LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : GCD00

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-BP101823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP017758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	26	29	37	rVB	16676	25450	1.72%	0.119%
2	3.705	102	105	111	rBV	27151	46154	3.11%	0.216%
3	3.799	119	121	124	rVB4	7367	7156	0.48%	0.034%
4	3.869	129	133	140	rVB	34749	51342	3.46%	0.240%
5	4.216	188	192	200	rVB4	15020	21930	1.48%	0.103%
6	4.375	217	219	223	rVB4	6525	6396	0.43%	0.030%
7	4.634	260	263	268	rVB5	9270	13837	0.93%	0.065%
8	4.922	307	312	320	rBV	55664	81652	5.51%	0.382%
9	5.452	397	402	404	rBV6	3614	6322	0.43%	0.030%
10	5.505	409	411	416	rVB5	3784	5285	0.36%	0.025%
11	6.028	497	500	503	rVB5	2314	3075	0.21%	0.014%
12	6.481	572	577	580	rBV5	8821	12563	0.85%	0.059%
13	7.046	667	673	684	rBV	214063	406482	27.42%	1.904%
14	7.228	698	704	717	rVV	209915	339383	22.90%	1.590%
15	7.405	728	734	750	rBV	260970	433755	29.26%	2.032%
16	7.693	781	783	788	rVB5	3708	5211	0.35%	0.024%
17	7.881	808	815	824	rBV	447877	729617	49.22%	3.418%
18	8.052	840	844	848	rVB5	12119	17590	1.19%	0.082%
19	8.610	931	939	955	rBV	201971	395845	26.71%	1.854%
20	8.746	957	962	969	rVB	61092	97855	6.60%	0.458%
21	9.093	1014	1021	1032	rVV	210924	369145	24.90%	1.729%
22	9.281	1050	1053	1058	rVB7	3881	5409	0.36%	0.025%
23	9.475	1080	1086	1088	rBV7	2293	4194	0.28%	0.020%
24	9.810	1136	1143	1156	rBV	147828	272918	18.41%	1.278%
25	10.010	1174	1177	1180	rBV5	2662	4035	0.27%	0.019%
26	10.181	1201	1206	1214	rVB5	6754	14660	0.99%	0.069%
27	10.340	1226	1233	1245	rBV	219721	447571	30.20%	2.096%
28	10.716	1290	1297	1305	rBV	619597	996848	67.25%	4.669%
29	10.898	1322	1328	1342	rBV2	89889	214513	14.47%	1.005%
30	11.775	1474	1477	1481	rVB6	3041	4508	0.30%	0.021%
31	12.228	1552	1554	1557	rVV4	2262	2947	0.20%	0.014%
32	12.269	1557	1561	1562	rVV4	2656	3184	0.21%	0.015%
33	12.316	1565	1569	1576	rVV8	5863	11720	0.79%	0.055%
34	12.634	1617	1623	1627	rVB9	2668	4615	0.31%	0.022%
35	12.816	1650	1654	1657	rBV6	2414	4394	0.30%	0.021%
36	12.857	1657	1661	1670	rVV2	22483	36214	2.44%	0.170%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
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Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

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-BP101823.MA.M
Title : SVOA CALIBRATION

37	13.140	1702	1709	1712	rBV9	1896	3757	0.25%	0.018%
38	13.269	1727	1731	1734	rVV6	3547	3373	0.23%	0.016%
39	13.387	1746	1751	1753	rBV2	22444	33498	2.26%	0.157%
40	13.416	1753	1756	1763	rVB2	27219	45688	3.08%	0.214%
41	13.751	1810	1813	1816	rBV5	2160	3500	0.24%	0.016%
42	13.792	1816	1820	1823	rVV6	3249	5136	0.35%	0.024%
43	13.840	1823	1828	1833	rVB9	5833	10705	0.72%	0.050%
44	13.998	1849	1855	1862	rBV	520128	720876	48.63%	3.377%
45	14.281	1896	1903	1912	rBV	566050	853213	57.56%	3.997%
46	14.487	1934	1938	1944	rBV9	6333	11776	0.79%	0.055%
47	14.581	1945	1954	1965	rVV	910661	1301565	87.81%	6.097%
48	14.781	1985	1988	1992	rBV5	9628	12306	0.83%	0.058%
49	14.851	1995	2000	2017	rVV3	40128	137746	9.29%	0.645%
50	14.969	2018	2020	2024	rVB5	6201	7677	0.52%	0.036%
51	15.163	2048	2053	2059	rBV8	13101	24600	1.66%	0.115%
52	15.328	2076	2081	2086	rVB8	5806	12230	0.83%	0.057%
53	15.369	2086	2088	2091	rBV4	3023	3540	0.24%	0.017%
54	15.416	2092	2096	2099	rVB6	3197	4688	0.32%	0.022%
55	15.586	2115	2125	2132	rBV	762079	1082248	73.01%	5.069%
56	15.657	2135	2137	2142	rVB5	7409	10873	0.73%	0.051%
57	15.734	2144	2150	2161	rBV	109613	188142	12.69%	0.881%
58	15.839	2163	2168	2173	rVB8	6503	12688	0.86%	0.059%
59	15.998	2189	2195	2204	rBV	69472	110735	7.47%	0.519%
60	16.228	2230	2234	2235	rVV4	2469	3476	0.23%	0.016%
61	16.245	2235	2237	2241	rVB5	4357	5673	0.38%	0.027%
62	16.381	2256	2260	2263	rVB6	2654	3055	0.21%	0.014%
63	16.433	2263	2269	2274	rBV10	7267	15350	1.04%	0.072%
64	16.722	2315	2318	2322	rBV6	6114	8100	0.55%	0.038%
65	16.892	2344	2347	2353	rVB8	2348	4120	0.28%	0.019%
66	17.004	2362	2366	2371	rBV6	20072	36717	2.48%	0.172%
67	17.092	2378	2381	2383	rBV3	3408	3271	0.22%	0.015%
68	17.222	2399	2403	2409	rBV3	25314	43358	2.93%	0.203%
69	17.292	2411	2415	2419	rVV6	14929	21614	1.46%	0.101%
70	17.375	2421	2429	2440	rVB	1028074	1482253	100.00%	6.943%
71	17.475	2440	2446	2459	rBV	745781	1075216	72.54%	5.036%
72	17.639	2472	2474	2478	rVB5	5155	5083	0.34%	0.024%
73	17.804	2499	2502	2504	rBV4	4628	5630	0.38%	0.026%
74	17.869	2510	2513	2519	rBV8	6836	9060	0.61%	0.042%
75	17.928	2520	2523	2526	rBV4	10806	13130	0.89%	0.062%
76	18.004	2533	2536	2540	rVB6	9134	12184	0.82%	0.057%

LSC Area Percent Report

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Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

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

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Title : SVOA CALIBRATION

77	18.116	2549	2555	2560	rBV7	23088	44925	3.03%	0.210%
78	18.169	2561	2564	2569	rVV3	36934	46380	3.13%	0.217%
79	18.227	2569	2574	2582	rVV	183892	275655	18.60%	1.291%
80	18.516	2621	2623	2632	rVB9	13820	23650	1.60%	0.111%
81	18.769	2664	2666	2671	rBV6	7031	10605	0.72%	0.050%
82	19.192	2734	2738	2742	rBV2	48446	65486	4.42%	0.307%
83	19.333	2759	2762	2764	rBV4	20991	25884	1.75%	0.121%
84	19.363	2764	2767	2768	rBV2	17396	20150	1.36%	0.094%
85	19.474	2782	2786	2794	rBV2	72129	108684	7.33%	0.509%
86	19.616	2807	2810	2815	rVB3	23994	31383	2.12%	0.147%
87	19.733	2824	2830	2837	rBV	1011151	1305754	88.09%	6.116%
88	20.198	2907	2909	2914	rBV6	20927	22965	1.55%	0.108%
89	20.863	3018	3022	3030	rBV5	112781	200223	13.51%	0.938%
90	21.157	3070	3072	3073	rBV2	40231	32323	2.18%	0.151%
91	21.186	3074	3077	3084	rVB5	74416	132860	8.96%	0.622%
92	21.516	3128	3133	3140	rVB	1053885	1348655	90.99%	6.317%
93	22.086	3228	3230	3236	rVB2	81186	98790	6.66%	0.463%
94	22.657	3323	3327	3337	rVB2	206482	332738	22.45%	1.559%
95	22.898	3365	3368	3373	rVB	126615	184568	12.45%	0.865%
96	23.204	3416	3420	3427	rVB	297204	478846	32.31%	2.243%
97	23.304	3432	3437	3449	rVB4	177176	478921	32.31%	2.243%
98	23.898	3531	3538	3548	rVB	590507	1254547	84.64%	5.876%
99	24.068	3561	3567	3580	rVB	640415	1379129	93.04%	6.460%
100	24.668	3663	3669	3679	rVB	438661	994208	67.07%	4.657%

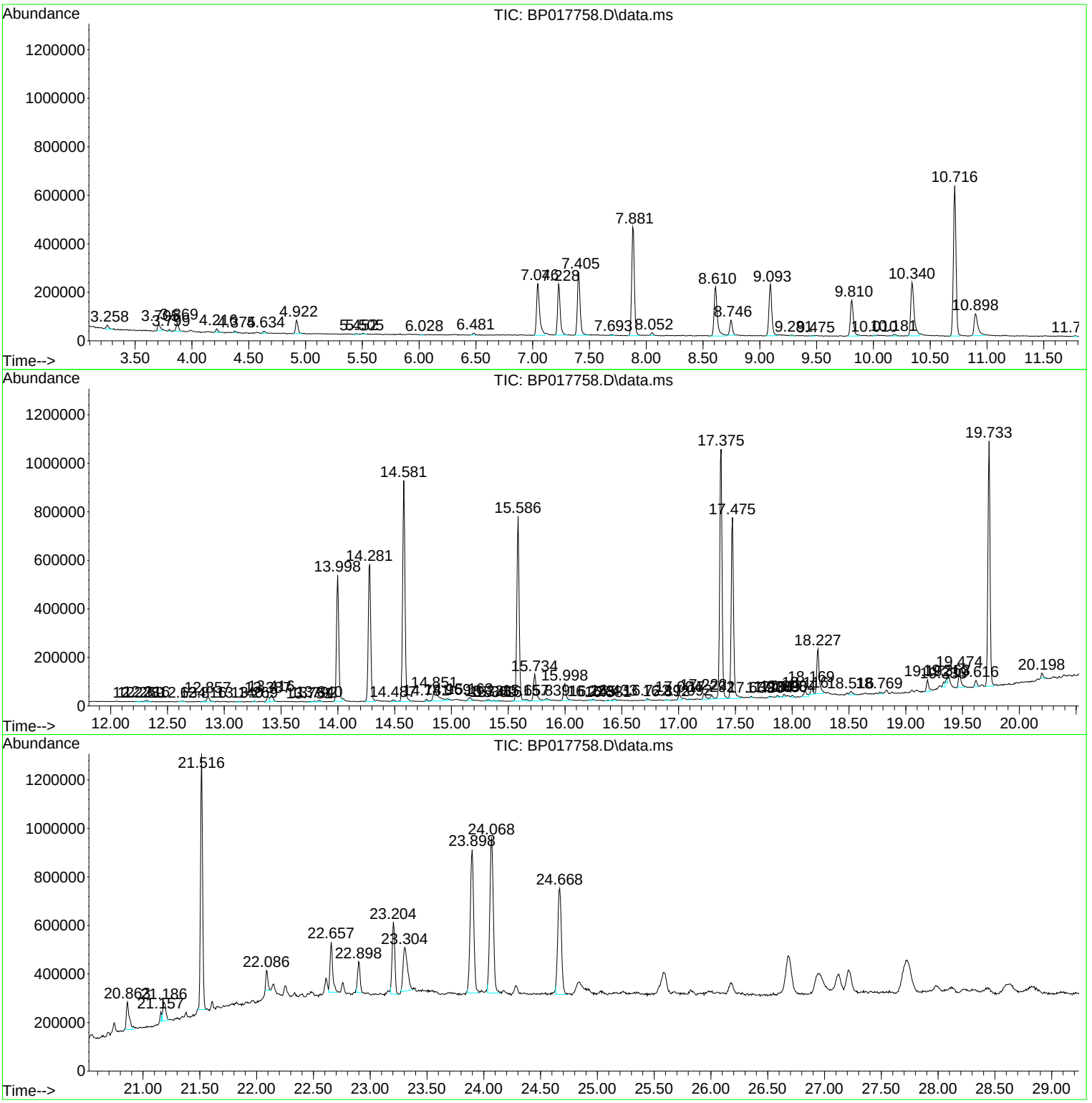
Sum of corrected areas: 21348954

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.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\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

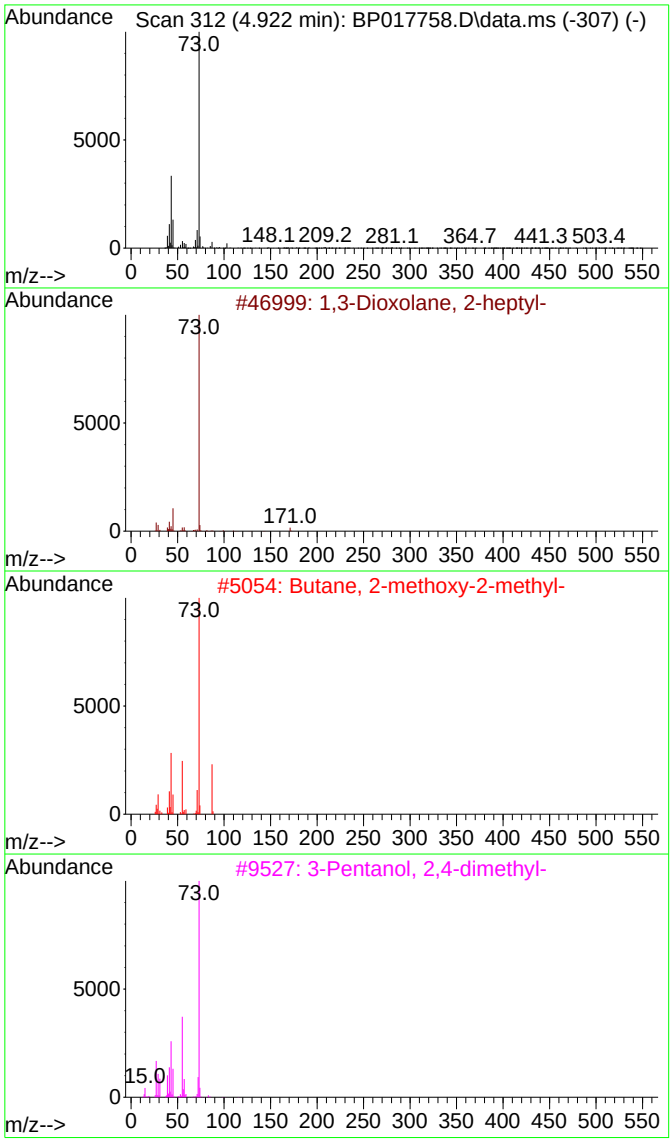
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

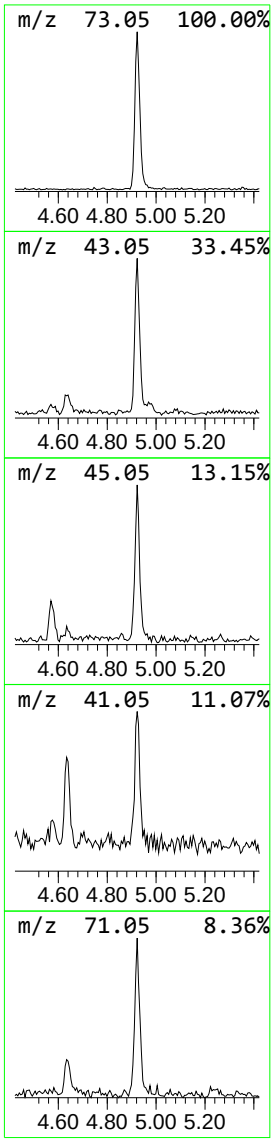
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	2.24 ng/ul	81652	1,4-Dichlorobenzene-d4	7.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	38
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	36
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	33
4	1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	28
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

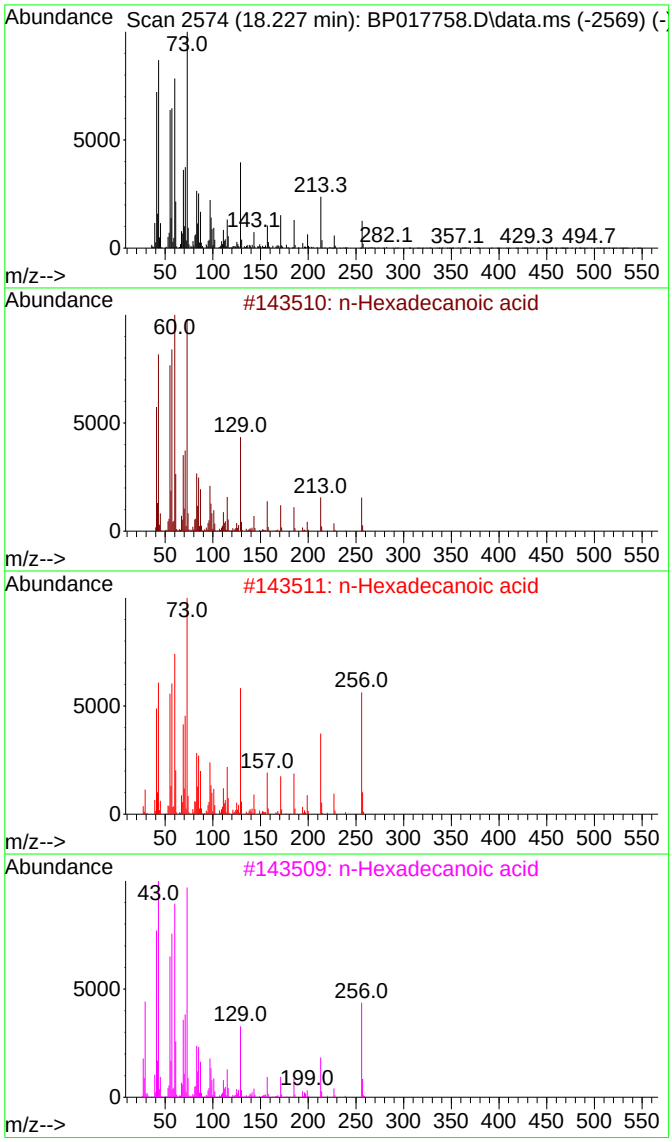
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

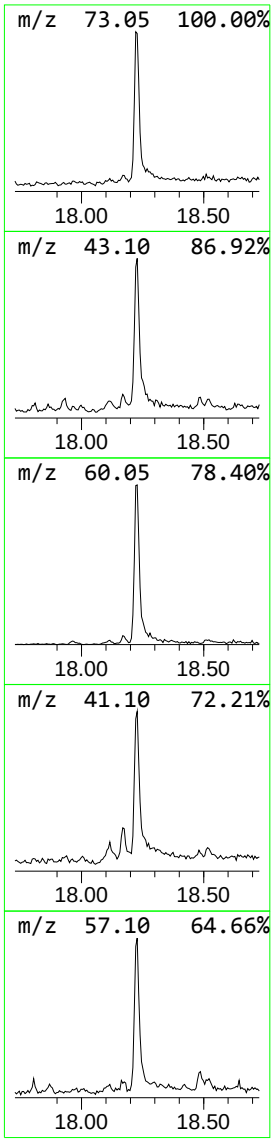
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	3.72 ng/ul	275655	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	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
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Acq On : 23 Oct 2023 20:01
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Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

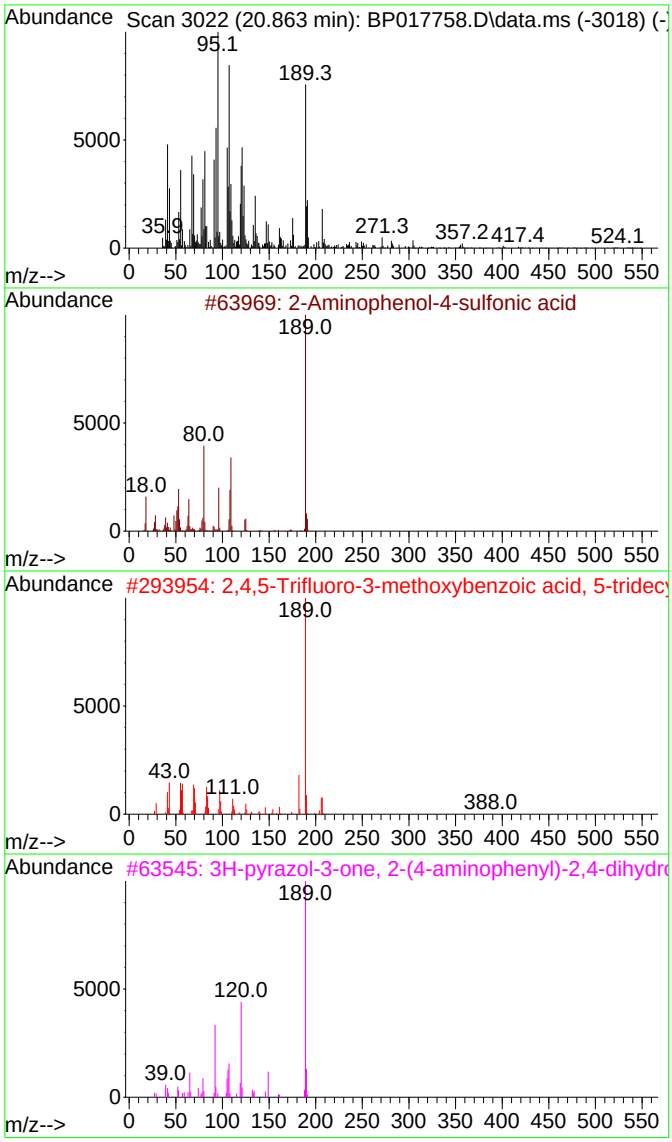
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

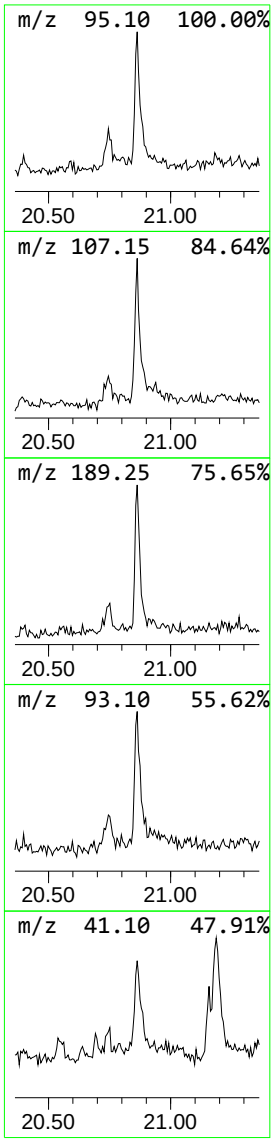
****

Peak Number 3 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.863	2.97 ng/ul	200223	Chrysene-d12	21.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminophenol-4-sulfonic acid	189	C6H7NO4S	000098-37-3	18
2	2,4,5-Trifluoro-3-methoxybenzoic...	388	C21H31F3O3	1000338-45-9	15
3	3H-pyrazol-3-one, 2-(4-aminophen...	189	C10H11N3O	1000400-19-6	14
4	Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	11
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	11





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

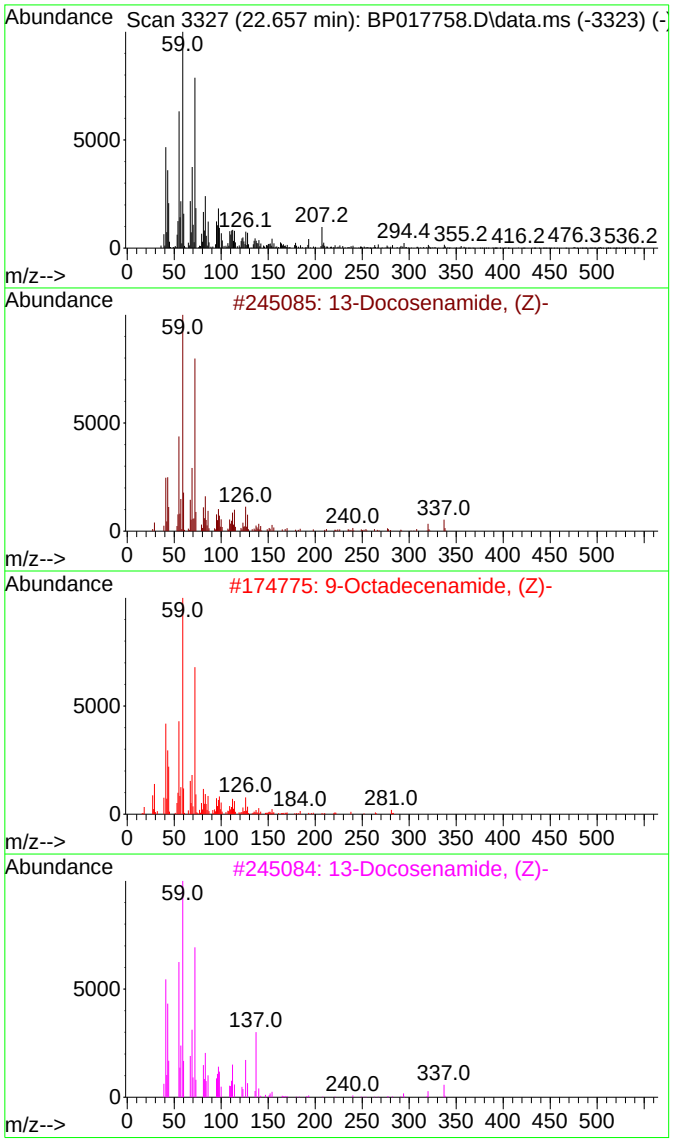
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

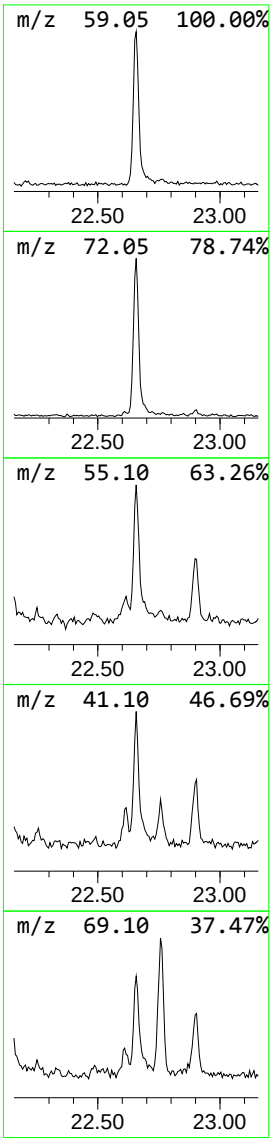
****

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.657	4.93 ng/ul	332738	Chrysene-d12	21.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
4	Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	43
5	7-Nonenamide	155	C9H17NO	090949-53-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

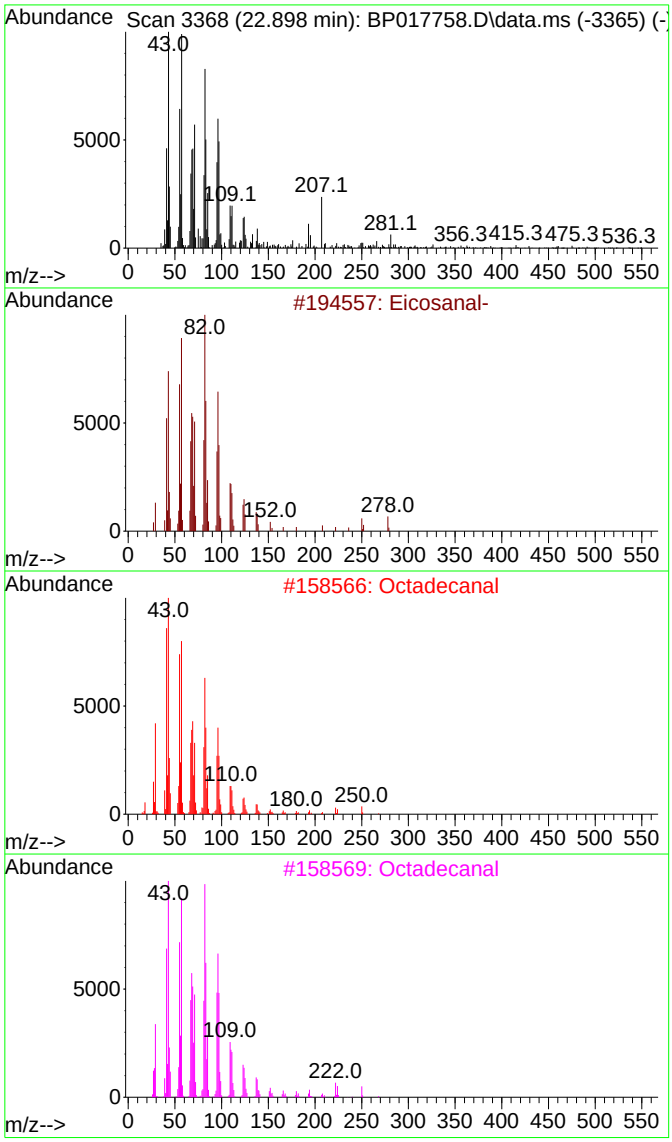
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

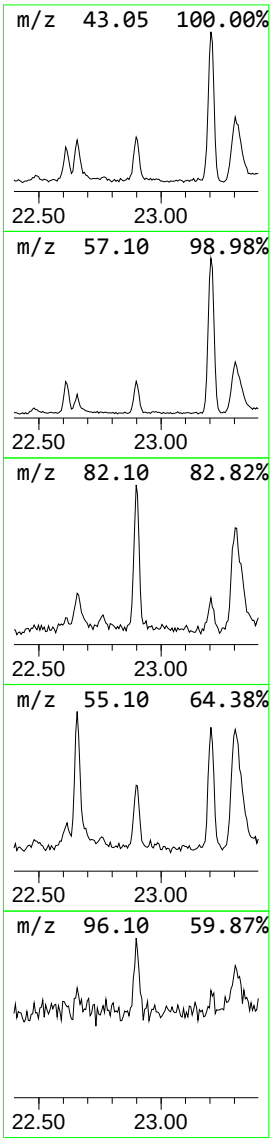
****

Peak Number 5 Eicosanal- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.898	2.68 ng/ul	184568	Perylene-d12	24.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanal-	296	C20H40O	002400-66-0	94
2	Octadecanal	268	C18H36O	000638-66-4	93
3	Octadecanal	268	C18H36O	000638-66-4	93
4	Octadecanal	268	C18H36O	000638-66-4	91
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90





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Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

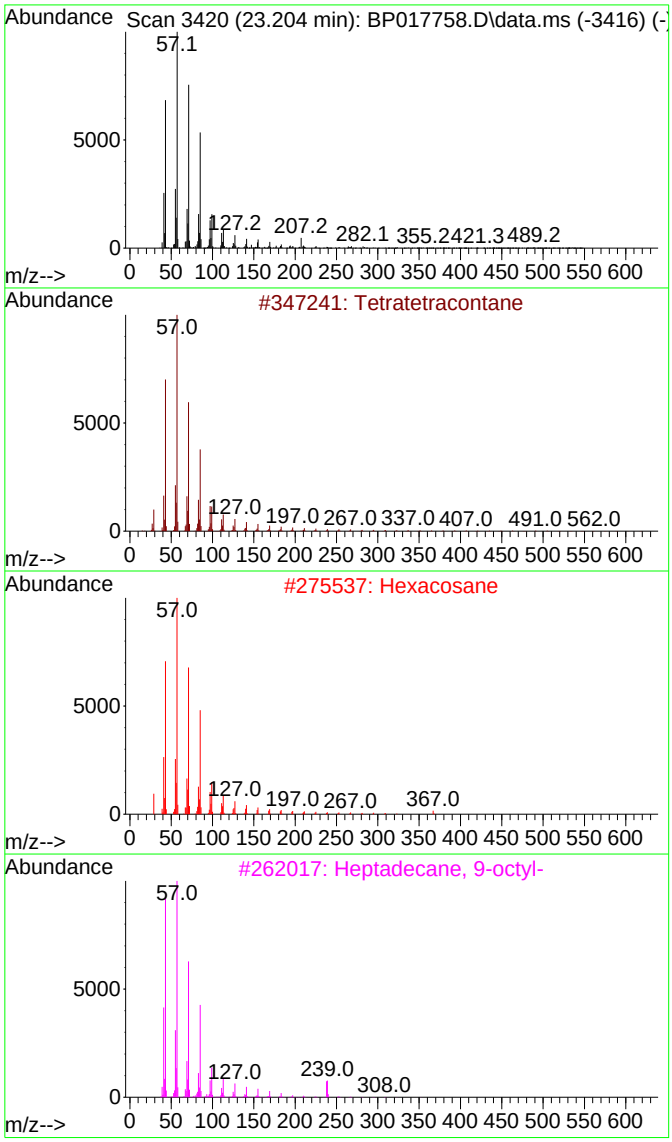
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

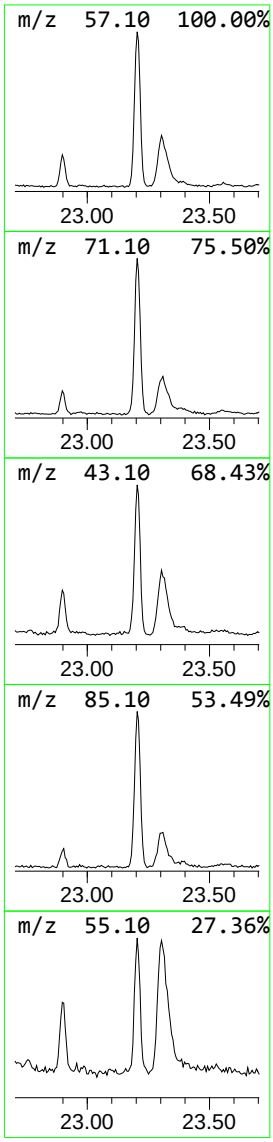
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.204	6.94 ng/ul	478846	Perylene-d12	24.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	83
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	83





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Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

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

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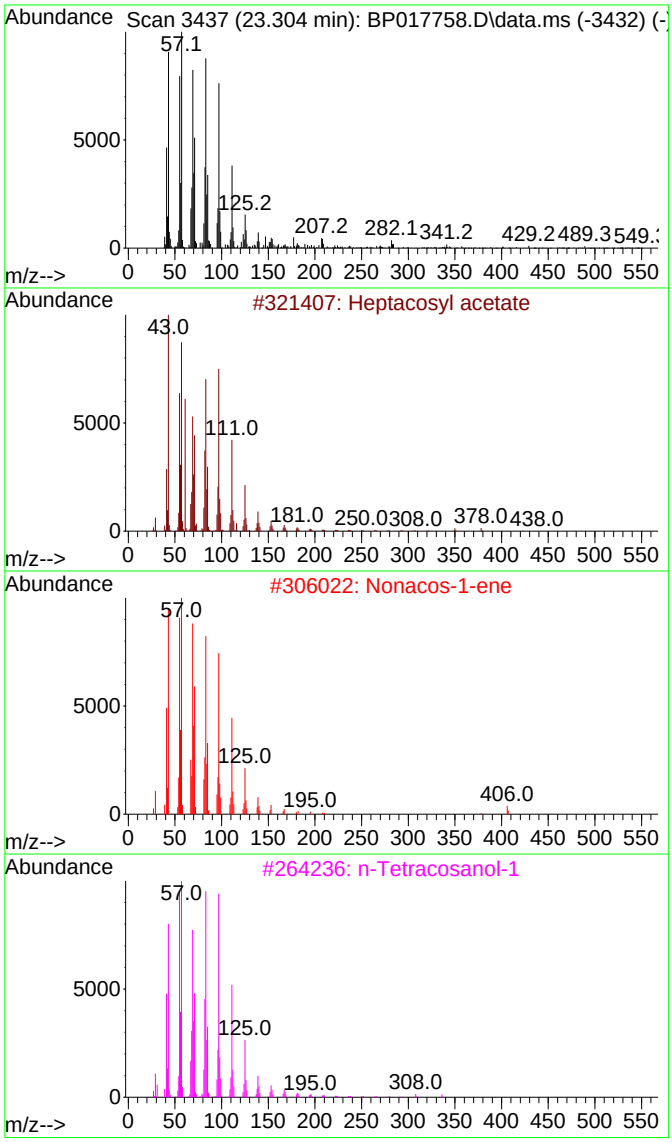
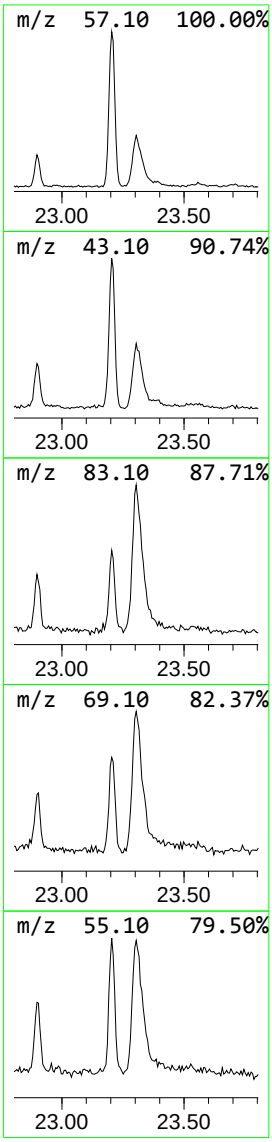
Peak Number 7 Heptacosyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.304	6.95 ng/ul	478921	Perylene-d12	24.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	95
2	Nonacos-1-ene	406	C29H58	018835-35-3	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Fumaric acid, pentadecyl pentafl...	492	C25H33F5O4	1000348-10-7	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.MA.M
Quant Title : SVOA CALIBRATION

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

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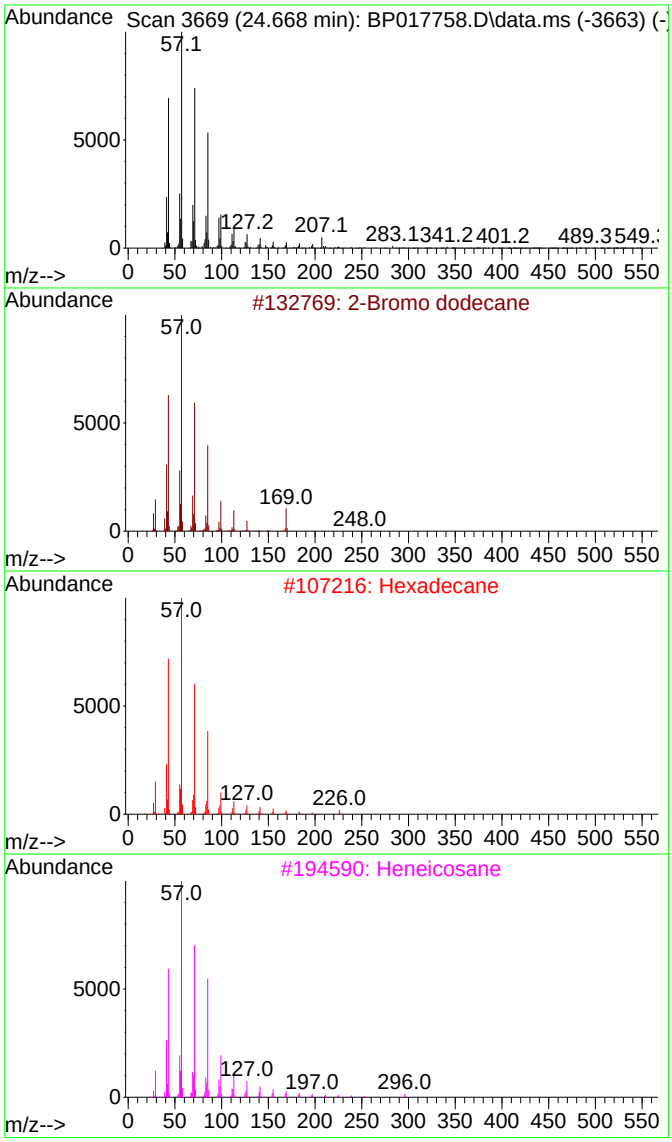
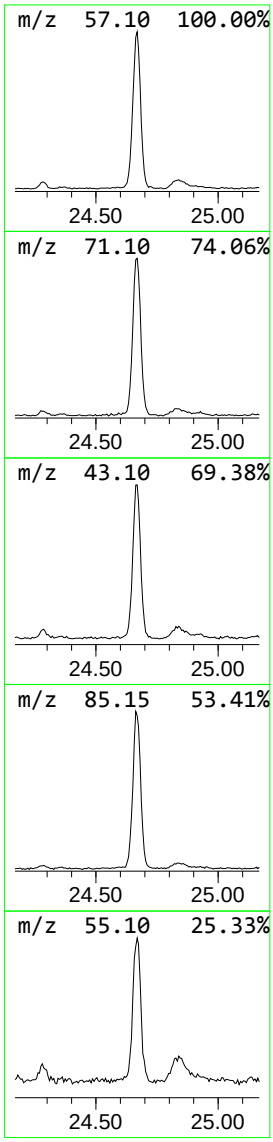
Peak Number 8 2-Bromo dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.668	14.42 ng/ul	994208	Perylene-d12	24.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Hexadecane	226	C16H34	000544-76-3	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heptacosane	380	C27H56	000593-49-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102323\
Data File : BP017758.D
Acq On : 23 Oct 2023 20:01
Operator : MA/JU
Sample : 04926-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCD00

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101823.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
unknown-01	4.922	2.2	ng/ul	81652	1	7.881	729617	20.0
n-Hexadecanoic ...	18.227	3.7	ng/ul	275655	4	17.375	1482250	20.0
unknown-02	20.863	3.0	ng/ul	200223	5	21.516	1348660	20.0
13-Docosenamide...	22.657	4.9	ng/ul	332738	5	21.516	1348660	20.0
Eicosanal-	22.898	2.7	ng/ul	184568	6	24.068	1379130	20.0
(DEL) Alkane: S...	23.204	6.9	ng/ul	478846	6	24.068	1379130	20.0
Heptacosyl acetate	23.304	7.0	ng/ul	478921	6	24.068	1379130	20.0
2-Bromo dodecane	24.668	14.4	ng/ul	994208	6	24.068	1379130	20.0