LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

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: BP020941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	41	45	51	rVB	34219	42923	0.83%	0.090%
2	3.346	59	61	66	rVB4	6096	5892	0.11%	0.012%
3	3.540	91	94	99	rVB2	5979	8338	0.16%	0.018%
4	3.669	114	116	129	rBV	128490	199965	3.88%	0.420%
5	3.975	164	168	172	rVB	13562	17825	0.35%	0.037%
6	4.328	225	228	234	rVB4	9224	14268	0.28%	0.030%
7	4.387	234	238	242	rVB4	5593	7956	0.15%	0.017%
8	4.434	242	246	250	rBV2	13236	17184	0.33%	0.036%
9	4.517	257	260	265	rVB6	3587	5990	0.12%	0.013%
10	4.869	316	320	328	rVB	11336	20294	0.39%	0.043%
11	5.752	465	470	474	rBV2	50009	72121	1.40%	0.152%
12	5.793	474	477	483	rVB3	10959	17723	0.34%	0.037%
13	6.158	534	539	543	rBV8	2905	5960	0.12%	0.013%
14	6.781	638	645	649	rBV5	7931	17983	0.35%	0.038%
15	6.828	649	653	656	rVV4	4356	6612	0.13%	0.014%
16	6.916	660	668	680	rVV	158684	300441	5.83%	0.631%
17	7.058	684	692	706	rBV	505919	807150	15.68%	1.696%
18	7.258	719	726	735	rBV	597786	1008877	19.59%	2.120%
19	7.405	748	751	758	rVB9	5606	11257	0.22%	0.024%
20	7.710	795	803	812	rBV	588916	947572	18.40%	1.991%
21	8.310	900	905	914	rBV5	7259	18677	0.36%	0.039%
22	8.428	917	925	938	rBV	490741	864609	16.79%	1.817%
23	8.599	951	954	962	rVB10	2728	7018	0.14%	0.015%
24	8.863	992	999	1011	rBV	623787	1020991	19.83%	2.146%
25	9.016	1018	1025	1029	rBV4	18218	33708	0.65%	0.071%
26	9.222	1053	1060	1067	rBV2	11342	19482	0.38%	0.041%
27	9.422	1090	1094	1098	rBV7	4239	7061	0.14%	0.015%
28	9.575	1114	1120	1136	rBV	504767	868825	16.87%	1.826%
29	9.834	1157	1164	1172	rBV3	30809	72285	1.40%	0.152%
30	10.116	1203	1212	1227	rBV	610426	1304117	25.33%	2.741%
31	10.475	1262	1273	1285	rBV	742941	1244337	24.17%	2.615%
32	10.634	1293	1300	1313	rBV	442288	918460	17.84%	1.930%
33	11.140	1382	1386	1392	rBV7	4384	8940	0.17%	0.019%
34	11.240	1396	1403	1406	rBV3	13431	29108	0.57%	0.061%
35	11.293	1406	1412	1425	rVB	79000	168374	3.27%	0.354%
36	12.069	1539	1544	1552	rBV	11665	21035	0.41%	0.044%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

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	12.622	1633	1638	1641	rBV7	3260	5331	0.10%	0.011%
38	12.798	1661	1668	1669	rBV6	4198	7467	0.15%	0.016%
39	13.181	1727	1733	1745	rBV	759084	1039502	20.19%	2.185%
40	13.751	1820	1830	1842	rBV	1205536	2037630	39.57%	4.282%
41	13.845	1842	1846	1852	rVB9	4094	8501	0.17%	0.018%
42	14.028	1863	1877	1891	rBV	1495075	2369469	46.02%	4.980%
43	14.340	1920	1930	1940	rBV	1056388	1604585	31.16%	3.372%
44	14.616	1971	1977	1992	rBV2	85979	236639	4.60%	0.497%
45	14.769	1997	2003	2011	rVV8	17245	45494	0.88%	0.096%
46	14.851	2015	2017	2023	rVB7	3348	5951	0.12%	0.013%
47	15.045	2047	2050	2056	rBV3	4467	8278	0.16%	0.017%
48	15.357	2093	2103	2111	rBV	2046576	3009280	58.44%	6.324%
49	15.422	2111	2114	2121	rVV9	13095	27814	0.54%	0.058%
50	15.492	2121	2126	2139	rVV	713300	1038040	20.16%	2.182%
51	15.598	2139	2144	2151	rVB5	11684	27246	0.53%	0.057%
52	15.698	2158	2161	2169	rVB10	4455	9131	0.18%	0.019%
53	15.922	2193	2199	2200	rBV6	6008	8435	0.16%	0.018%
54	15.986	2206	2210	2214	rVB	8132	10574	0.21%	0.022%
55	16.151	2234	2238	2244	rVB8	5183	8350	0.16%	0.018%
56	16.239	2249	2253	2258	rBV7	9256	15580	0.30%	0.033%
57	16.539	2300	2304	2311	rBV	51672	78127	1.52%	0.164%
58	16.898	2363	2365	2368	rBV4	6459	6251	0.12%	0.013%
59	17.069	2390	2394	2397	rVB6	10487	14852	0.29%	0.031%
60	17.151	2399	2408	2417	rBV	1120730	1946696	37.81%	4.091%
61	17.257	2420	2426	2435	rVV2	2498706	3528236	68.52%	7.415%
62	17.328	2435	2438	2451	rVB6	36514	83669	1.62%	0.176%
63	17.663	2491	2495	2497	rBV5	8344	12735	0.25%	0.027%
64	17.816	2517	2521	2522	rBV4	7367	8549	0.17%	0.018%
65	17.845	2523	2526	2535	rVB7	18030	30090	0.58%	0.063%
66	17.957	2540	2545	2549	rBV2	58287	91553	1.78%	0.192%
67	18.080	2560	2566	2577	rBV	442437	745738	14.48%	1.567%
68	19.098	2737	2739	2746	rVB	30051	37861	0.74%	0.080%
69	19.186	2750	2754	2758	rBV	38907	55550	1.08%	0.117%
70	19.263	2763	2767	2769	rVV2	36497	55389	1.08%	0.116%
71	19.292	2770	2772	2781	rVB3	51873	96077	1.87%	0.202%
72	19.422	2790	2794	2805	rBV	232528	406077	7.89%	0.853%
73	19.639	2825	2831	2839	rBV	3167201	4433540	86.10%	9.318%
74	20.557	2984	2987	2992	rBV4	60944	93664	1.82%	0.197%
75	21.598	3159	3164	3177	rVB2	1499927	2291036	44.49%	4.815%
76	21.869	3205	3210	3217	rVB	654729	1062119	20.63%	2.232%

LSC Area Percent Report

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Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

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

77	22.327	3284	3288	3294	rVB	218706	356079	6.92%	0.748%
78	23.380	3460	3467	3478	rVB2	1208548	2834315	55.05%	5.957%
79	24.704	3683	3692	3706	rVB2	1734083	5149042	100.00%	10.821%
80	24.933	3723	3731	3741	rBV	972030	2498689	48.53%	5.251%

Sum of corrected areas: 47582589

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
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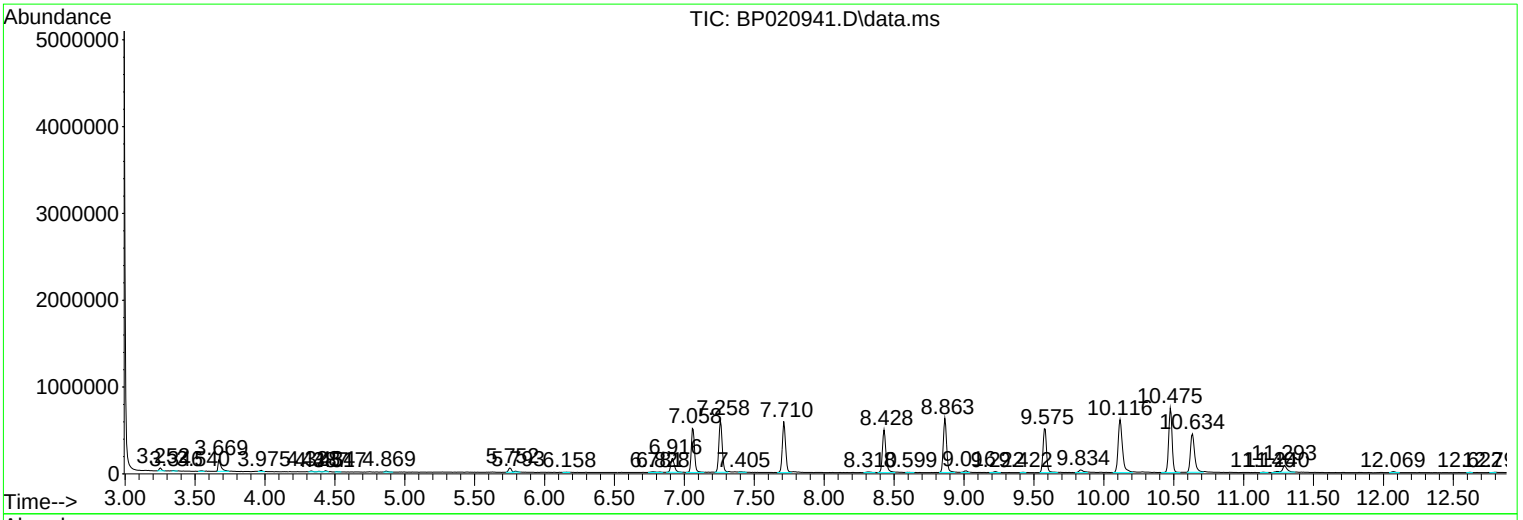
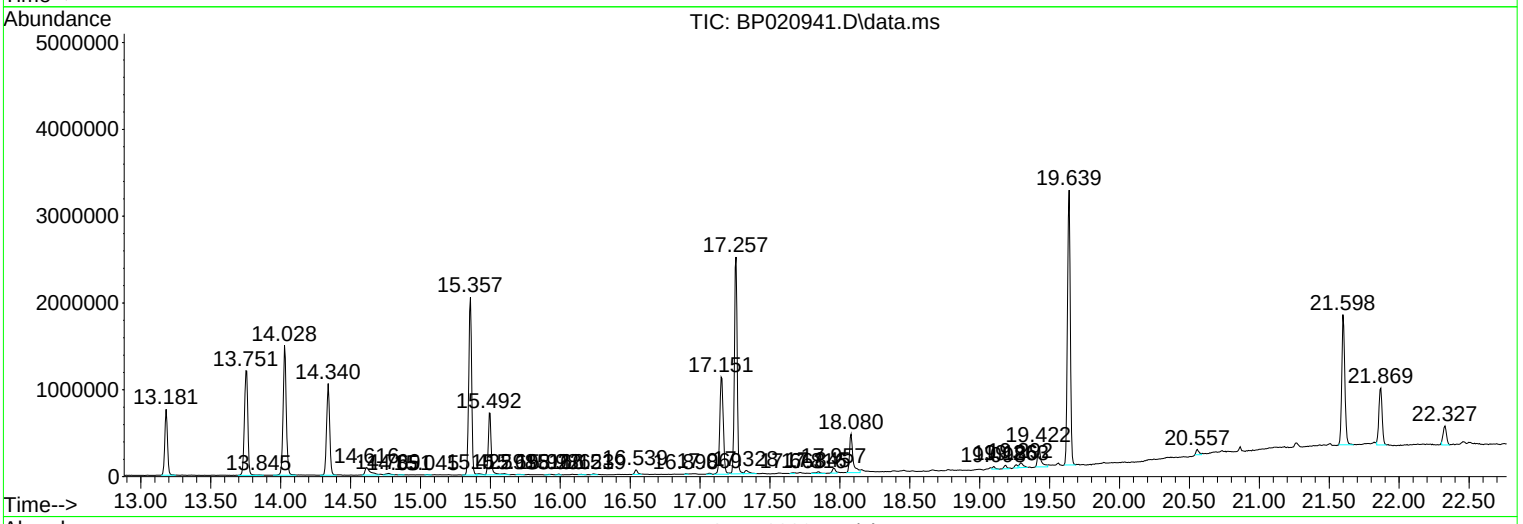
Misc :
ALS Vial : 49 Sample Multiplier: 1

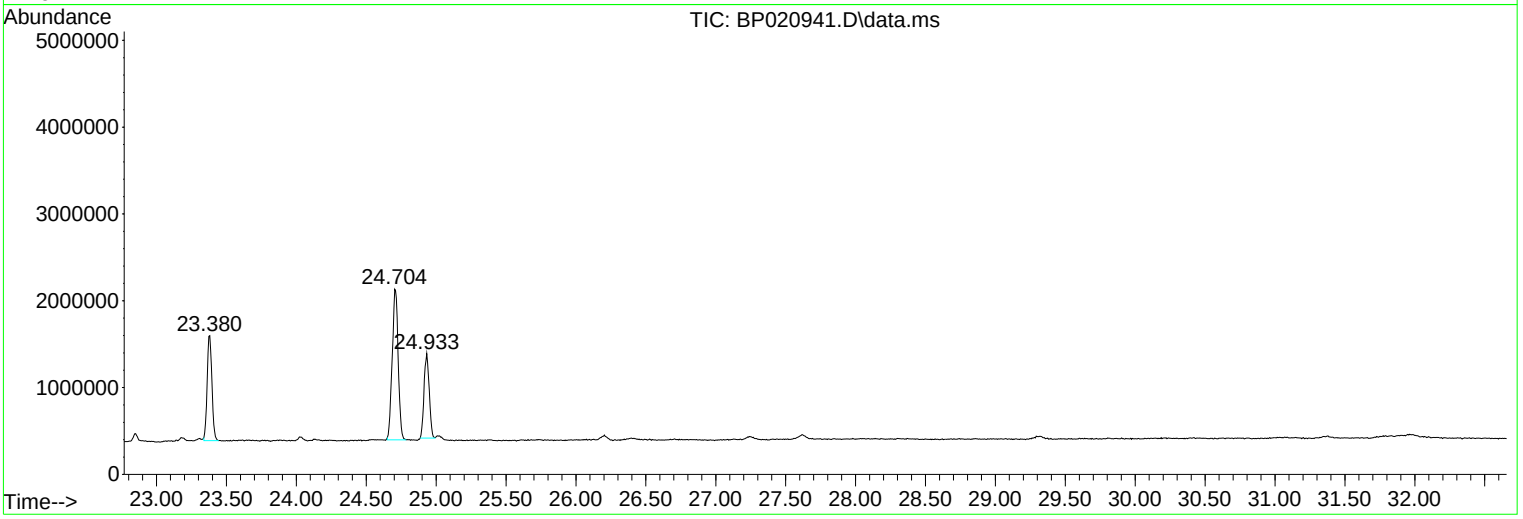
Instrument :
BNA_P
ClientSampleId :
E08E9

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\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

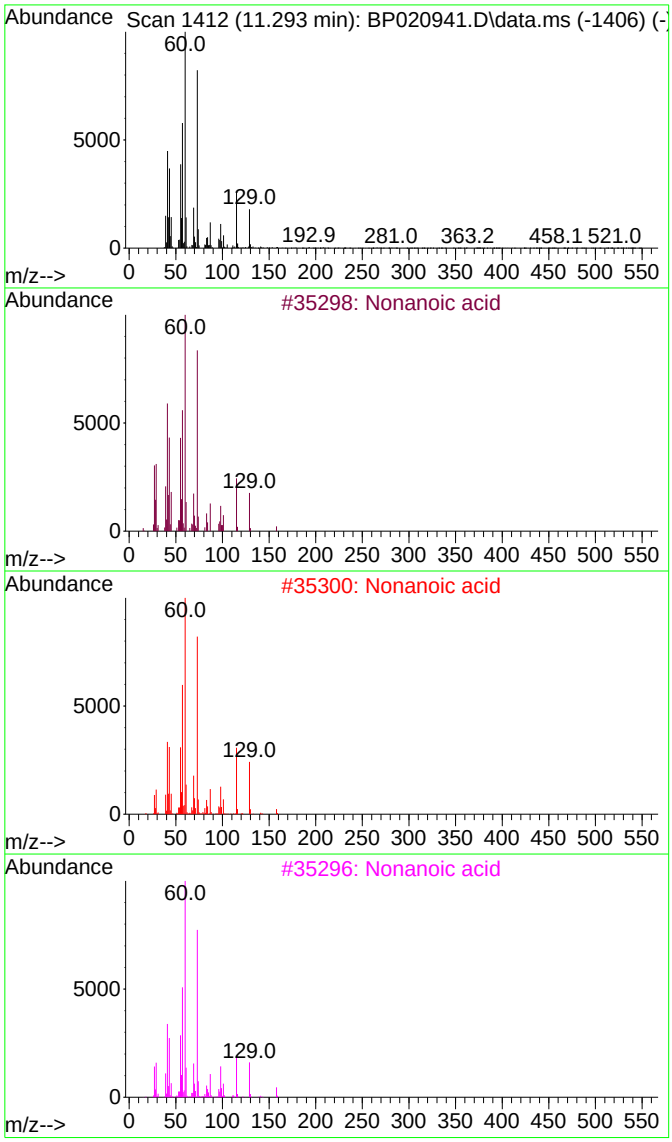
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

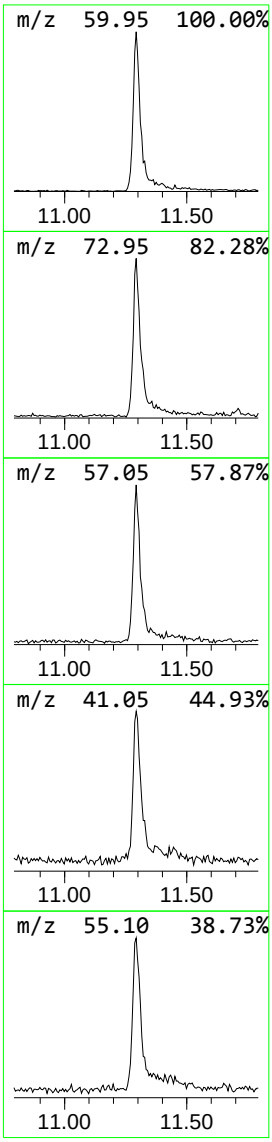
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.293	2.71 ng/ul	168374	Naphthalene-d8	10.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	91
2	Nonanoic acid	158	C9H18O2	000112-05-0	91
3	Nonanoic acid	158	C9H18O2	000112-05-0	86
4	Nonanoic acid	158	C9H18O2	000112-05-0	78
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

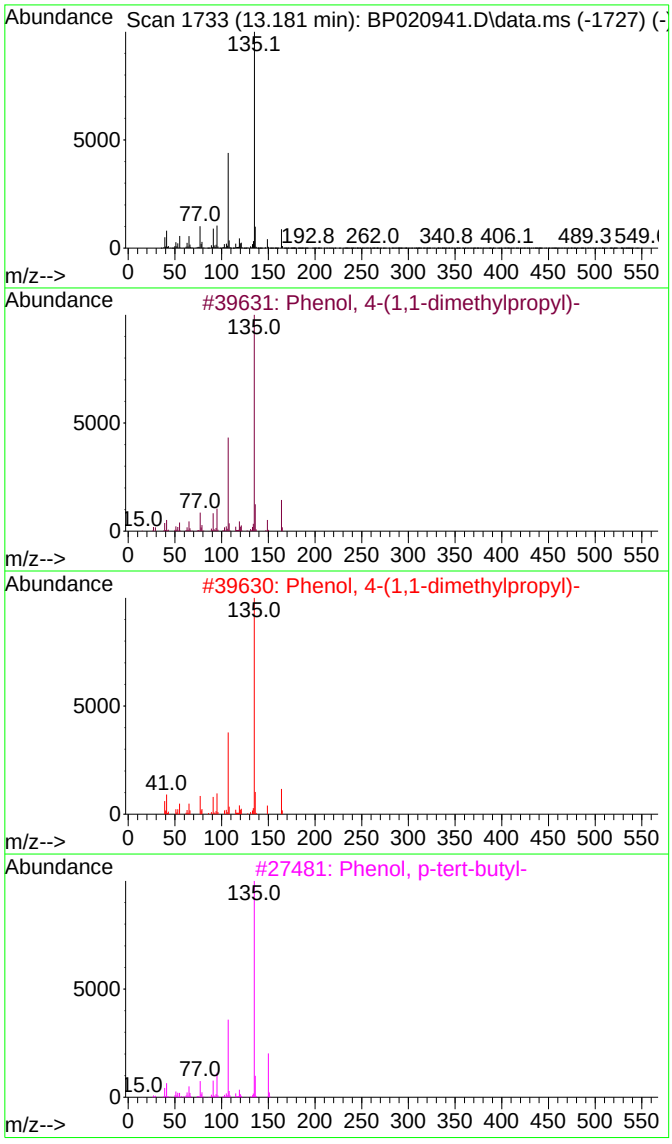
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

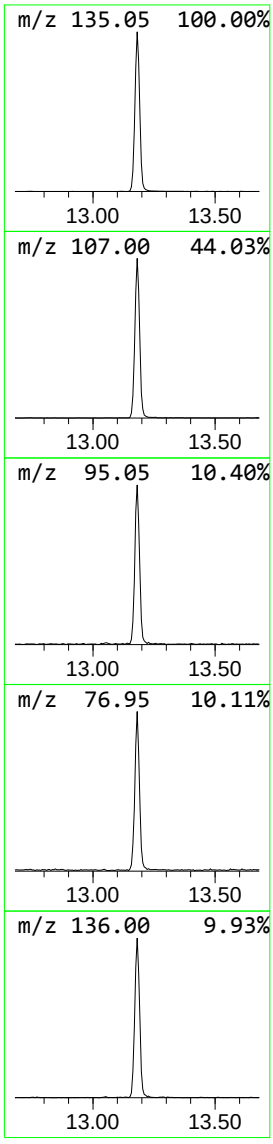
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.181	12.96 ng/ul	1039500	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
5	Hexestrol	270	C18H22O2	000084-16-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

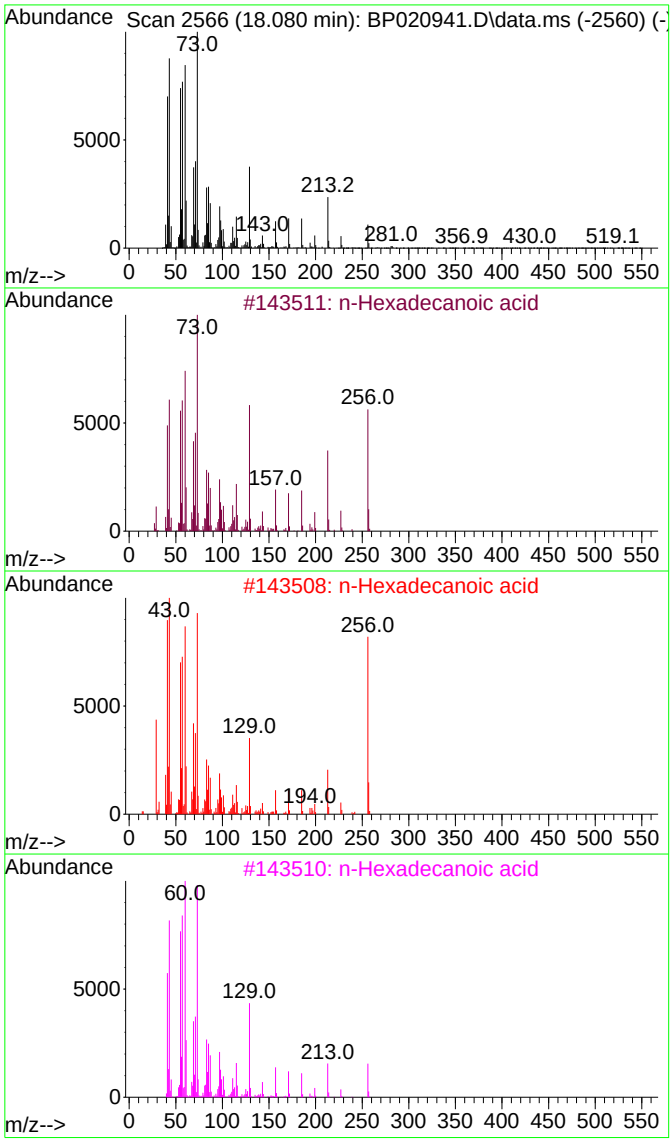
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

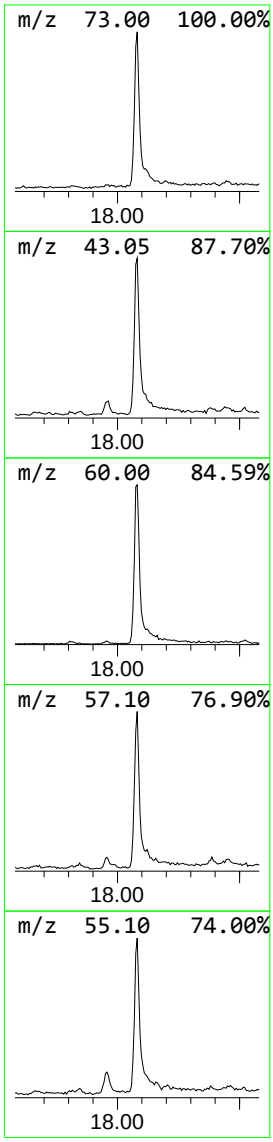
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.081	7.66 ng/ul	745738	Phenanthrene-d10	17.151

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	99
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





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Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
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Misc :
ALS Vial : 49 Sample Multiplier: 1

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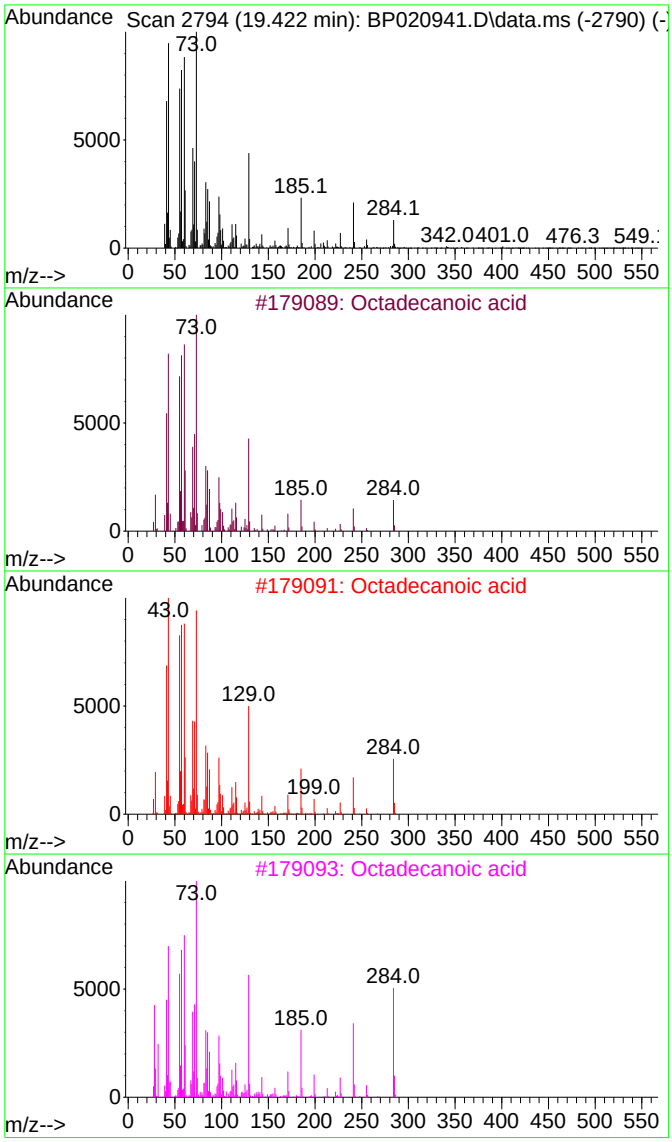
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

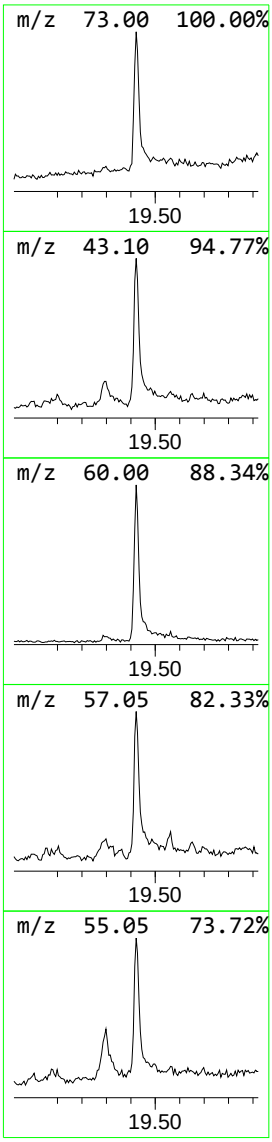
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	3.54 ng/ul	406077	Chrysene-d12	21.598

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	96
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	89





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Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

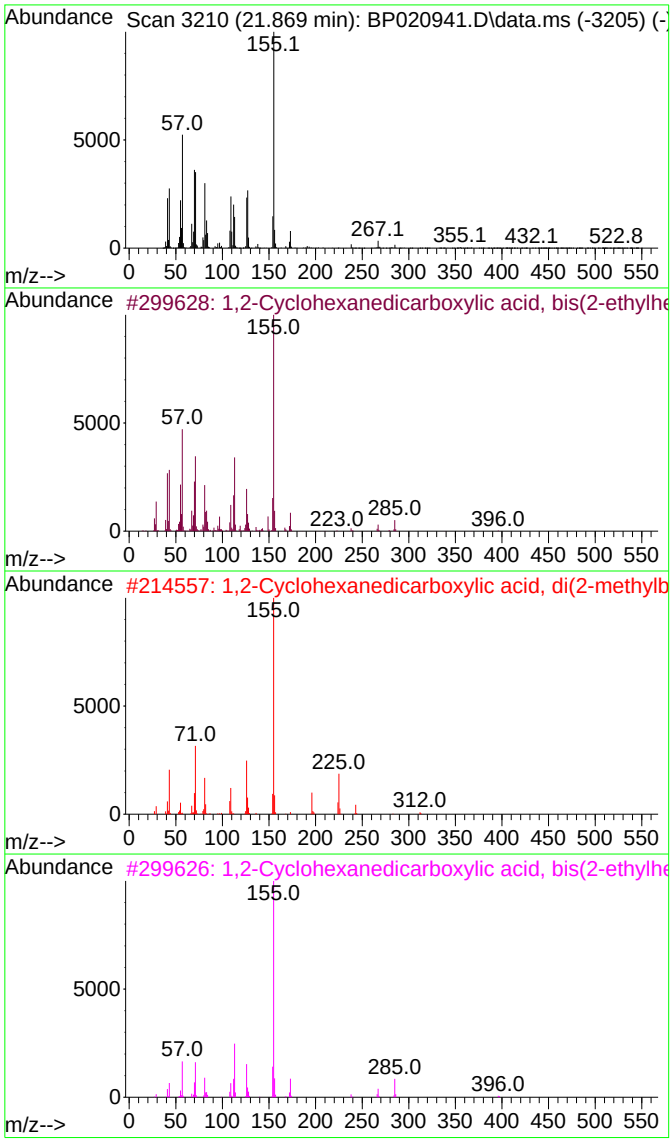
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

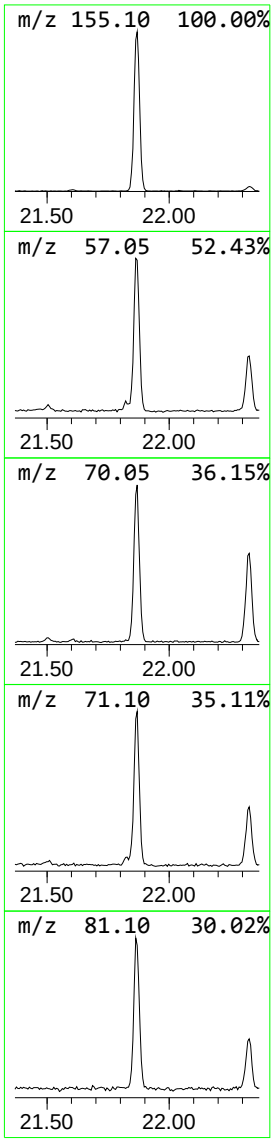
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,2-Cyclohexanedicarboxylic... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.869	9.27 ng/ul	1062120	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	80
2	1,2-Cyclohexanedicarboxylic acid...	312	C18H32O4	1000339-55-6	53
3	1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	53
4	1,2-Cyclohexanedicarboxylic acid...	438	C27H50O4	1000339-46-0	50
5	1,2-Cyclohexanedicarboxylic acid...	300	C16H28O5	1000339-90-7	49





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Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

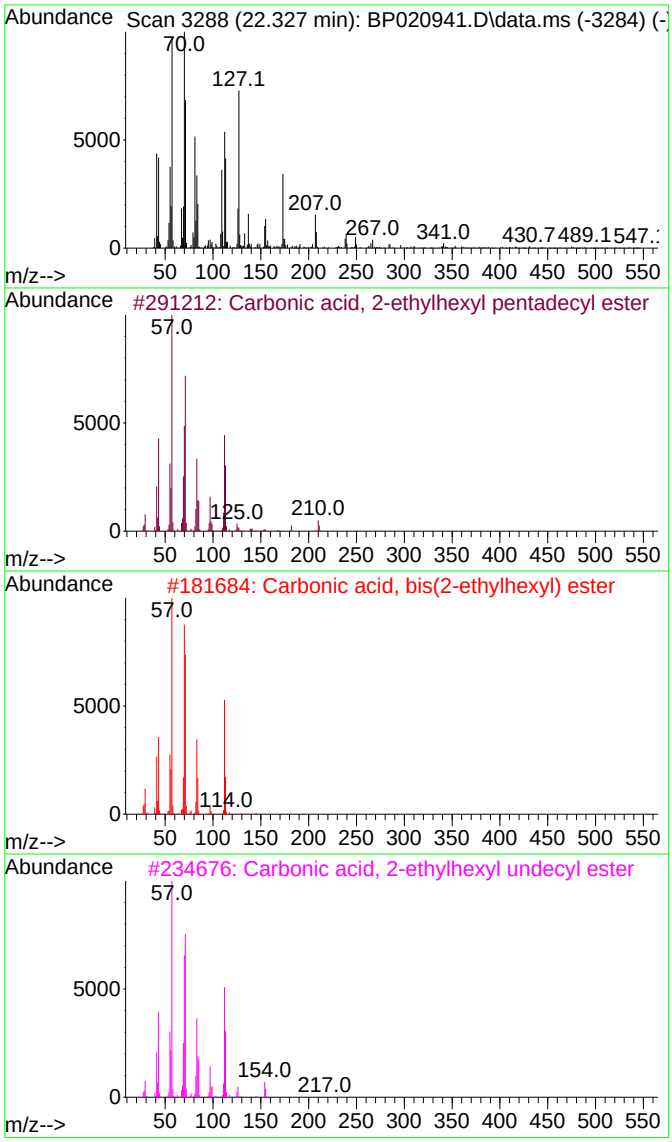
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

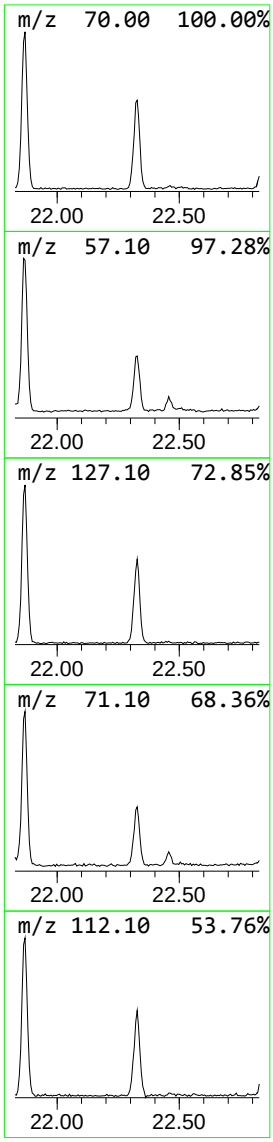
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.327	3.11 ng/ul	356079	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-ethylhexyl pent...	384	C24H48O3	1000383-14-2	47
2	Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	47
3	Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	38
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	27
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

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

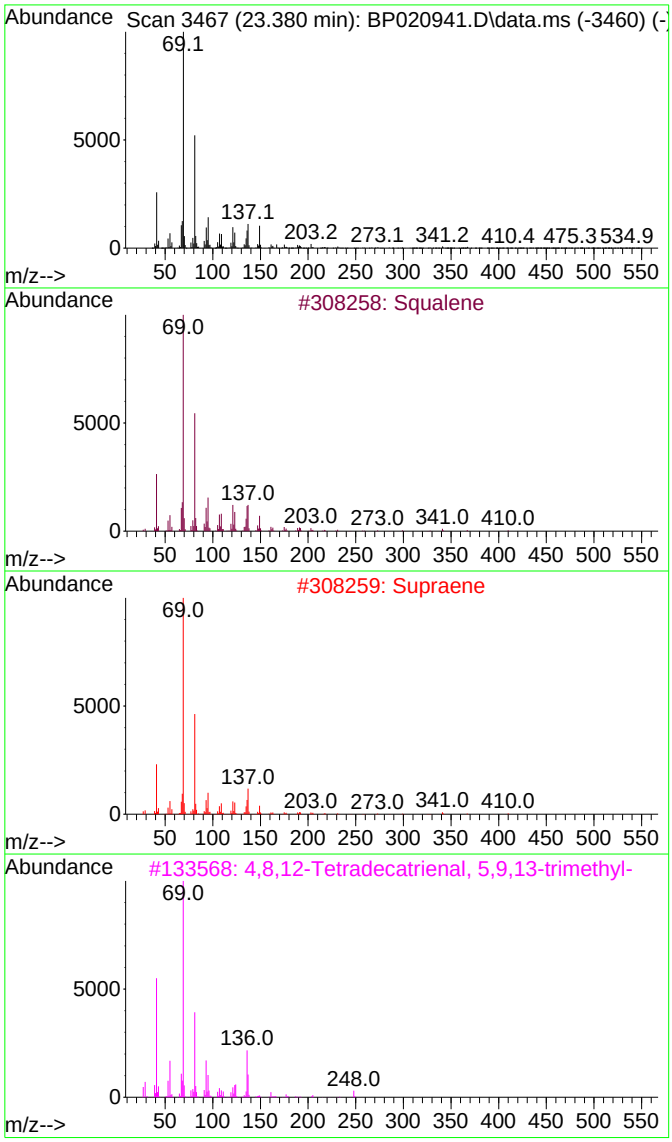
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

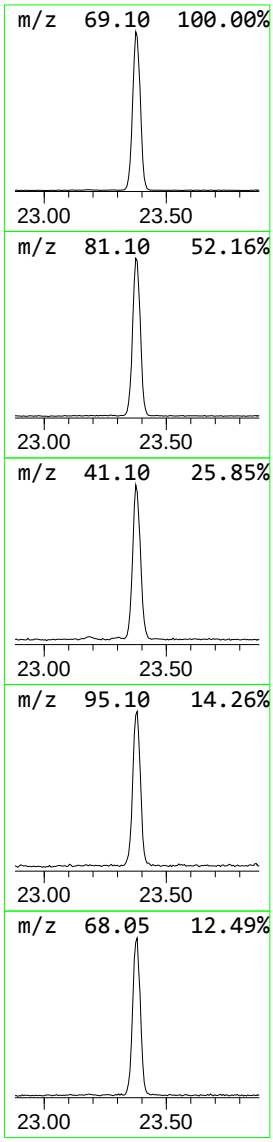
****

Peak Number 7 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.380	22.69 ng/ul	2834320	Perylene-d12	24.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	89
2	Supraene	410	C30H50	007683-64-9	83
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	68
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020941.D
Acq On : 12 Jul 2024 20:11
Operator : MA/JU
Sample : P3231-01
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E08E9

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
Nonanoic acid	11.293	2.7	ng/ul	168374	2	10.475	1244340	20.0
Phenol, 4-(1,1-...	13.181	13.0	ng/ul	1039500	3	14.339	1604590	20.0
n-Hexadecanoic ...	18.081	7.7	ng/ul	745738	4	17.151	1946700	20.0
Octadecanoic acid	19.422	3.5	ng/ul	406077	5	21.598	2291040	20.0
1,2-Cyclohexane...	21.869	9.3	ng/ul	1062120	5	21.598	2291040	20.0
unknown-01	22.327	3.1	ng/ul	356079	5	21.598	2291040	20.0
Squalene	23.380	22.7	ng/ul	2834320	6	24.933	2498690	20.0