LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

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_M\Methods\SFAM-EPA-BM110724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM048559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	20	24	32	rVB	35020	56828	1.29%	0.109%
2	3.552	92	96	112	rBV	188597	340495	7.74%	0.655%
3	3.769	129	133	141	rVB5	13631	27435	0.62%	0.053%
4	3.869	145	150	155	rVB2	11419	19439	0.44%	0.037%
5	4.228	208	211	218	rVB5	13283	22877	0.52%	0.044%
6	5.175	369	372	377	rBV2	14725	23412	0.53%	0.045%
7	5.722	460	465	467	rBV2	33173	51774	1.18%	0.100%
8	5.757	467	471	482	rVB	104846	169206	3.85%	0.326%
9	6.316	561	566	573	rBV	51658	82293	1.87%	0.158%
10	6.687	623	629	635	rBV2	17077	29508	0.67%	0.057%
11	6.845	646	656	666	rVB	171561	330373	7.51%	0.636%
12	6.998	676	682	693	rBV	514308	827050	18.80%	1.592%
13	7.198	705	716	726	rBV	596499	987553	22.44%	1.901%
14	7.457	754	760	768	rBV6	10700	26260	0.60%	0.051%
15	7.663	787	795	801	rBV	621729	1017389	23.12%	1.959%
16	7.734	801	807	817	rVB	112408	198632	4.51%	0.382%
17	7.822	818	822	829	rVB7	10473	19578	0.44%	0.038%
18	7.916	830	838	843	rBV	53616	100980	2.29%	0.194%
19	8.281	892	900	906	rBV8	9502	24809	0.56%	0.048%
20	8.381	911	917	925	rVV	534261	927929	21.09%	1.786%
21	8.451	925	929	933	rVV2	51733	89496	2.03%	0.172%
22	8.487	933	935	939	rVV	25379	35984	0.82%	0.069%
23	8.757	975	981	986	rBV2	72537	132849	3.02%	0.256%
24	8.816	986	991	1001	rVV	579285	987525	22.44%	1.901%
25	8.910	1001	1007	1013	rVV	129032	207573	4.72%	0.400%
26	8.992	1016	1021	1035	rVB	80941	161779	3.68%	0.311%
27	9.239	1052	1063	1075	rVB3	46765	95307	2.17%	0.183%
28	9.392	1082	1089	1094	rVB8	9987	20954	0.48%	0.040%
29	9.539	1104	1114	1130	rBV	474386	873626	19.85%	1.682%
30	9.716	1136	1144	1154	rVV4	95529	228599	5.20%	0.440%
31	9.792	1154	1157	1166	rVV4	19550	42048	0.96%	0.081%
32	9.928	1174	1180	1189	rBV2	88851	209956	4.77%	0.404%
33	10.081	1198	1206	1223	rBV	816320	1464246	33.28%	2.819%
34	10.239	1226	1233	1240	rBV4	27200	61435	1.40%	0.118%
35	10.310	1241	1245	1249	rVB6	12581	18629	0.42%	0.036%
36	10.363	1249	1254	1261	rVB6	11833	23113	0.53%	0.044%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
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Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A4EC3

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_M\Methods\SFAM-EPA-BM110724.MA.M
Title : SVOA CALIBRATION

37	10.445	1261	1268	1277	rBV	843643	1473995	33.50%	2.838%
38	10.510	1277	1279	1286	rVB3	32228	37706	0.86%	0.073%
39	10.592	1286	1293	1307	rBV	348054	756150	17.18%	1.456%
40	10.745	1313	1319	1330	rVB2	57592	121470	2.76%	0.234%
41	10.845	1330	1336	1345	rBV3	28312	61809	1.40%	0.119%
42	10.992	1356	1361	1367	rBV2	17099	35709	0.81%	0.069%
43	11.057	1368	1372	1376	rVV2	16818	30241	0.69%	0.058%
44	11.110	1376	1381	1390	rVB	22394	44355	1.01%	0.085%
45	11.263	1397	1407	1416	rBV7	28384	69889	1.59%	0.135%
46	11.475	1437	1443	1449	rVB5	11484	20730	0.47%	0.040%
47	11.733	1480	1487	1492	rBV2	34861	56523	1.28%	0.109%
48	11.869	1503	1510	1518	rVB10	13194	31589	0.72%	0.061%
49	12.045	1536	1540	1546	rVB2	14475	21244	0.48%	0.041%
50	12.598	1628	1634	1640	rBV5	8796	18078	0.41%	0.035%
51	12.663	1640	1645	1658	rVV2	58836	124761	2.84%	0.240%
52	12.916	1682	1688	1694	rBV	112009	156604	3.56%	0.301%
53	13.239	1734	1743	1761	rBV	95210	240034	5.46%	0.462%
54	13.551	1790	1796	1805	rVB4	30527	56074	1.27%	0.108%
55	13.721	1818	1825	1836	rBV	1360813	1943305	44.16%	3.741%
56	13.845	1841	1846	1851	rBV4	23093	31567	0.72%	0.061%
57	13.963	1861	1866	1868	rBV	109406	165520	3.76%	0.319%
58	14.004	1868	1873	1883	rVB	1544468	2335277	53.07%	4.496%
59	14.186	1900	1904	1911	rBV4	16470	34647	0.79%	0.067%
60	14.263	1911	1917	1921	rBV2	1145778	1789167	40.66%	3.444%
61	14.310	1921	1925	1944	rVB2	1570282	2925632	66.49%	5.632%
62	14.551	1960	1966	1980	rBV4	63712	176084	4.00%	0.339%
63	14.751	1994	2000	2009	rBV2	43661	83926	1.91%	0.162%
64	14.998	2036	2042	2045	rBV6	14634	26987	0.61%	0.052%
65	15.063	2049	2053	2058	rVV	25986	37644	0.86%	0.072%
66	15.139	2058	2066	2076	rVB3	34333	73981	1.68%	0.142%
67	15.304	2088	2094	2107	rVB	2120999	3009140	68.39%	5.793%
68	15.445	2111	2118	2131	rBV	542617	840017	19.09%	1.617%
69	15.674	2152	2157	2173	rVB	45830	81846	1.86%	0.158%
70	15.868	2184	2190	2196	rVB4	47132	70511	1.60%	0.136%
71	16.021	2204	2216	2221	rBV4	8771	31575	0.72%	0.061%
72	16.080	2221	2226	2227	rVV	184471	214098	4.87%	0.412%
73	16.104	2227	2230	2247	rVV	325311	619275	14.07%	1.192%
74	16.233	2249	2252	2257	rVV2	19057	30928	0.70%	0.060%
75	17.057	2383	2392	2398	rBV	1453702	2064078	46.91%	3.973%
76	17.157	2402	2409	2419	rVV	2215719	3251235	73.89%	6.259%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

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_M\Methods\SFAM-EPA-BM110724.MA.M
Title : SVOA CALIBRATION

77	17.345	2437	2441	2445	rVV2	15689	21062	0.48%	0.041%
78	17.615	2482	2487	2489	rBV	24253	31265	0.71%	0.060%
79	17.639	2489	2491	2499	rVV	17247	39330	0.89%	0.076%
80	17.727	2500	2506	2517	rVB	1990687	2540476	57.74%	4.891%
81	17.957	2539	2545	2553	rBV2	264602	412807	9.38%	0.795%
82	18.027	2553	2557	2561	rVB	37201	53904	1.23%	0.104%
83	18.168	2577	2581	2584	rBV	26991	33865	0.77%	0.065%
84	18.204	2584	2587	2592	rVV5	17878	25120	0.57%	0.048%
85	18.451	2624	2629	2633	rBV4	26924	42347	0.96%	0.082%
86	18.709	2670	2673	2681	rBV5	14303	27126	0.62%	0.052%
87	18.898	2701	2705	2710	rBV8	10620	20751	0.47%	0.040%
88	19.015	2721	2725	2729	rBV2	35361	55035	1.25%	0.106%
89	19.086	2733	2737	2740	rVV	35099	49163	1.12%	0.095%
90	19.121	2740	2743	2752	rVB5	28265	49328	1.12%	0.095%
91	19.239	2757	2763	2781	rBV	555299	973625	22.13%	1.874%
92	19.380	2784	2787	2793	rVB4	18625	25360	0.58%	0.049%
93	19.451	2793	2799	2807	rBV	3027402	4086373	92.87%	7.866%
94	19.686	2836	2839	2844	rVB7	21465	30499	0.69%	0.059%
95	19.833	2861	2864	2873	rVB7	21377	31920	0.73%	0.061%
96	20.945	3050	3053	3060	rVB	132975	194974	4.43%	0.375%
97	21.280	3104	3110	3123	rBV	1618326	2426852	55.15%	4.672%
98	22.627	3334	3339	3348	rVB4	204138	396152	9.00%	0.763%
99	23.991	3562	3571	3583	rVB	1816500	4400199	100.00%	8.471%
100	24.191	3596	3605	3617	rVB	1118609	2848950	64.75%	5.484%

Sum of corrected areas: 51946823

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
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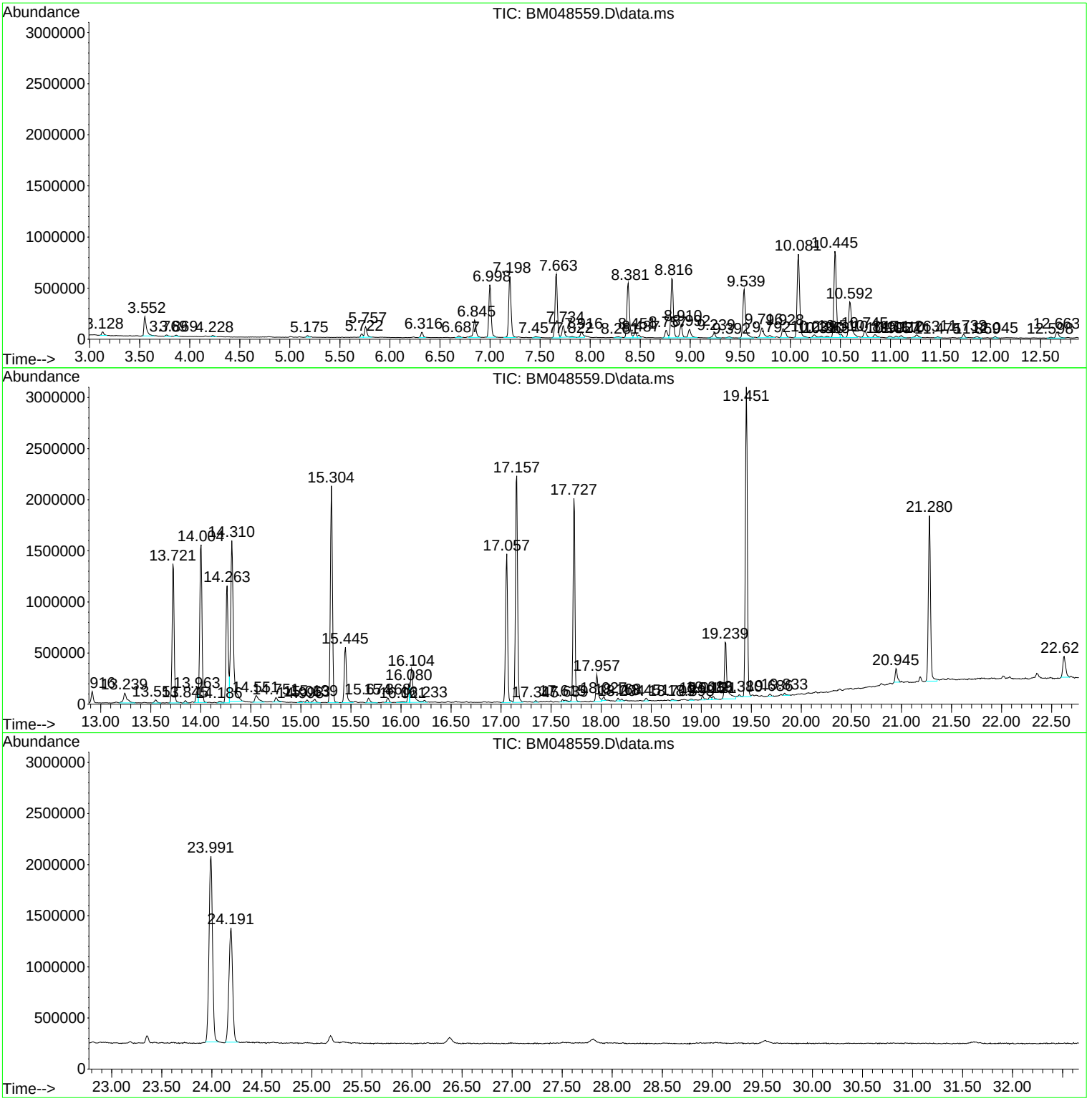
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

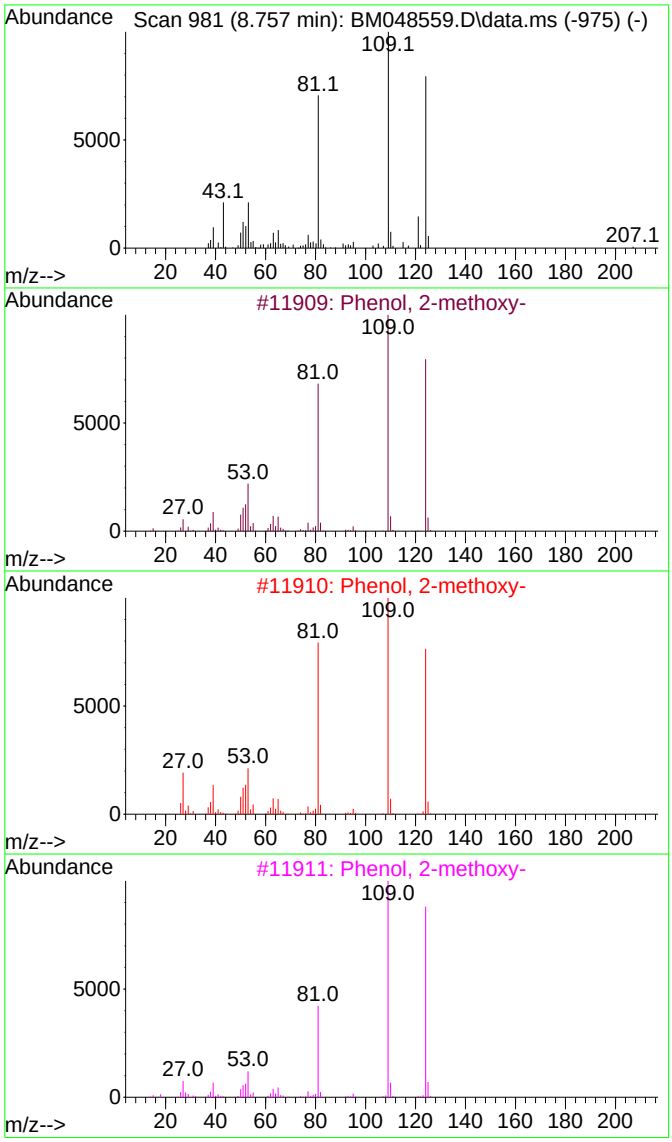
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

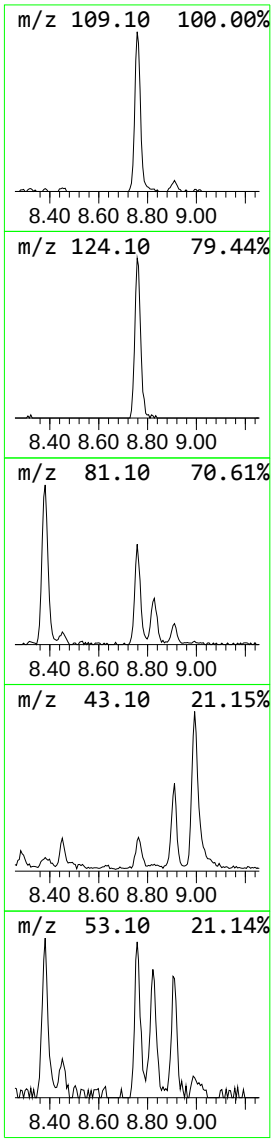
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 2-methoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.757	2.61 ng/ul	132849	1,4-Dichlorobenzene-d4	7.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
4	Mequinol	124	C7H8O2	000150-76-5	87
5	Mequinol	124	C7H8O2	000150-76-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

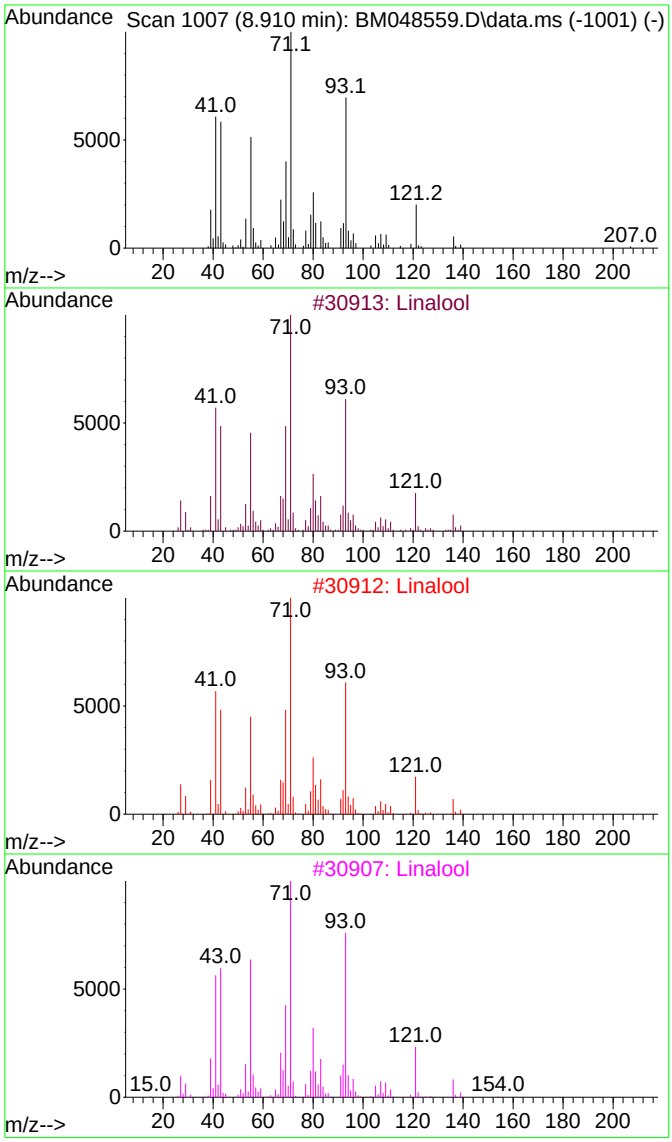
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

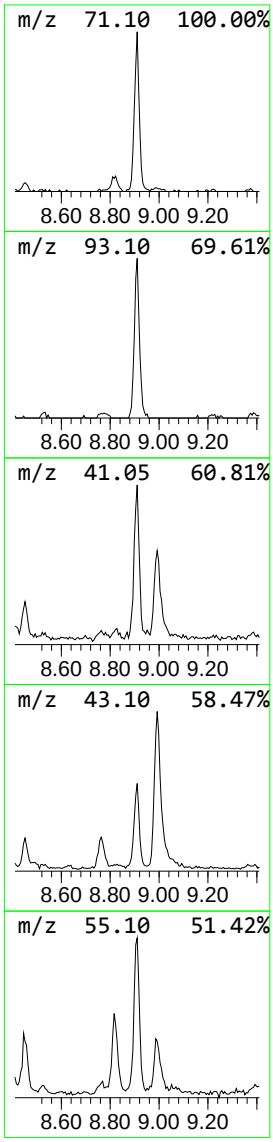
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Linalool Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	4.08 ng/ul	207573	1,4-Dichlorobenzene-d4	7.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linalool	154	C10H18O	000078-70-6	86
2	Linalool	154	C10H18O	000078-70-6	86
3	Linalool	154	C10H18O	000078-70-6	58
4	1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H18O2	000115-99-1	49
5	1,5-Dimethyl-1-vinyl-4-hexenyl b...	224	C14H24O2	000078-36-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

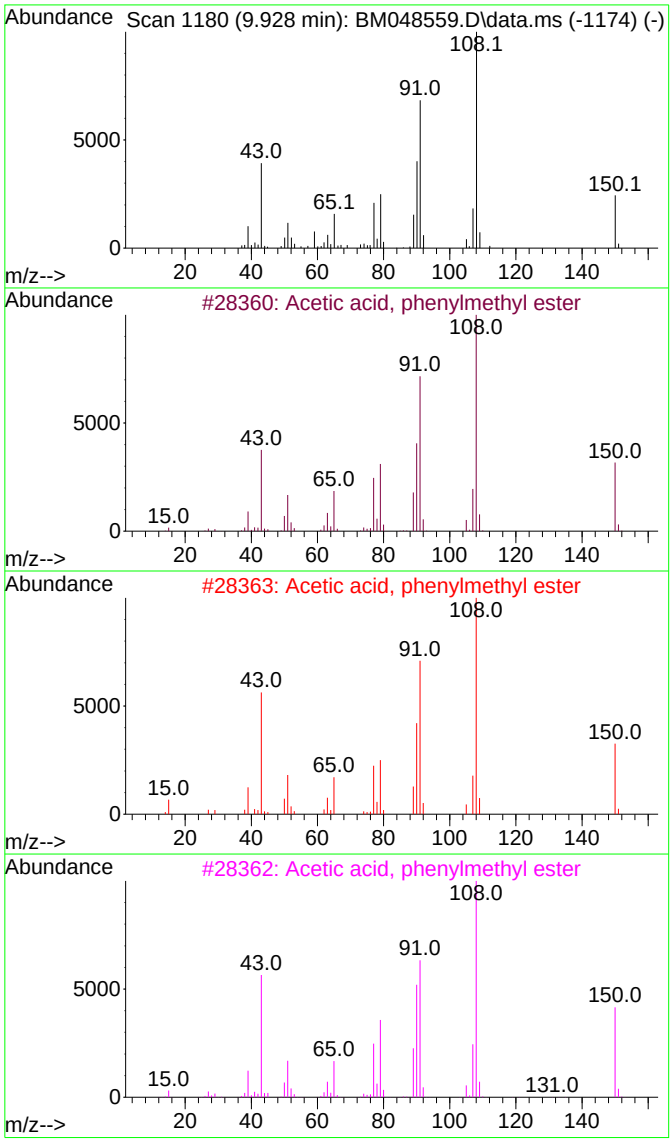
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

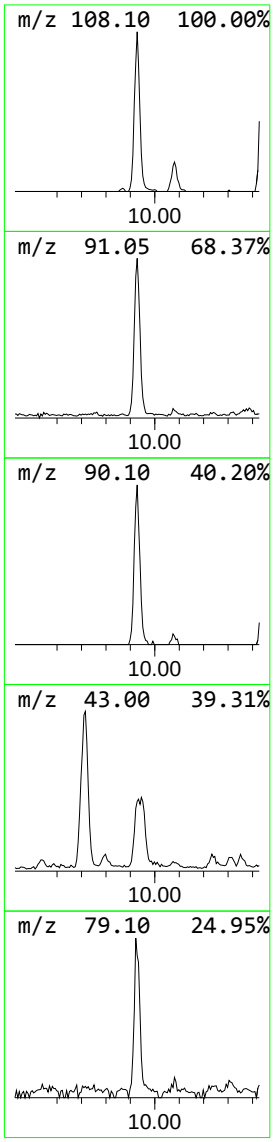
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, phenylmethyl e... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	2.85 ng/ul	209956	Naphthalene-d8	10.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
2	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
3	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	94
4	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	94
5	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
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Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

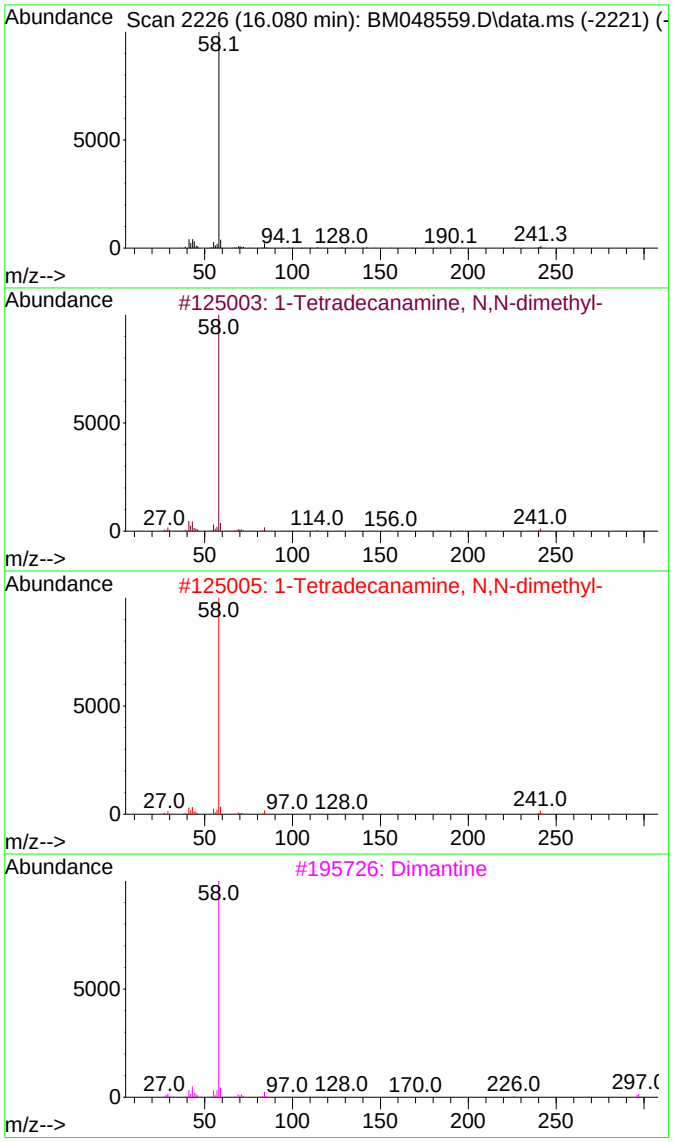
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

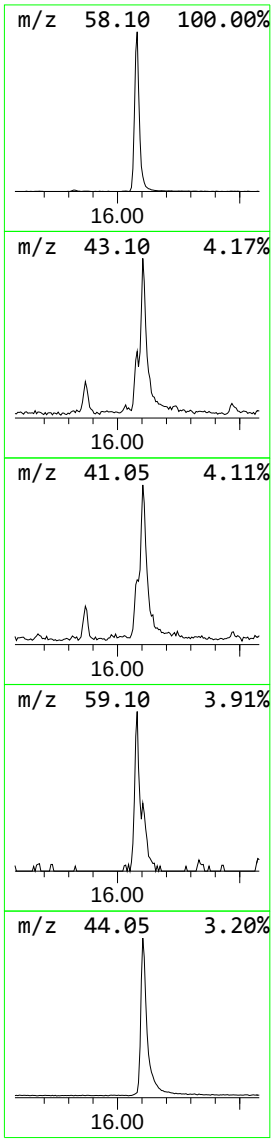
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Tetradecanamine, N,N-dime... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	2.07 ng/ul	214098	Phenanthrene-d10	17.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	90
2	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	90
3	Dimantine	297	C20H43N	000124-28-7	78
4	Tetradonium Bromide	335	C17H38BrN	001119-97-7	78
5	Dimantine	297	C20H43N	000124-28-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

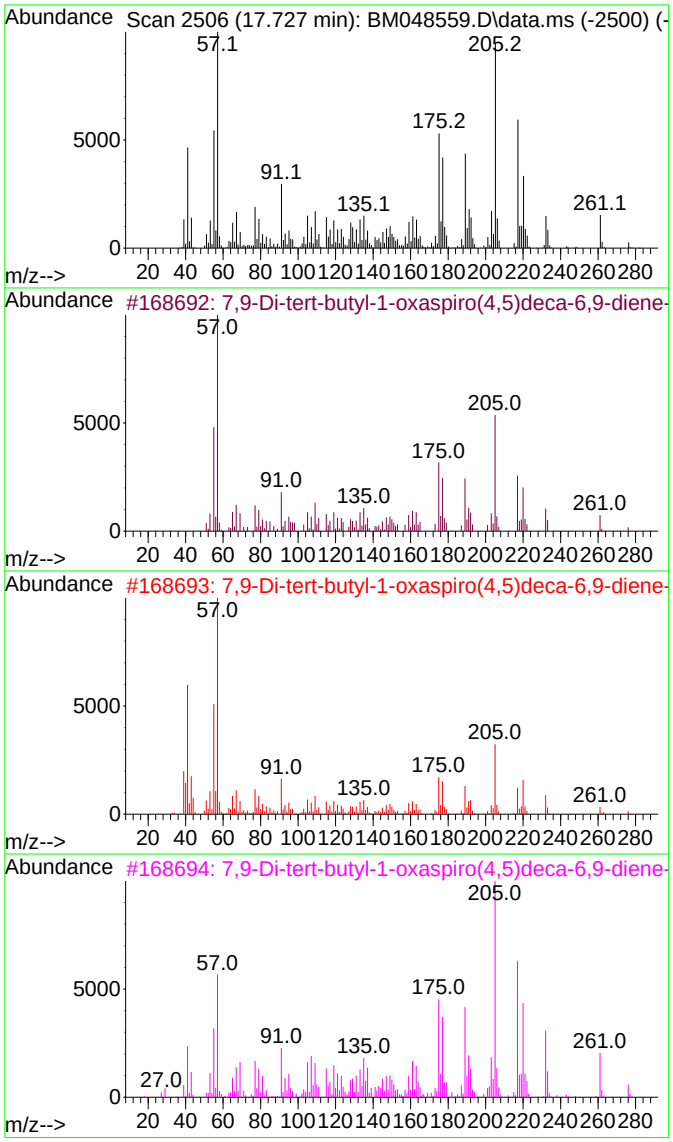
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

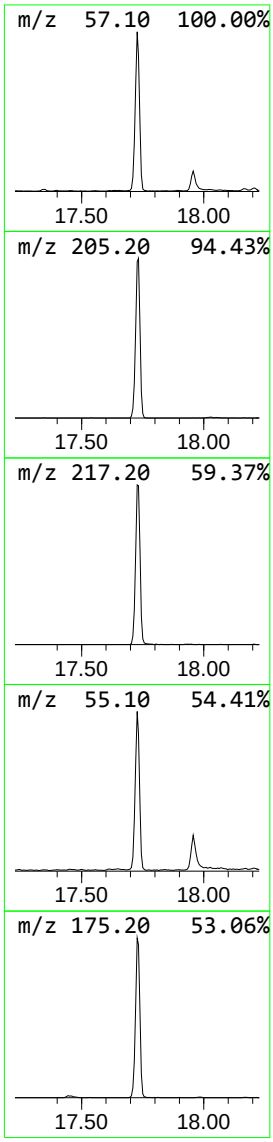
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	24.62 ng/ul	2540480	Phenanthrene-d10	17.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	64
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	50
4	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	50
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	49





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Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

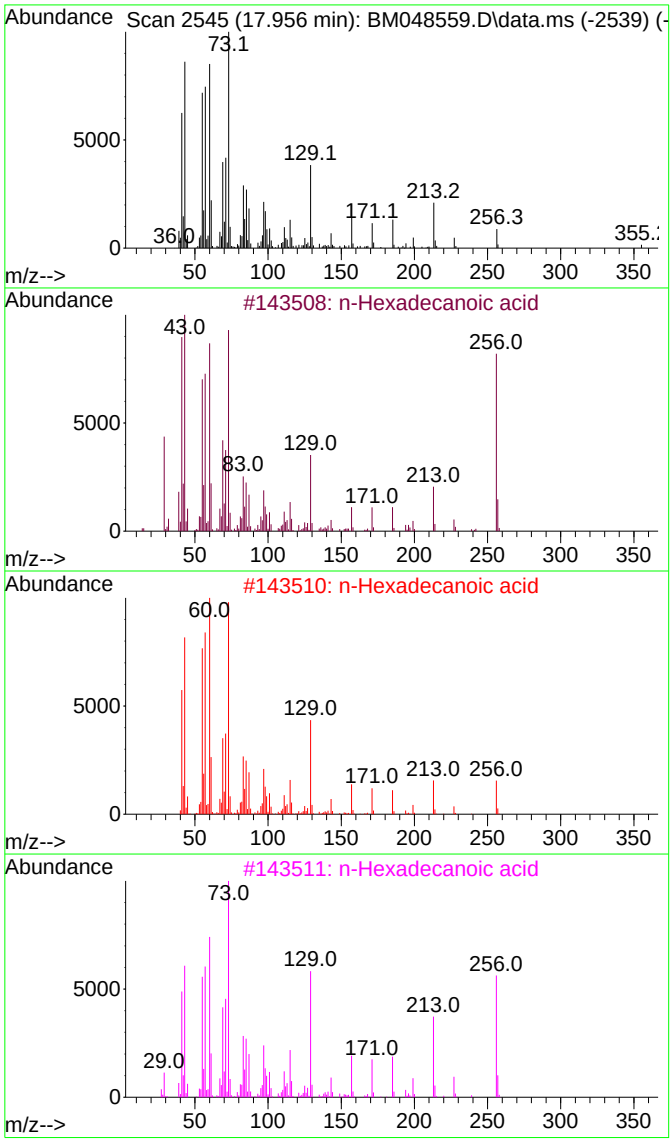
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

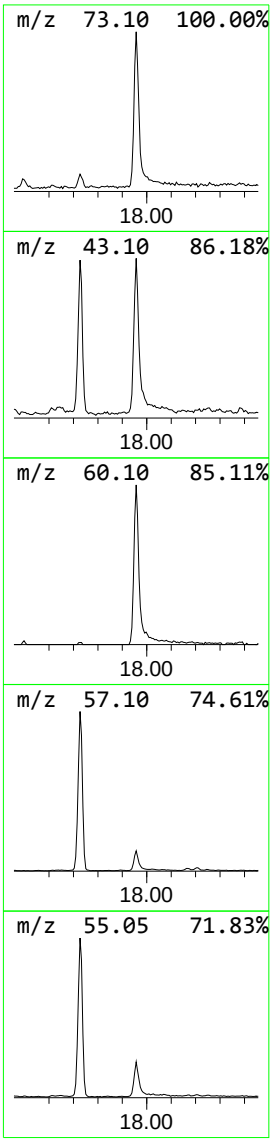
****

Peak Number 11 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.956	4.00 ng/ul	412807	Phenanthrene-d10	17.057

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

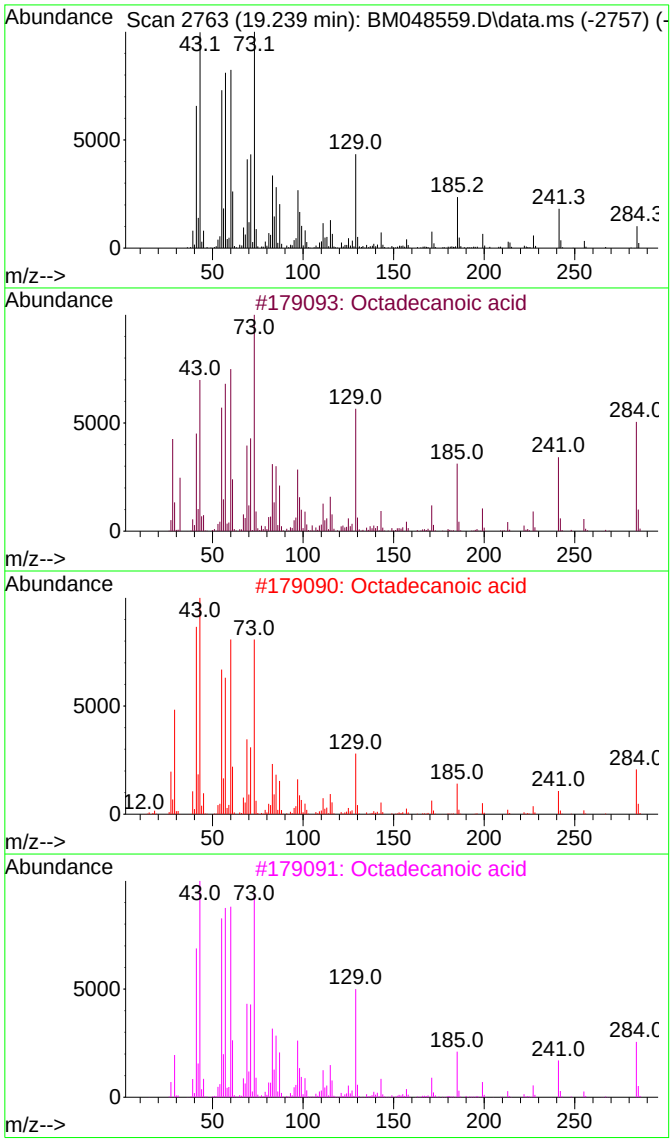
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

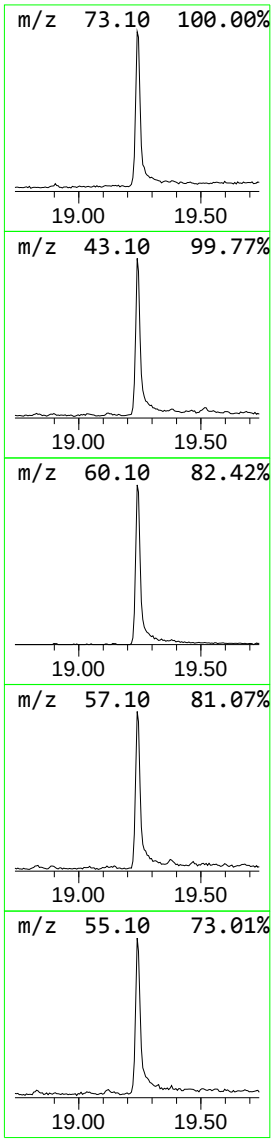
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.239	8.02 ng/ul	973625	Chrysene-d12	21.280

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	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

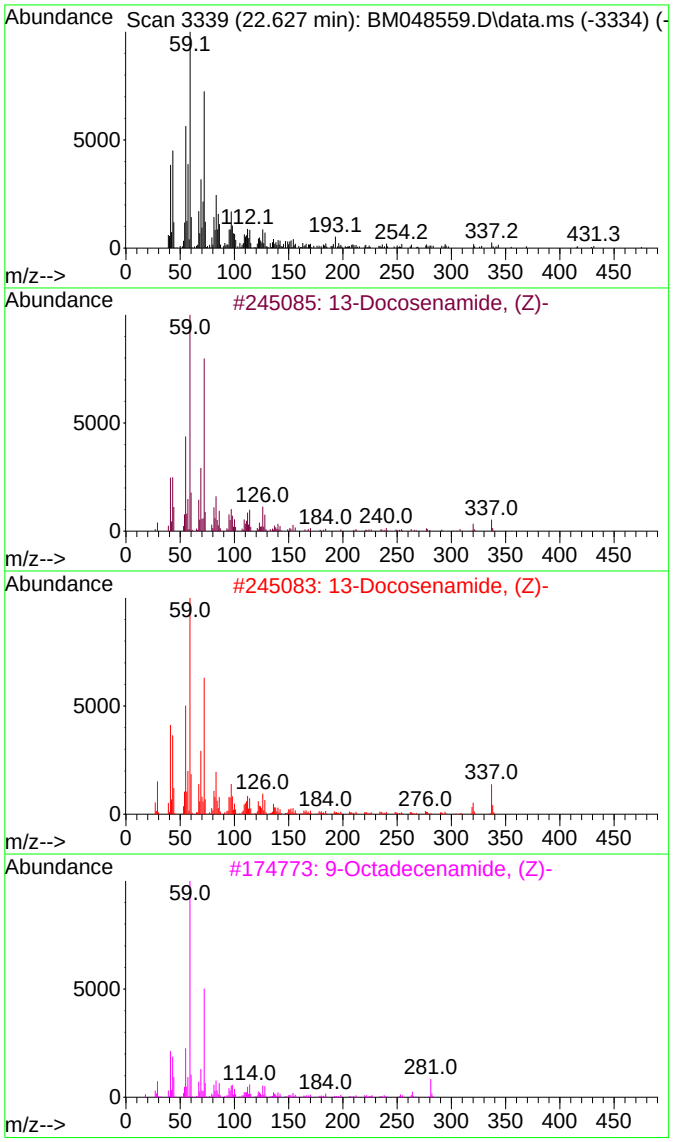
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.MA.M
Quant Title : SVOA CALIBRATION

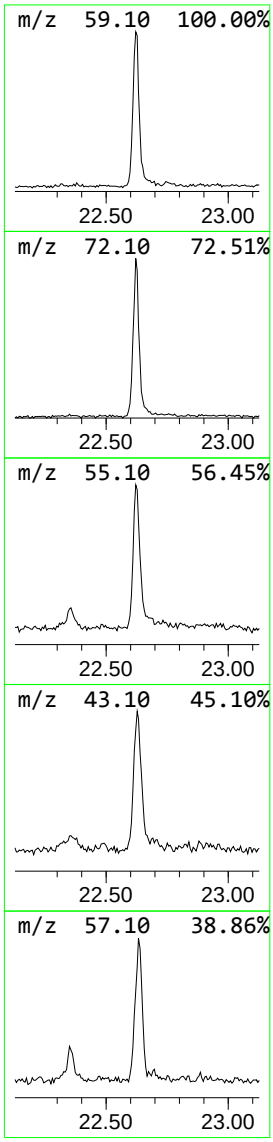
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.627	3.26 ng/ul	396152	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	92
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	76
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110824\
Data File : BM048559.D
Acq On : 09 Nov 2024 10:40
Operator : RC/JU
Sample : P4585-03
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM110724.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
Phenol, 2-methoxy-	8.757	2.6	ng/ul	132849	1	7.663	1017390	20.0
Linalool	8.910	4.1	ng/ul	207573	1	7.663	1017390	20.0
Acetic acid, ph...	9.928	2.9	ng/ul	209956	2	10.445	1474000	20.0
1-Tetradecanami...	16.080	2.1	ng/ul	214098	4	17.057	2064080	20.0
7,9-Di-tert-but...	17.727	24.6	ng/ul	2540480	4	17.057	2064080	20.0
n-Hexadecanoic ...	17.956	4.0	ng/ul	412807	4	17.057	2064080	20.0
Octadecanoic acid	19.239	8.0	ng/ul	973625	5	21.280	2426850	20.0
13-Docosenamide...	22.627	3.3	ng/ul	396152	5	21.280	2426850	20.0