LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A46Q9

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-BP071223.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP016332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	12	16	21	rVB3	11507	17082	0.76%	0.073%
2	3.746	93	95	107	rBV	79019	183191	8.16%	0.780%
3	4.040	141	145	149	rBV	20224	29796	1.33%	0.127%
4	4.258	178	182	183	rBV3	18359	22899	1.02%	0.097%
5	4.581	234	237	243	rVB6	6744	8619	0.38%	0.037%
6	5.152	333	334	338	rVB4	2068	2383	0.11%	0.010%
7	5.193	338	341	342	rBV3	2813	2403	0.11%	0.010%
8	5.305	358	360	362	rBV3	2186	2695	0.12%	0.011%
9	5.363	366	370	373	rVB5	5331	7880	0.35%	0.034%
10	5.822	438	448	459	rBV2	133606	335634	14.95%	1.429%
11	5.910	460	463	469	rVB3	12095	26812	1.19%	0.114%
12	6.187	505	510	521	rVB	32657	58392	2.60%	0.249%
13	6.581	571	577	598	rBV	213775	614702	27.38%	2.617%
14	7.005	648	649	654	rBV5	2562	2727	0.12%	0.012%
15	7.193	674	681	695	rBV3	66955	284311	12.67%	1.210%
16	7.305	695	700	710	rVV	66884	158432	7.06%	0.674%
17	7.510	729	735	755	rBV2	112649	316519	14.10%	1.348%
18	7.957	803	811	828	rBV2	134970	453131	20.19%	1.929%
19	8.199	843	852	857	rBV2	11866	33603	1.50%	0.143%
20	8.263	857	863	875	rBV	231439	505255	22.51%	2.151%
21	8.669	929	932	935	rBV5	2322	3249	0.14%	0.014%
22	8.763	942	948	949	rBV	48946	73769	3.29%	0.314%
23	9.057	994	998	1008	rVB	2942	7732	0.34%	0.033%
24	9.193	1015	1021	1035	rBV2	84798	312237	13.91%	1.329%
25	9.934	1137	1147	1148	rBV	55188	93507	4.17%	0.398%
26	10.287	1204	1207	1209	rVB4	2598	2529	0.11%	0.011%
27	10.487	1234	1241	1242	rBV6	4185	6862	0.31%	0.029%
28	10.546	1243	1251	1273	rVV3	70302	397617	17.71%	1.693%
29	10.787	1284	1292	1313	rVB	231202	718234	32.00%	3.058%
30	11.069	1330	1340	1353	rBV4	32144	157387	7.01%	0.670%
31	11.428	1400	1401	1406	rVB5	3366	3576	0.16%	0.015%
32	11.504	1412	1414	1418	rVB5	2190	2935	0.13%	0.012%
33	12.081	1507	1512	1518	rBV10	2564	6509	0.29%	0.028%
34	12.140	1520	1522	1526	rVB5	1948	2572	0.11%	0.011%
35	12.181	1526	1529	1532	rBV5	1990	2589	0.12%	0.011%
36	12.269	1538	1544	1546	rBV7	1322	2549	0.11%	0.011%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

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-BP071223.MA.M
Title : SVOA CALIBRATION

37	12.328	1548	1554	1555	rVB6	1539	2851	0.13%	0.012%
38	12.381	1560	1563	1567	rBV5	1951	2984	0.13%	0.013%
39	12.463	1572	1577	1580	rVV6	4689	8539	0.38%	0.036%
40	12.751	1619	1626	1628	rBV8	3704	5517	0.25%	0.023%
41	12.816	1630	1637	1639	rBV3	10418	18886	0.84%	0.080%
42	12.845	1640	1642	1649	rVB3	9696	17110	0.76%	0.073%
43	13.057	1675	1678	1681	rVB5	1849	2965	0.13%	0.013%
44	13.492	1746	1752	1759	rBV3	10387	22579	1.01%	0.096%
45	13.898	1816	1821	1824	rVB7	1643	2529	0.11%	0.011%
46	14.039	1838	1845	1869	rBV	348606	926036	41.25%	3.942%
47	14.304	1883	1890	1906	rBV2	483153	980183	43.67%	4.173%
48	14.445	1911	1914	1923	rVB10	7147	17149	0.76%	0.073%
49	14.610	1935	1942	1955	rBV	629577	1123024	50.03%	4.781%
50	15.063	2008	2019	2029	rBV8	32979	164386	7.32%	0.700%
51	15.404	2076	2077	2083	rBV5	3383	4314	0.19%	0.018%
52	15.622	2107	2114	2137	rBV2	554076	1368941	60.99%	5.828%
53	15.851	2146	2153	2173	rBV5	54039	259202	11.55%	1.104%
54	16.004	2174	2179	2192	rVB	87997	173356	7.72%	0.738%
55	16.498	2259	2263	2264	rBV4	3098	3906	0.17%	0.017%
56	16.551	2268	2272	2279	rVB10	6066	10123	0.45%	0.043%
57	16.704	2297	2298	2301	rVB3	3445	2386	0.11%	0.010%
58	16.792	2307	2313	2315	rBV7	4488	8068	0.36%	0.034%
59	16.922	2330	2335	2341	rBV7	9090	20972	0.93%	0.089%
60	17.075	2356	2361	2375	rBV7	29044	88410	3.94%	0.376%
61	17.257	2388	2392	2397	rVB7	8642	11811	0.53%	0.050%
62	17.375	2405	2412	2424	rBV	892014	1506119	67.10%	6.412%
63	17.480	2424	2430	2450	rVB2	598345	1373987	61.21%	5.850%
64	18.080	2529	2532	2535	rBV5	8355	13575	0.60%	0.058%
65	18.227	2552	2557	2567	rBV2	218157	406080	18.09%	1.729%
66	18.439	2590	2593	2594	rBV3	6113	6315	0.28%	0.027%
67	19.286	2734	2737	2740	rBV4	17286	23257	1.04%	0.099%
68	19.316	2740	2742	2744	rVV2	16580	17875	0.80%	0.076%
69	19.363	2748	2750	2753	rVV	24210	32719	1.46%	0.139%
70	19.398	2753	2756	2761	rVB	38809	53892	2.40%	0.229%
71	19.451	2761	2765	2776	rBV	159122	284356	12.67%	1.211%
72	19.710	2803	2809	2823	rBV	1220815	2205244	98.24%	9.388%
73	20.174	2886	2888	2892	rVB3	30278	30266	1.35%	0.129%
74	20.657	2968	2970	2973	rBV2	39446	39361	1.75%	0.168%
75	21.063	3036	3039	3045	rBV4	154376	252225	11.24%	1.074%
76	21.110	3045	3047	3050	rVV	75931	70518	3.14%	0.300%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

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-BP071223.MA.M
Title : SVOA CALIBRATION

77	21.474	3104	3109	3120	rBV	1073103	2101866	93.64%	8.948%
78	22.016	3198	3201	3206	rVB	164709	200352	8.93%	0.853%
79	23.086	3380	3383	3393	rVB	212166	331291	14.76%	1.410%
80	23.792	3497	3503	3523	rVB2	902360	2244680	100.00%	9.556%
81	23.957	3525	3531	3550	rVB	793996	2188378	97.49%	9.317%

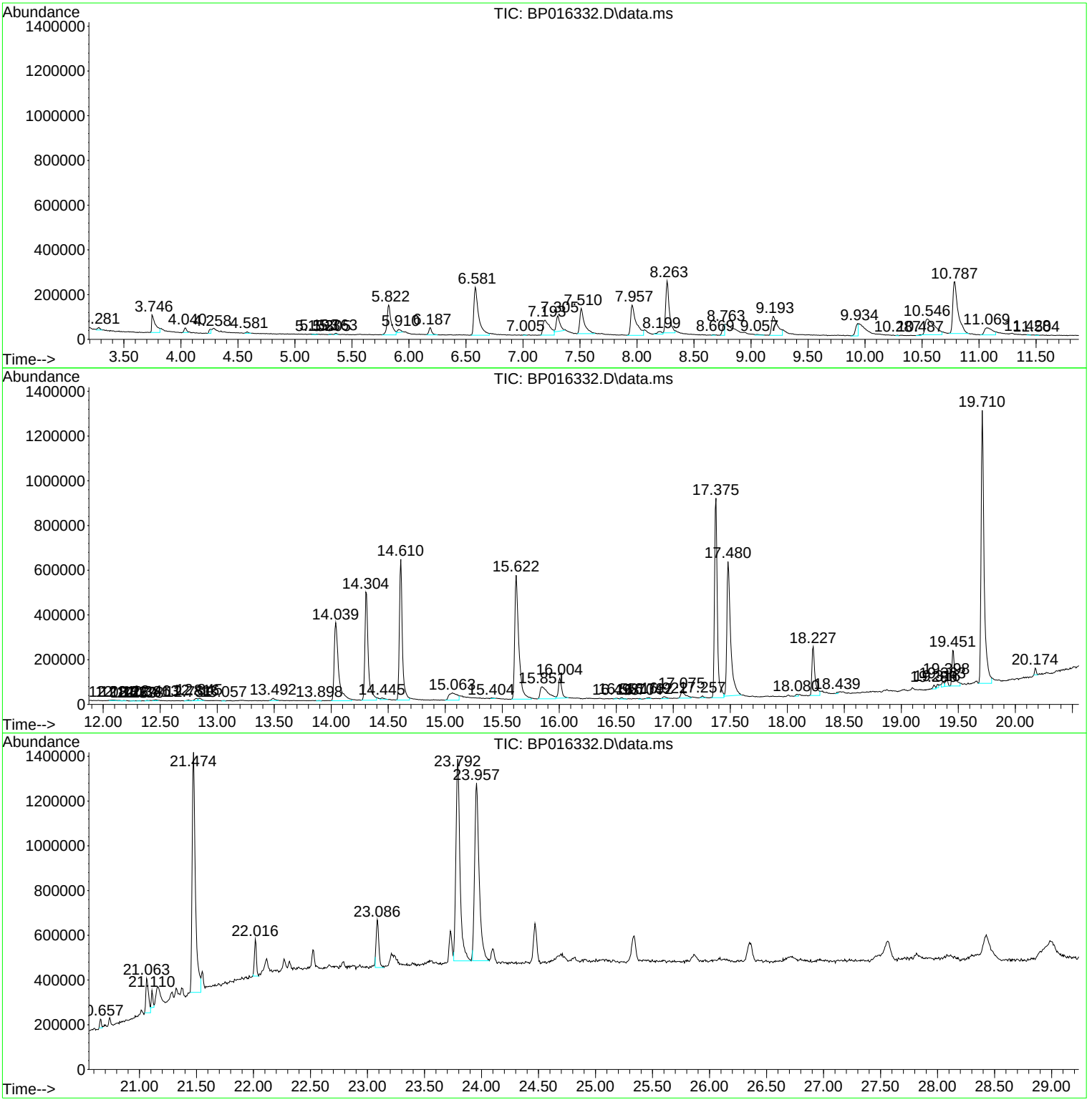
Sum of corrected areas: 23488902

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.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\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

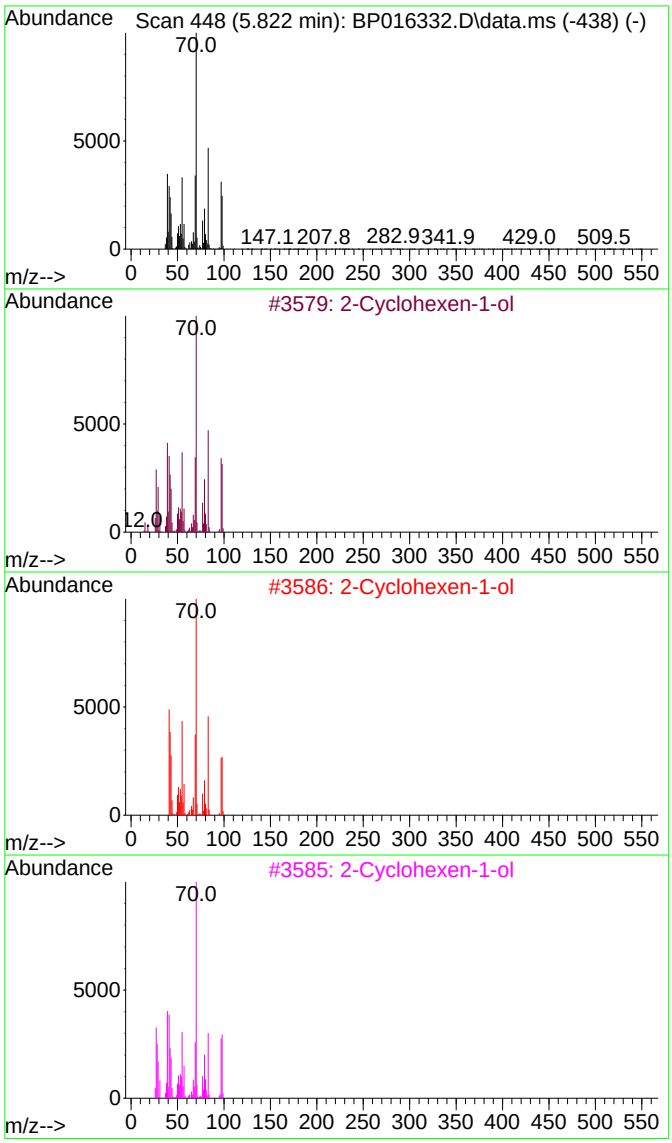
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

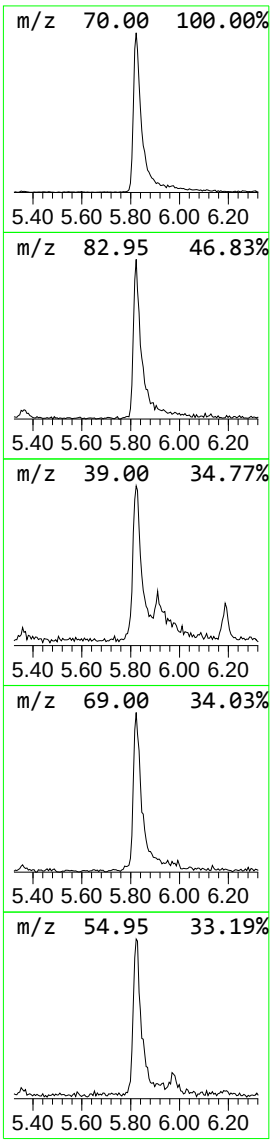
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Cyclohexen-1-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	14.81 ng/ul	335634	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	96
2	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	95
3	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	87
4	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	52
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

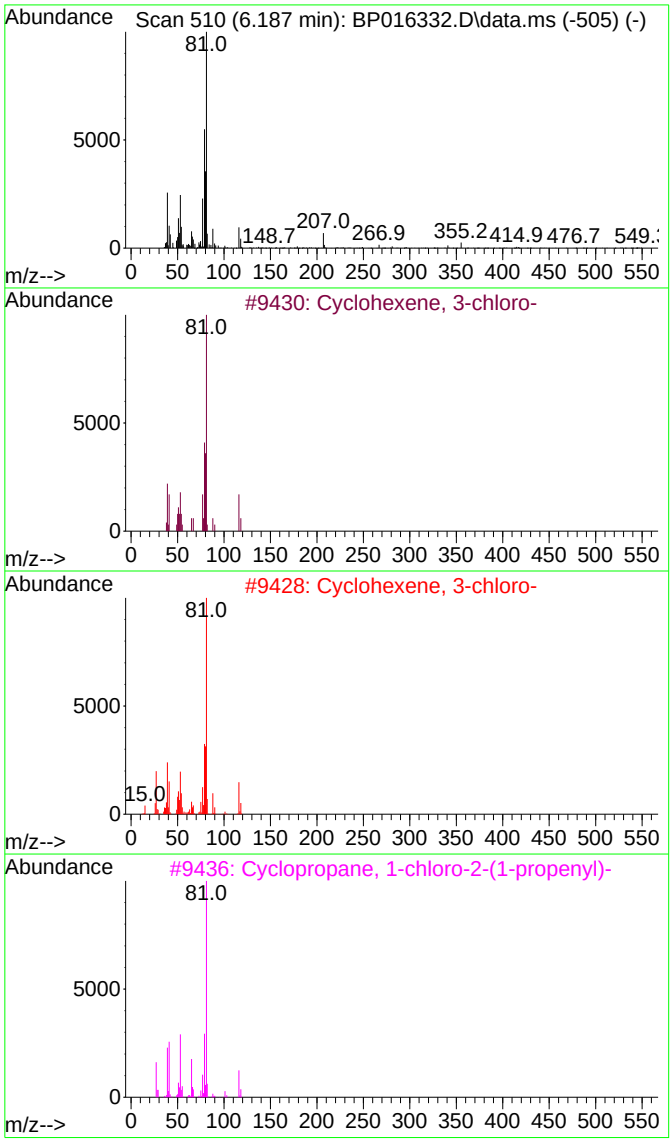
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

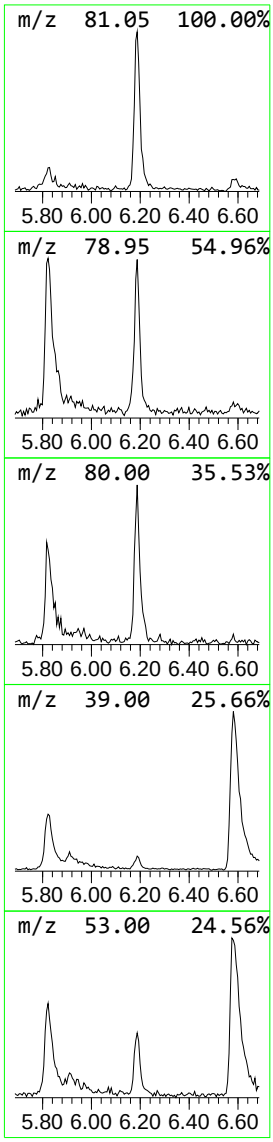
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexene, 3-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.187	2.58 ng/ul	58392	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 3-chloro-	116	C6H9Cl	002441-97-6	94
2	Cyclohexene, 3-chloro-	116	C6H9Cl	002441-97-6	59
3	Cyclopropane, 1-chloro-2-(1-prop...	116	C6H9Cl	074752-94-6	53
4	2-Pentyne, 4,4-dimethyl-	96	C7H12	000999-78-0	47
5	2,3-Dimethyl-1,4-pentadiene	96	C7H12	000758-86-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

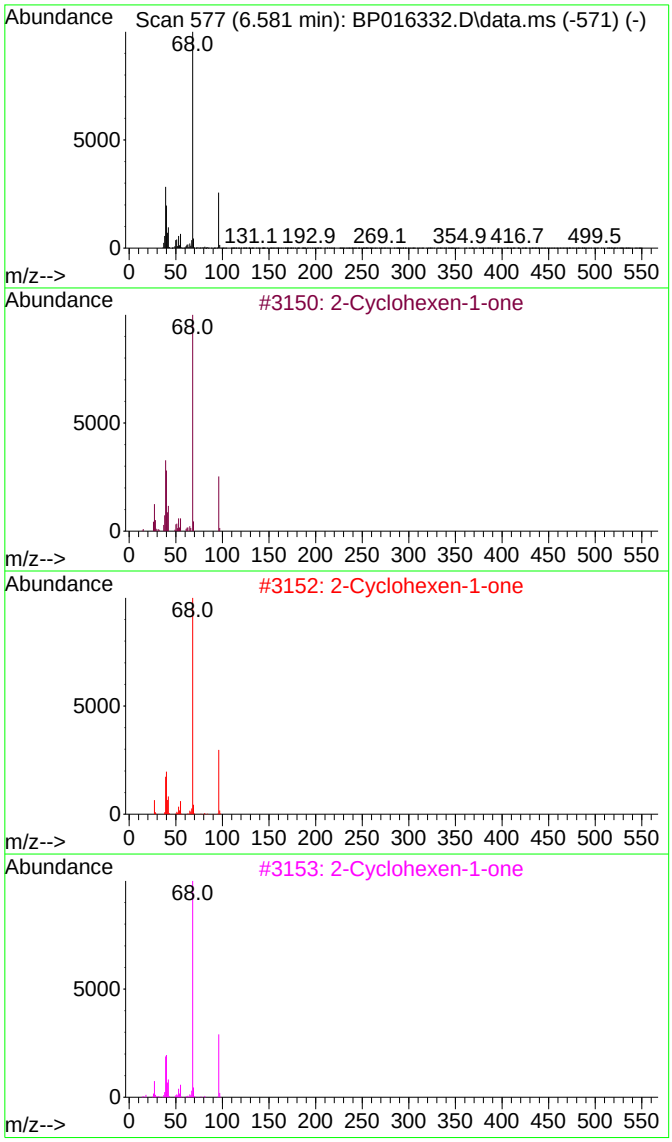
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

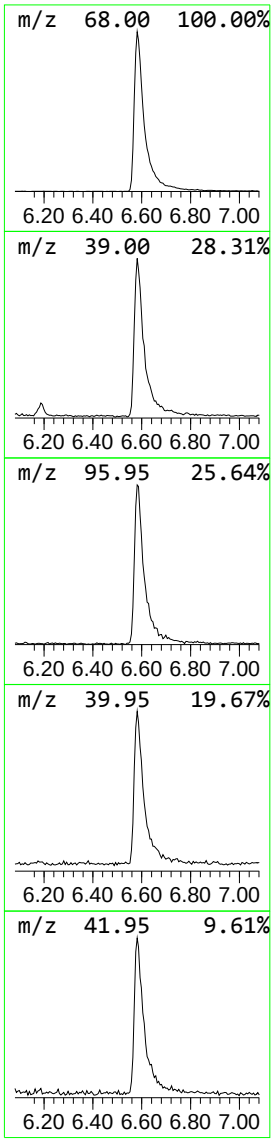
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Cyclohexen-1-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	27.13 ng/ul	614702	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	94
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	62
5	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

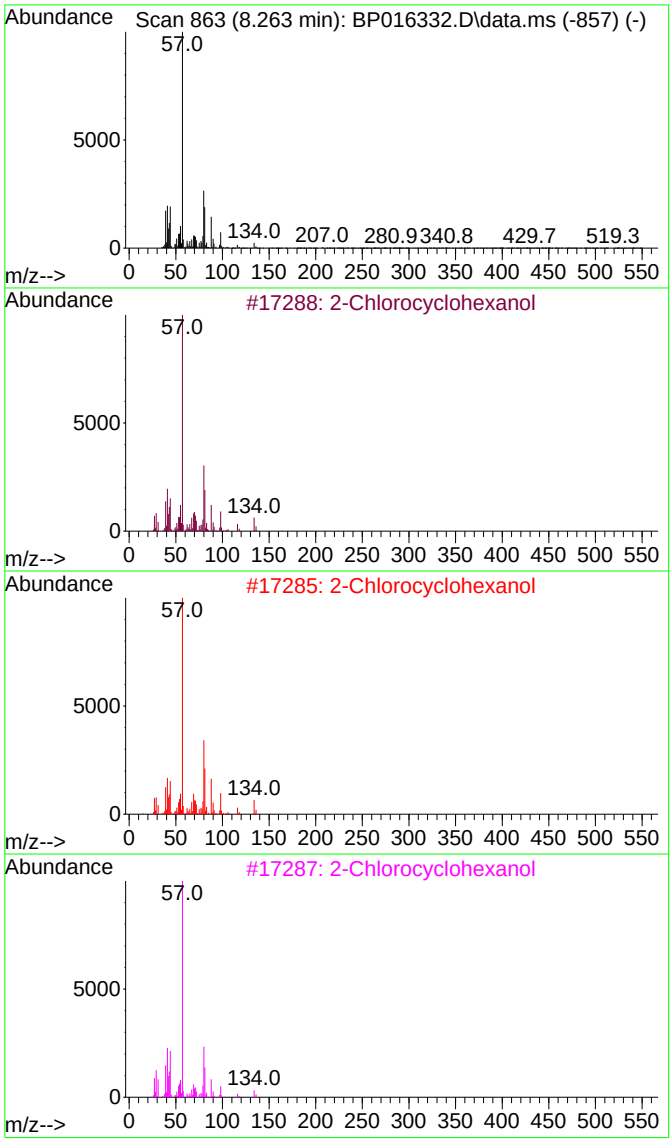
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

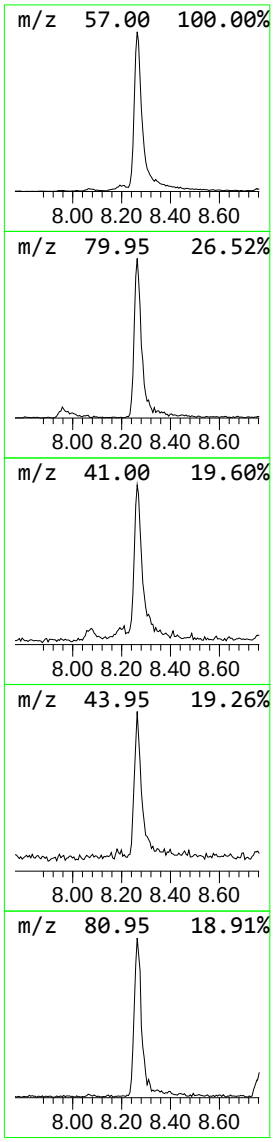
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.263	22.30 ng/ul	505255	1,4-Dichlorobenzene-d4	7.957

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	81
3	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	58
4	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	52
5	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

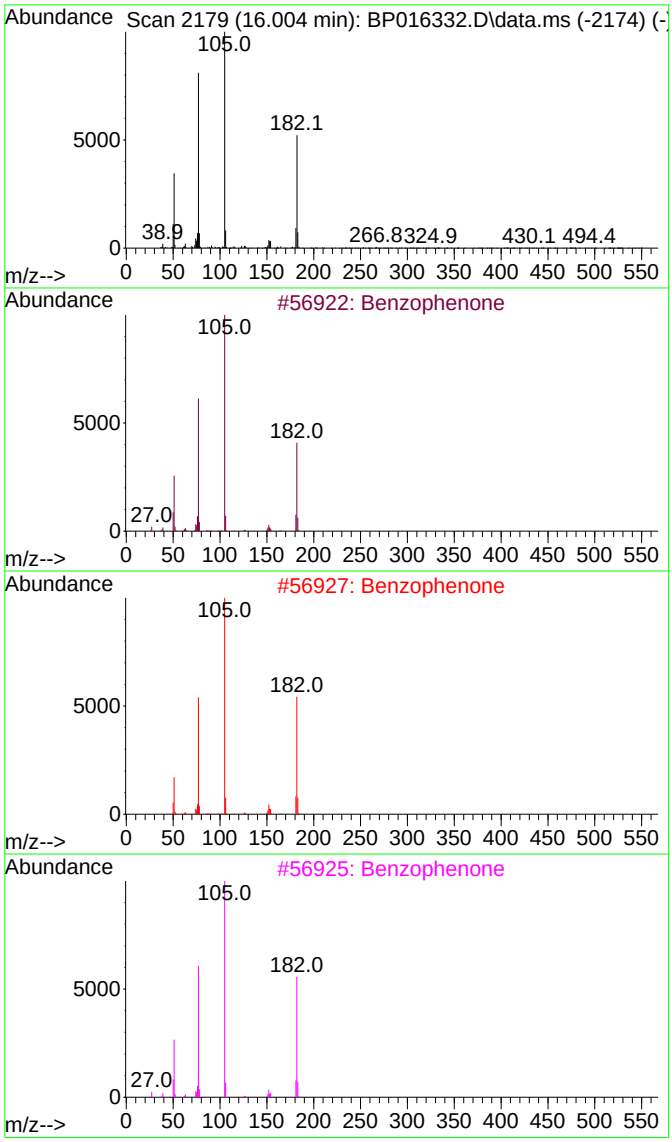
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

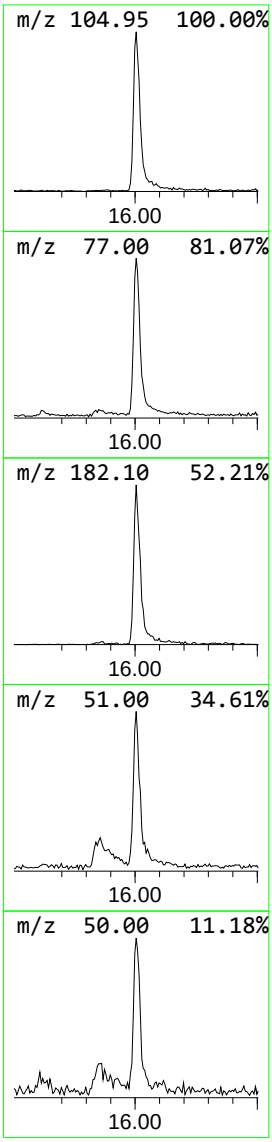
****

Peak Number 5 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	2.30 ng/ul	173356	Phenanthrene-d10	17.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	97
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

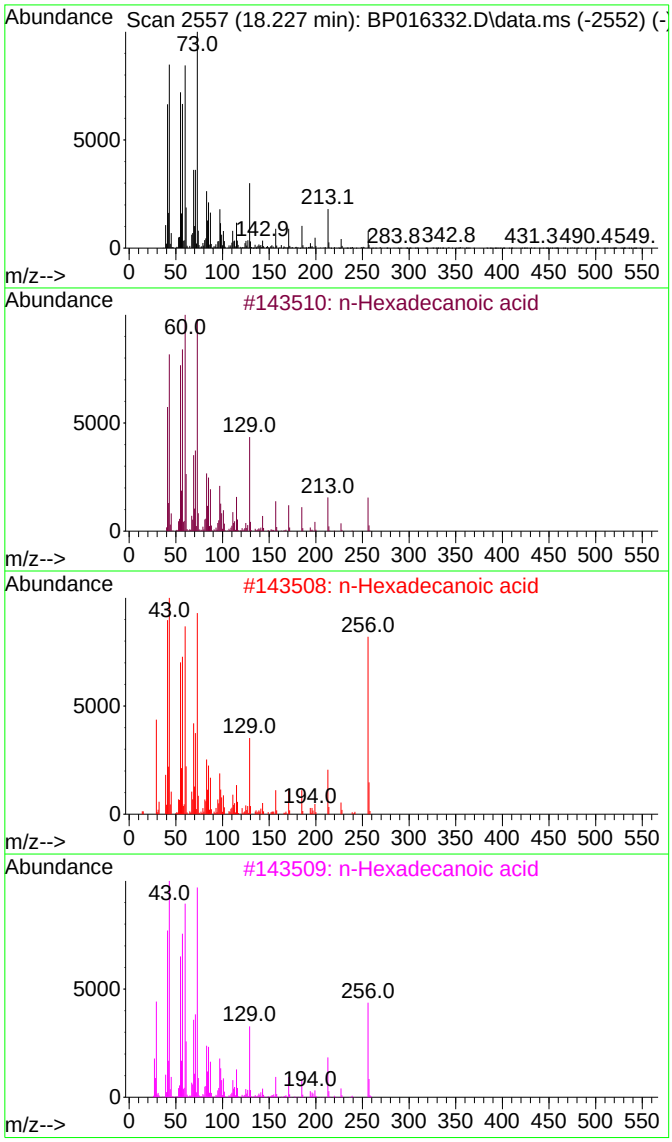
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

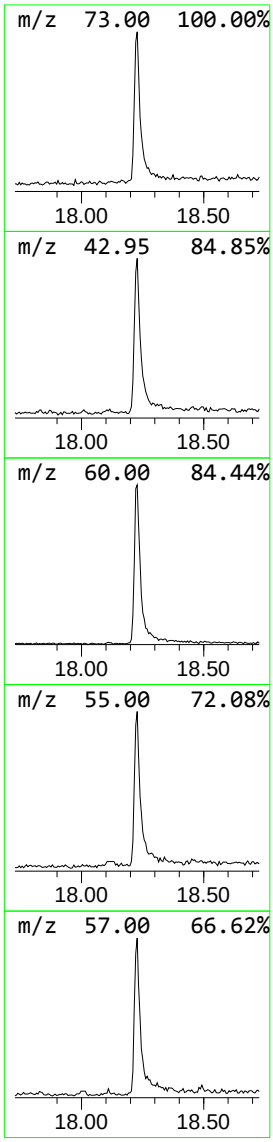
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	5.39 ng/ul	406080	Phenanthrene-d10	17.375

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	92
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





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Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

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

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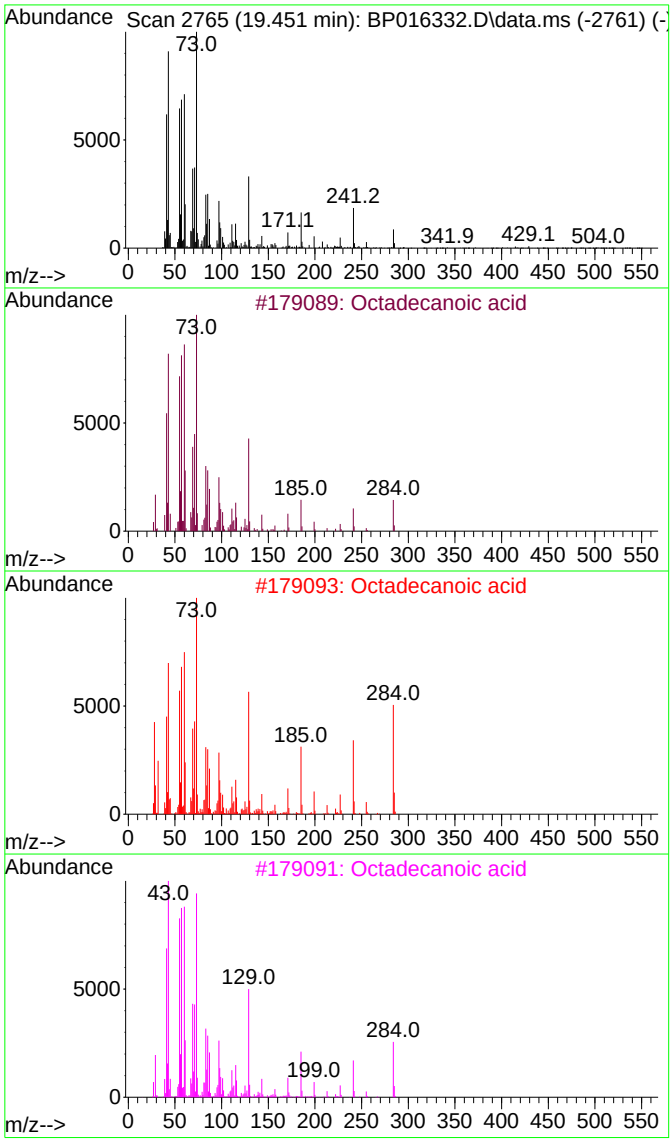
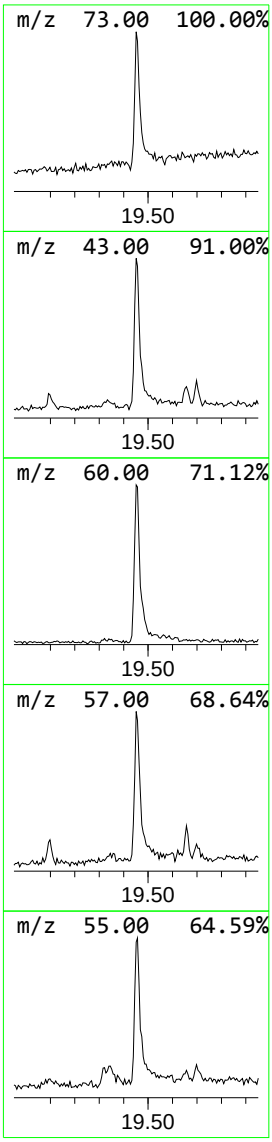
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.71 ng/ul	284356	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	97
5	Octadecanoic acid	284	C18H36O2	000057-11-4	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

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

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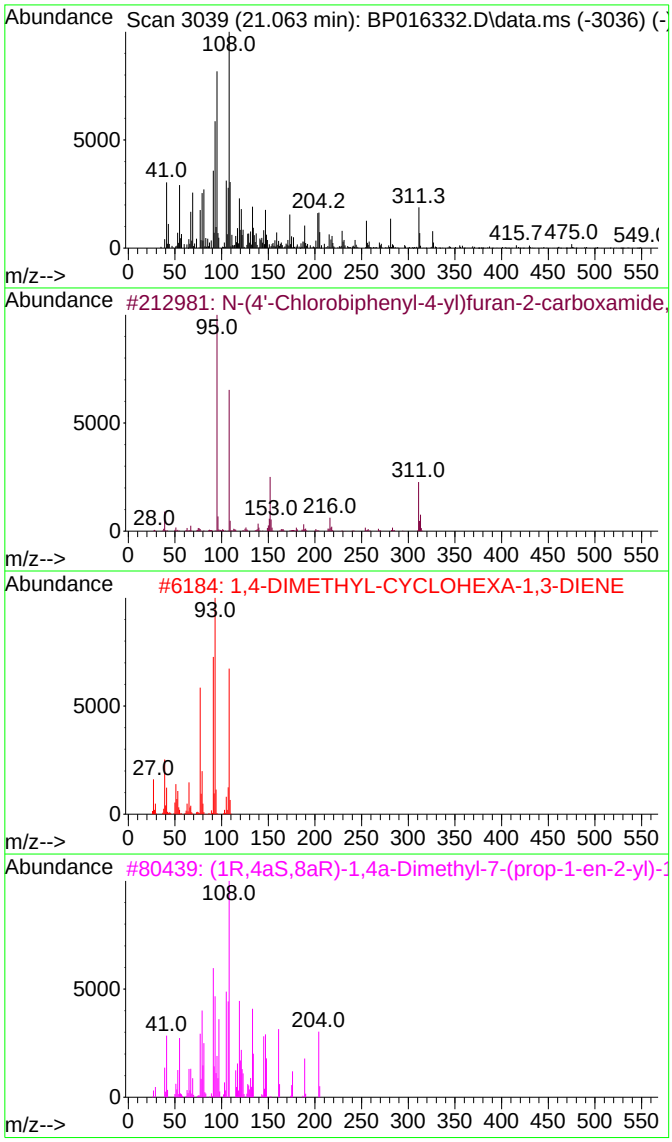
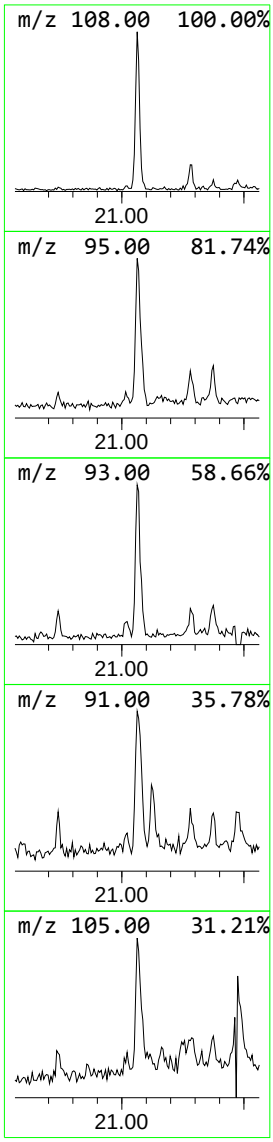
Peak Number 8 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	2.40 ng/ul	252225	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(4'-Chlorobiphenyl-4-yl)furan-...	311	C18H14ClNO2	1000510-86-1	38
2	1,4-DIMETHYL-CYCLOHEXA-1,3-DIENE	108	C8H12	026120-52-5	38
3	(1R,4aS,8aR)-1,4a-Dimethyl-7-(pr...	204	C15H24	194607-93-7	38
4	1,7,7-Trimethylbicyclo[2.2.1]hep...	152	C10H16O	1000190-98-1	35
5	4-[4-[(2-Hydroxybenzoyl)amino]an...	326	C17H14N2O5	1000272-26-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

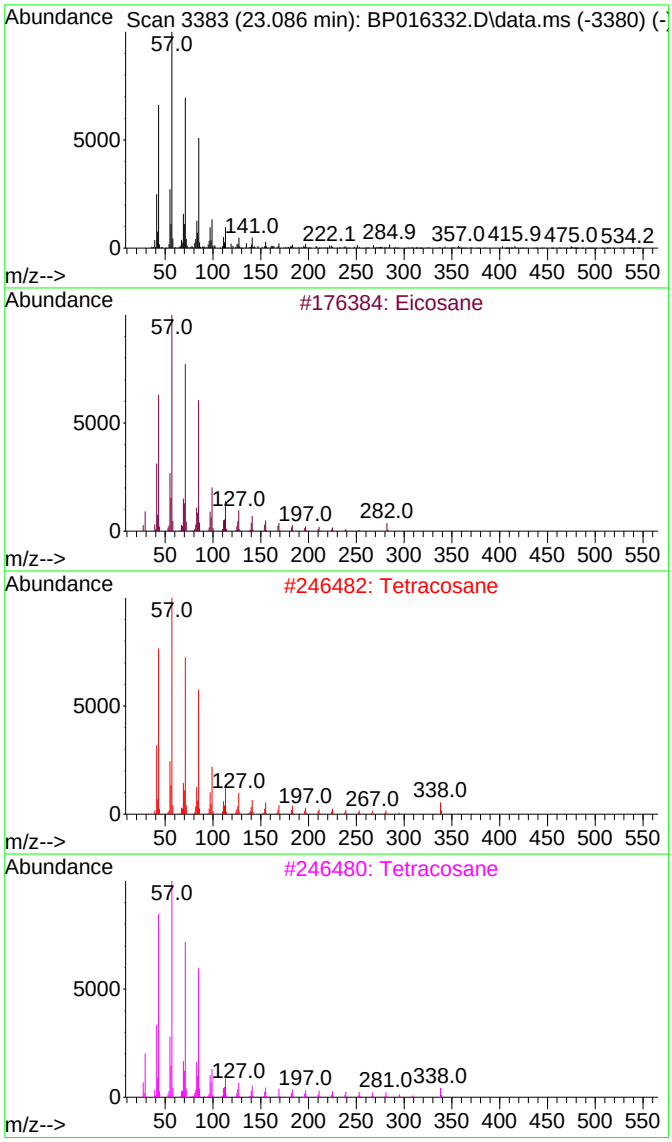
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

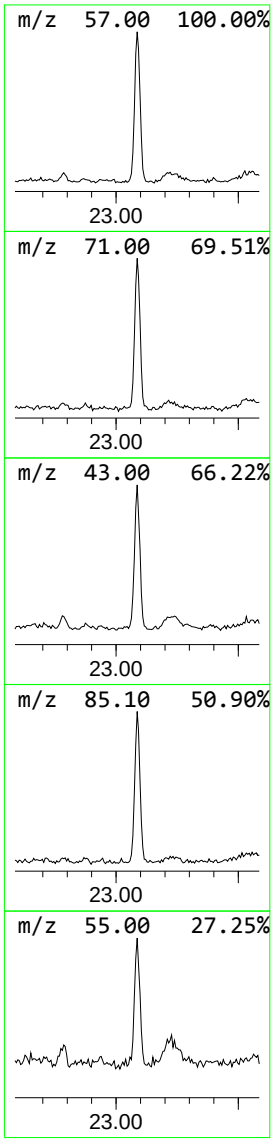
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	3.03 ng/ul	331291	Perylene-d12	23.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tetracosane	338	C24H50	000646-31-1	93
3	Tetracosane	338	C24H50	000646-31-1	93
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071923\
Data File : BP016332.D
Acq On : 19 Jul 2023 19:54
Operator : MA/JU
Sample : 03472-18
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46Q9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.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-ol	5.822	14.8	ng/ul	335634	1	7.957	453131	20.0
Cyclohexene, 3-...	6.187	2.6	ng/ul	58392	1	7.957	453131	20.0
2-Cyclohexen-1-one	6.581	27.1	ng/ul	614702	1	7.957	453131	20.0
2-Chlorocyclohe...	8.263	22.3	ng/ul	505255	1	7.957	453131	20.0
Benzophenone	16.004	2.3	ng/ul	173356	4	17.375	1506120	20.0
n-Hexadecanoic ...	18.227	5.4	ng/ul	406080	4	17.375	1506120	20.0
Octadecanoic acid	19.451	2.7	ng/ul	284356	5	21.474	2101870	20.0
unknown-01	21.063	2.4	ng/ul	252225	5	21.474	2101870	20.0
(DEL) Alkane: S...	23.086	3.0	ng/ul	331291	6	23.957	2188380	20.0