB	16781	24923	0.99%	0.120%
18	4.928	320	330	334	rBV10	5219	12931	0.51%	0.062%
19	5.605	439	445	449	rBV3	38126	66832	2.66%	0.323%
20	5.652	449	453	459	rVB	70644	111755	4.45%	0.540%
21	5.758	467	471	475	rVB3	11858	16480	0.66%	0.080%
22	5.975	497	508	511	rBV6	15878	43759	1.74%	0.211%
23	6.005	511	513	518	rVB3	11280	15127	0.60%	0.073%
24	6.322	560	567	578	rBV	642084	1003950	39.93%	4.849%
25	6.522	593	601	609	rBV5	42497	82691	3.29%	0.399%
26	6.857	653	658	666	rVV	72422	120312	4.79%	0.581%
27	6.922	666	669	677	rVB7	8919	16804	0.67%	0.081%
28	7.010	678	684	691	rVB	61097	98470	3.92%	0.476%
29	7.210	710	718	725	rBV	87671	149246	5.94%	0.721%
30	7.363	739	744	751	rBV3	28674	57490	2.29%	0.278%
31	7.422	752	754	762	rVB9	8206	14030	0.56%	0.068%
32	7.669	789	796	804	rVB	372145	595399	23.68%	2.876%
33	7.840	820	825	832	rBV	54179	89792	3.57%	0.434%
34	7.922	832	839	843	rVV2	57677	105576	4.20%	0.510%
35	7.981	843	849	863	rVB	322637	561787	22.35%	2.713%
36	8.375	905	916	921	rBV2	46484	89954	3.58%	0.434%

LSC Area Percent Report

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Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

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	8.428	921	925	930	rVV5	15815	33622	1.34%	0.162%
38	8.481	930	934	945	rVB	21094	36771	1.46%	0.178%
39	8.640	956	961	965	rBV3	7500	13768	0.55%	0.066%
40	8.804	983	989	1000	rBV	77344	139322	5.54%	0.673%
41	8.899	1000	1005	1009	rVV2	47426	77598	3.09%	0.375%
42	8.940	1009	1012	1019	rVB4	20583	34873	1.39%	0.168%
43	9.222	1051	1060	1069	rBV9	10126	29668	1.18%	0.143%
44	9.522	1105	1111	1118	rVB	64541	111732	4.44%	0.540%
45	9.693	1135	1140	1144	rBV7	7211	13427	0.53%	0.065%
46	9.799	1154	1158	1163	rVB7	8185	13411	0.53%	0.065%
47	10.057	1193	1202	1219	rBV3	108357	324135	12.89%	1.565%
48	10.293	1233	1242	1248	rBV2	14005	26837	1.07%	0.130%
49	10.428	1256	1265	1277	rBV	480356	845449	33.63%	4.083%
50	10.810	1324	1330	1334	rBV5	8870	21459	0.85%	0.104%
51	10.881	1334	1342	1350	rVV3	66852	127712	5.08%	0.617%
52	10.957	1350	1355	1362	rVB10	6538	13760	0.55%	0.066%
53	11.069	1368	1374	1375	rBV2	10506	18783	0.75%	0.091%
54	11.093	1375	1378	1383	rVV2	14840	26136	1.04%	0.126%
55	11.151	1383	1388	1395	rVV3	13105	30235	1.20%	0.146%
56	11.234	1395	1402	1409	rVB8	19580	40047	1.59%	0.193%
57	11.340	1414	1420	1427	rBV8	8259	16136	0.64%	0.078%
58	12.310	1580	1585	1590	rBV8	6717	12845	0.51%	0.062%
59	12.375	1590	1596	1602	rVB3	28107	49739	1.98%	0.240%
60	12.481	1609	1614	1617	rBV3	17109	29606	1.18%	0.143%
61	12.669	1643	1646	1651	rVB5	9527	13554	0.54%	0.065%
62	13.681	1811	1818	1826	rBV	239991	349964	13.92%	1.690%
63	13.969	1858	1867	1880	rBV	227359	359536	14.30%	1.736%
64	14.139	1886	1896	1901	rVB	6908	14468	0.58%	0.070%
65	14.281	1912	1920	1927	rBV	822215	1319967	52.50%	6.375%
66	14.345	1927	1931	1937	rVB	10441	16022	0.64%	0.077%
67	14.510	1953	1959	1969	rBV	54488	117975	4.69%	0.570%
68	14.651	1979	1983	1985	rBV3	9918	13699	0.54%	0.066%
69	15.092	2050	2058	2065	rBV8	9244	18809	0.75%	0.091%
70	15.281	2084	2090	2097	rBV	323824	526073	20.93%	2.541%
71	15.339	2097	2100	2105	rVB3	15924	23402	0.93%	0.113%
72	15.416	2107	2113	2120	rBV	84247	117031	4.66%	0.565%
73	15.663	2147	2155	2162	rBV	43346	76235	3.03%	0.368%
74	15.810	2178	2180	2187	rVB4	11431	16632	0.66%	0.080%
75	15.963	2195	2206	2212	rBV	103989	163960	6.52%	0.792%
76	16.022	2212	2216	2223	rVB9	7200	14418	0.57%	0.070%

LSC Area Percent Report

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Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

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

77	16.763	2338	2342	2347	rVB2	22507	29904	1.19%	0.144%
78	16.886	2360	2363	2369	rVB2	8931	14460	0.58%	0.070%
79	16.957	2370	2375	2379	rBV8	8091	13577	0.54%	0.066%
80	17.075	2388	2395	2400	rBV	1302352	1804545	71.78%	8.715%
81	17.116	2400	2402	2407	rVB	202795	231885	9.22%	1.120%
82	17.175	2407	2412	2417	rBV	361060	541270	21.53%	2.614%
83	17.698	2497	2501	2508	rVB7	11320	20706	0.82%	0.100%
84	18.016	2547	2555	2564	rBV2	113935	214801	8.54%	1.037%
85	18.110	2568	2571	2577	rVB3	18913	28642	1.14%	0.138%
86	18.180	2578	2583	2587	rBV2	39993	57160	2.27%	0.276%
87	18.504	2635	2638	2643	rVB3	19146	22182	0.88%	0.107%
88	19.210	2753	2758	2765	rVB	410334	499845	19.88%	2.414%
89	19.345	2778	2781	2787	rVB5	40255	57266	2.28%	0.277%
90	19.557	2812	2817	2820	rBV	487235	681646	27.11%	3.292%
91	19.586	2820	2822	2827	rVB	208445	235294	9.36%	1.136%
92	19.851	2864	2867	2873	rVB2	25468	40455	1.61%	0.195%
93	20.216	2926	2929	2933	rBV	42171	50580	2.01%	0.244%
94	21.180	3090	3093	3102	rVB6	75010	131429	5.23%	0.635%
95	21.421	3132	3134	3138	rVB	59617	63288	2.52%	0.306%
96	21.504	3141	3148	3154	rVV2	1494616	2514034	100.00%	12.142%
97	21.551	3154	3156	3162	rVB	131021	181712	7.23%	0.878%
98	23.898	3551	3555	3564	rVB2	123646	274608	10.92%	1.326%
99	24.539	3659	3664	3671	rVB	155601	342531	13.62%	1.654%
100	24.768	3694	3703	3714	rVB2	892310	2391977	95.14%	11.552%

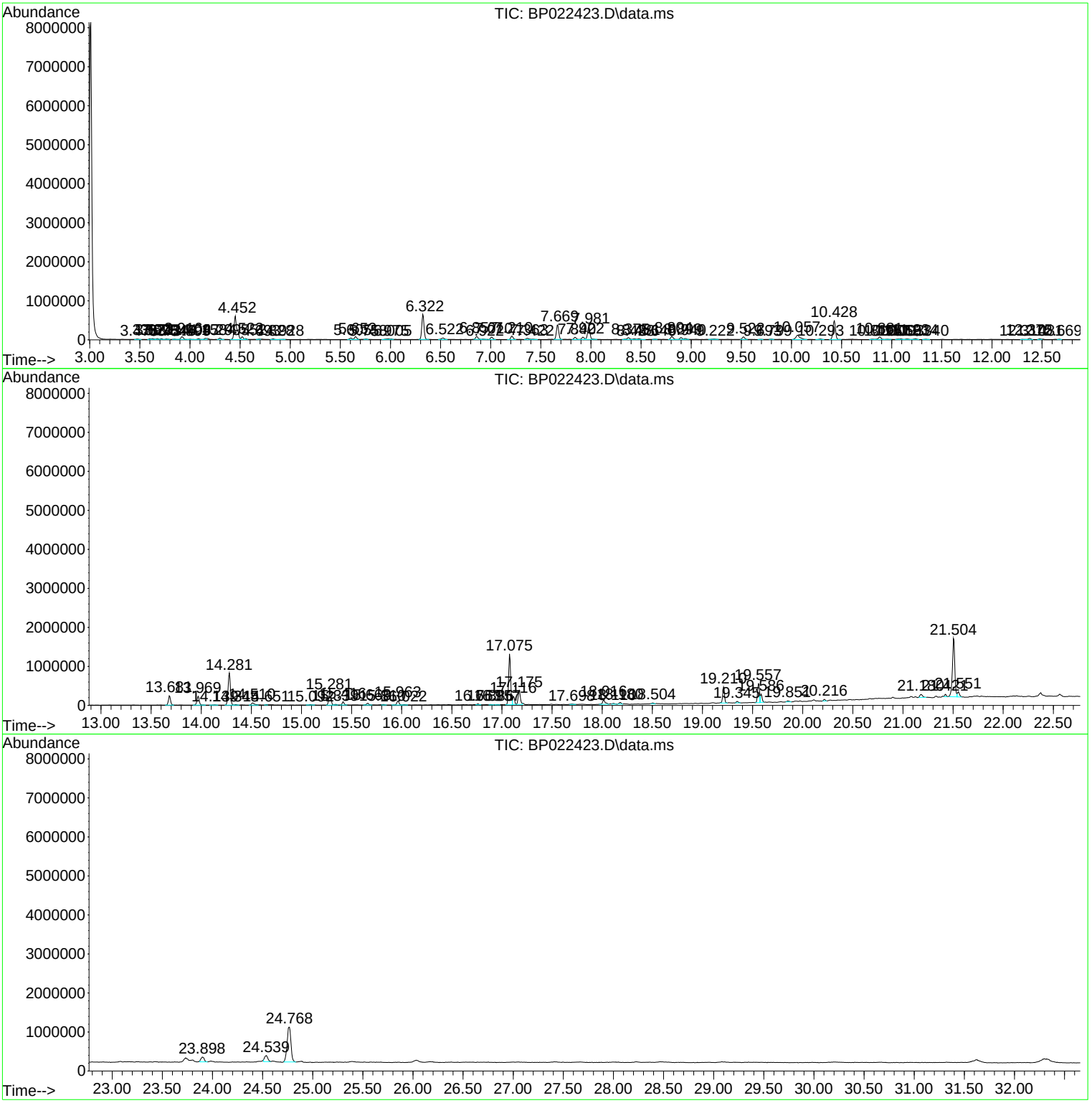
Sum of corrected areas: 20705285

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

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 : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

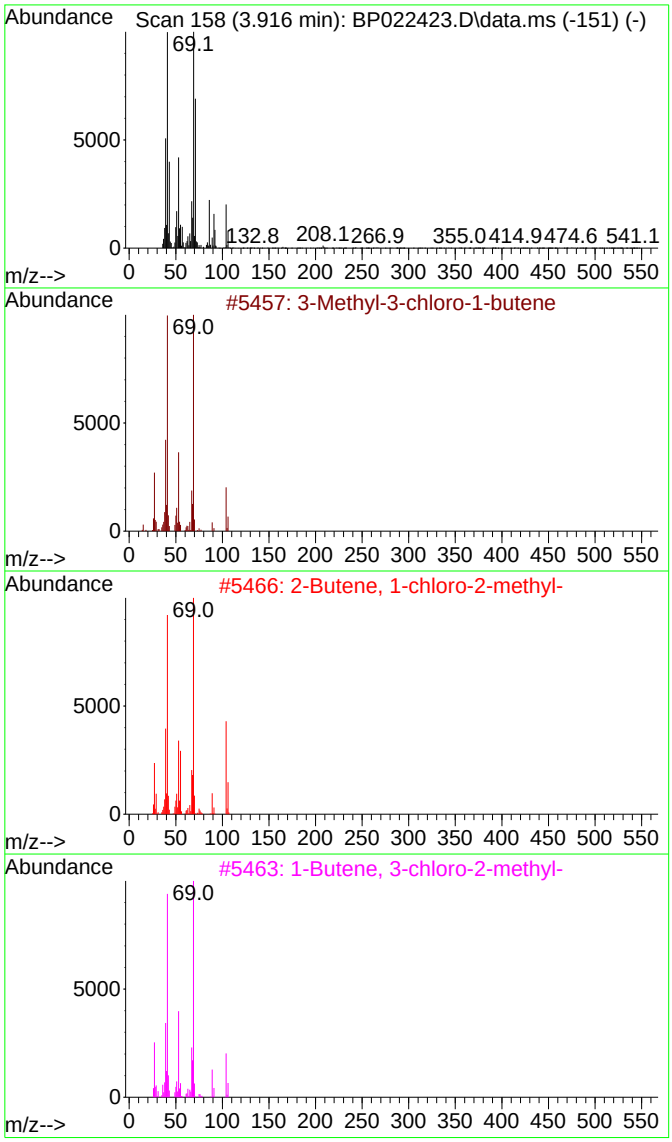
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

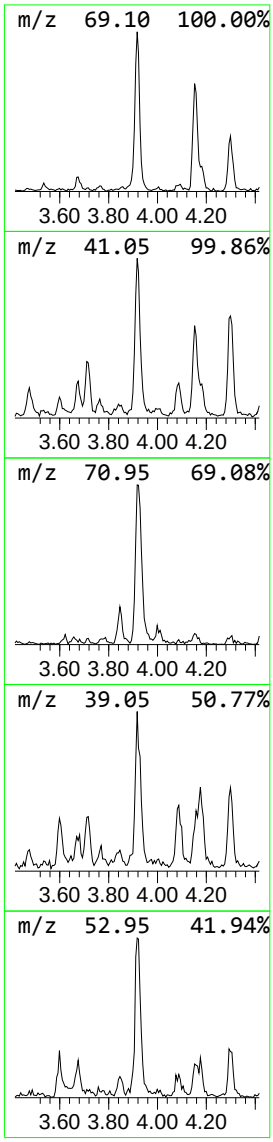
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Methyl-3-chloro-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.916	4.26 ng/ul	126893	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	93
2	2-Butene, 1-chloro-2-methyl-	104	C5H9Cl	013417-43-1	64
3	1-Butene, 3-chloro-2-methyl-	104	C5H9Cl	005166-35-8	62
4	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	53
5	Butanoic acid , but-3-yn-2-yl ester	140	C8H12O2	1000299-11-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

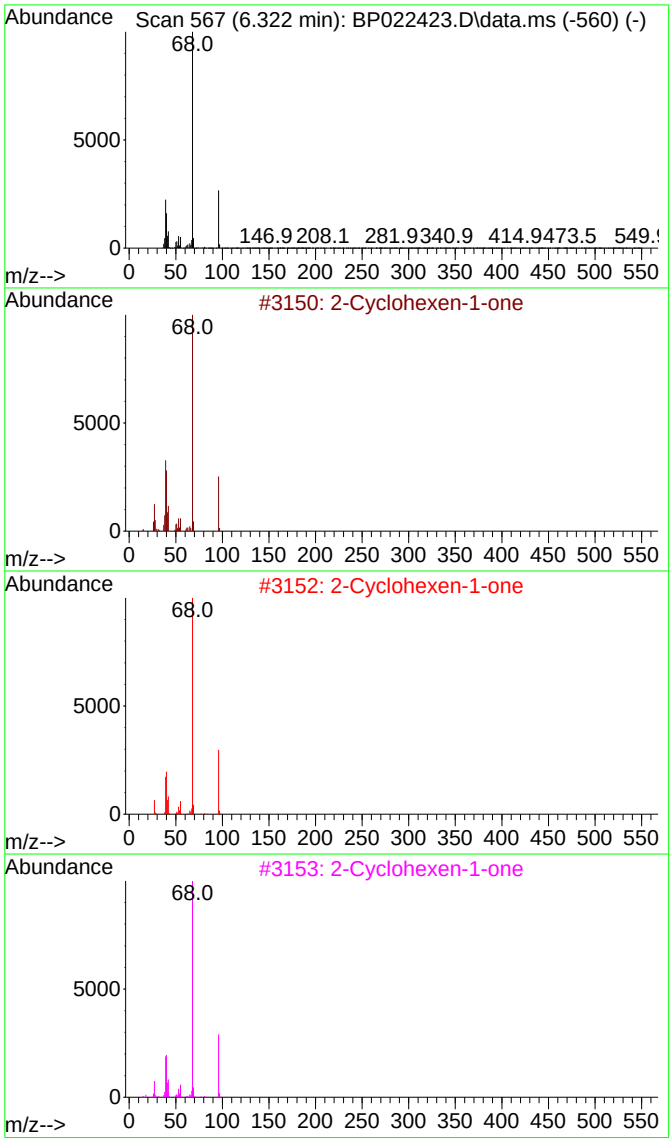
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

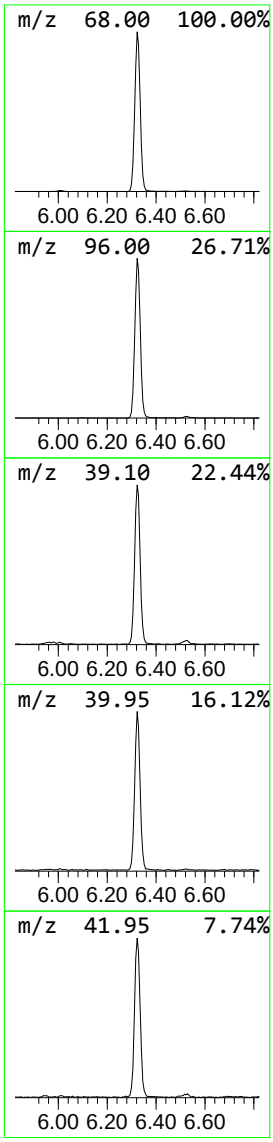
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.322	33.72 ng/ul	1003950	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 : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

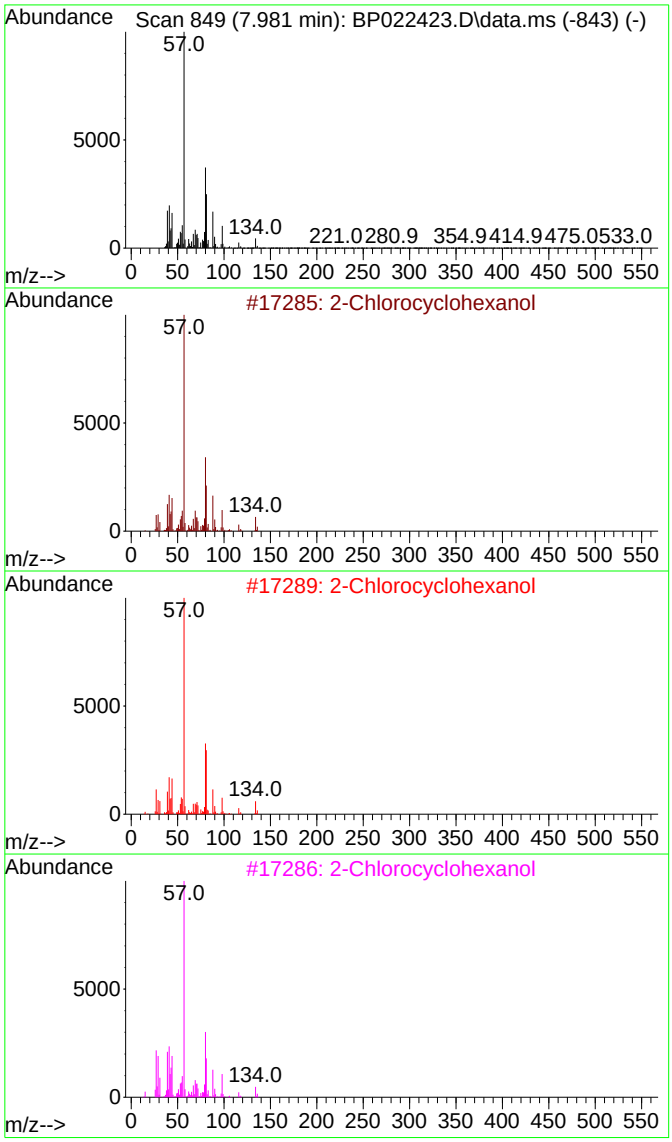
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

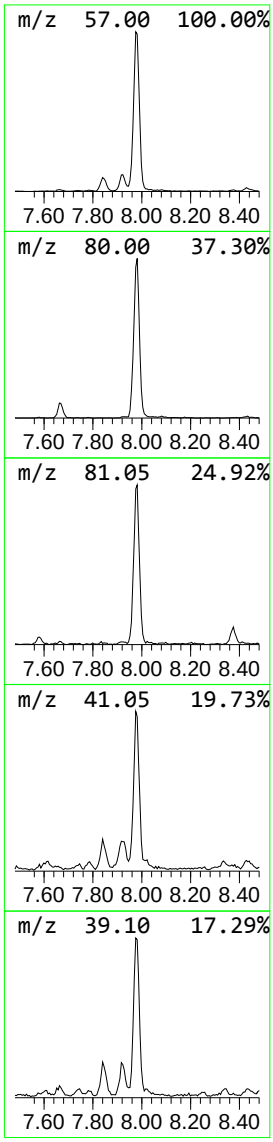
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.981	18.87 ng/ul	561787	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	87
3	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	81
4	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	80
5	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

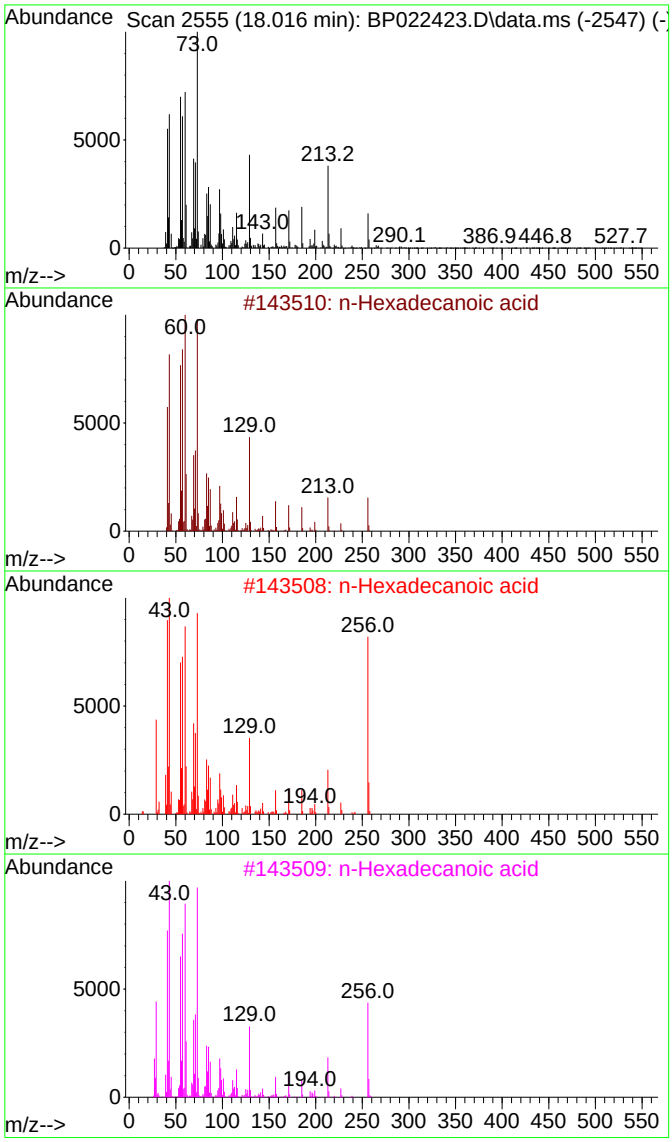
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

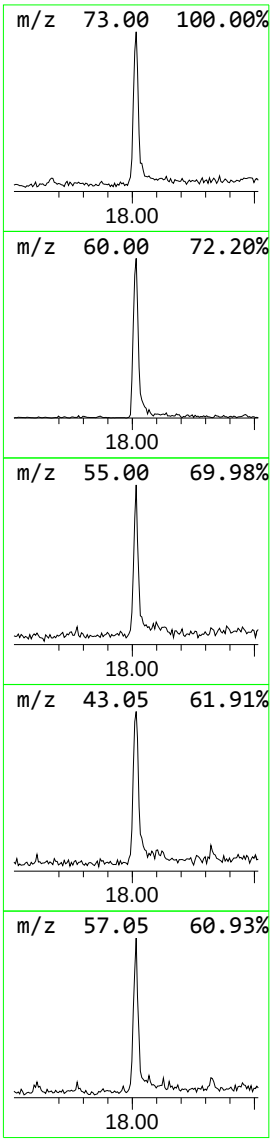
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	2.38 ng/ul	214801	Phenanthrene-d10	17.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

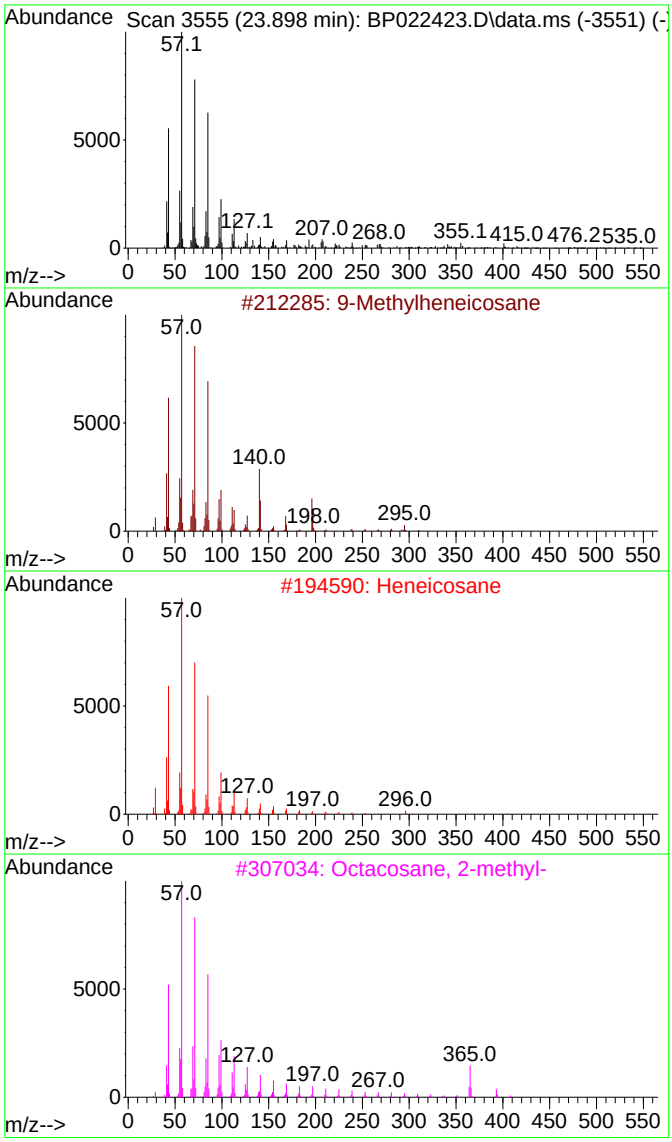
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

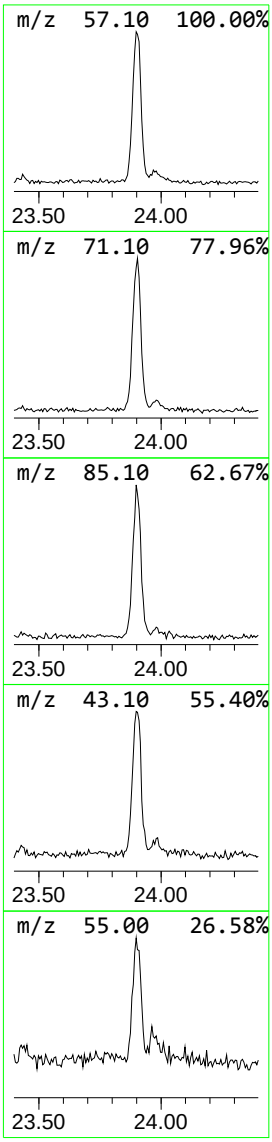
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.898	2.30 ng/ul	274608	Perylene-d12	24.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methylheneicosane	310	C22H46	070475-51-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	11-Methylpentacosane	366	C26H54	015689-71-1	91
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101624\
Data File : BP022423.D
Acq On : 16 Oct 2024 21:12
Operator : RC/JU
Sample : P4284-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4EW3

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
3-Methyl-3-chlo...	3.916	4.3	ng/ul	126893	1	7.669	595399	20.0
2-Cyclohexen-1-one	6.322	33.7	ng/ul	1003950	1	7.669	595399	20.0
2-Chlorocyclohe...	7.981	18.9	ng/ul	561787	1	7.669	595399	20.0
n-Hexadecanoic ...	18.016	2.4	ng/ul	214801	4	17.075	1804550	20.0
(DEL) Alkane: S...	23.898	2.3	ng/ul	274608	6	24.762	2391980	20.0