LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029562.D
Acq On : 08 Feb 2024 01:17
Operator : MA/JU
Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : C0FJ4

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_N\Methods\SFAM-EPA-BN020724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN029562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	37	41	47	rBV	79791	96754	2.05%	0.159%
2	3.740	107	111	118	rBV	433116	653660	13.86%	1.077%
3	3.804	119	122	127	rVV	88900	123316	2.61%	0.203%
4	3.857	128	131	135	rVB	31236	36836	0.78%	0.061%
5	3.969	146	150	157	rVB4	19170	34963	0.74%	0.058%
6	4.057	161	165	174	rVB2	34899	62876	1.33%	0.104%
7	4.287	201	204	211	rVB6	11760	18930	0.40%	0.031%
8	4.440	227	230	235	rVB	21017	27506	0.58%	0.045%
9	4.628	257	262	266	rVV	64586	93292	1.98%	0.154%
10	4.675	266	270	283	rVV	28842	54973	1.17%	0.091%
11	4.887	301	306	311	rVB7	7019	11728	0.25%	0.019%
12	4.981	318	322	333	rVB	46966	79462	1.68%	0.131%
13	5.093	339	341	350	rVB9	6211	12381	0.26%	0.020%
14	5.775	454	457	461	rVB6	7486	9643	0.20%	0.016%
15	6.863	638	642	646	rBV4	6753	9867	0.21%	0.016%
16	7.051	666	674	683	rVV	1153717	1913122	40.56%	3.151%
17	7.228	697	704	716	rBV	1003720	1537766	32.60%	2.533%
18	7.410	729	735	747	rBV	1191314	1848720	39.19%	3.045%
19	7.581	760	764	772	rVB9	11412	23622	0.50%	0.039%
20	7.704	782	785	792	rVB6	5435	9565	0.20%	0.016%
21	7.887	807	816	822	rBV	789772	1270390	26.93%	2.092%
22	7.951	822	827	833	rVB2	11865	19444	0.41%	0.032%
23	8.128	849	857	861	rBV9	8094	16128	0.34%	0.027%
24	8.592	927	936	949	rBV	1220082	1972385	41.82%	3.249%
25	8.716	951	957	966	rVB	76024	130294	2.76%	0.215%
26	9.051	1007	1014	1026	rBV	1093553	1784042	37.82%	2.938%
27	9.445	1077	1081	1085	rBV3	10076	16540	0.35%	0.027%
28	9.769	1128	1136	1146	rBV	780589	1314407	27.87%	2.165%
29	9.898	1154	1158	1166	rVB4	12297	22303	0.47%	0.037%
30	10.134	1195	1198	1203	rVB5	10706	15336	0.33%	0.025%
31	10.304	1219	1227	1239	rBV	1237724	2068724	43.86%	3.407%
32	10.551	1265	1269	1277	rBV9	4770	9164	0.19%	0.015%
33	10.686	1284	1292	1299	rBV	997261	1719908	36.46%	2.833%
34	10.828	1308	1316	1332	rBV	1041046	1854812	39.32%	3.055%
35	11.233	1379	1385	1393	rVB	7210	18435	0.39%	0.030%
36	11.445	1417	1421	1424	rBV6	8541	11174	0.24%	0.018%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_N
ClientSampleId :
C0FJ4

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Title : SVOA CALIBRATION

37	12.110	1529	1534	1540	rVB3	9352	17002	0.36%	0.028%
38	12.275	1556	1562	1568	rBV2	22627	38930	0.83%	0.064%
39	12.933	1669	1674	1680	rVB9	6942	12325	0.26%	0.020%
40	13.357	1741	1746	1752	rBV2	23204	36846	0.78%	0.061%
41	13.433	1753	1759	1767	rVV	49523	85188	1.81%	0.140%
42	13.498	1767	1770	1780	rVB8	4360	9267	0.20%	0.015%
43	13.780	1809	1818	1823	rBV9	12248	28473	0.60%	0.047%
44	13.863	1826	1832	1835	rVB9	5525	9674	0.21%	0.016%
45	13.951	1840	1847	1858	rBV	2028168	2840897	60.23%	4.679%
46	14.222	1882	1893	1905	rBV	2351702	3474060	73.65%	5.722%
47	14.527	1938	1945	1953	rBV	1326737	1931676	40.95%	3.182%
48	14.680	1967	1971	1974	rBV	32561	47341	1.00%	0.078%
49	14.727	1974	1979	1983	rVV	916598	1290082	27.35%	2.125%
50	14.786	1983	1989	2003	rVV	1730336	2690108	57.03%	4.431%
51	14.892	2005	2007	2012	rVV5	21578	38604	0.82%	0.064%
52	14.957	2012	2018	2025	rVB5	39637	74374	1.58%	0.122%
53	15.392	2088	2092	2097	rVB7	7364	12087	0.26%	0.020%
54	15.521	2107	2114	2121	rBV	2895140	4206118	89.17%	6.928%
55	15.580	2123	2124	2129	rVV5	8201	13190	0.28%	0.022%
56	15.645	2129	2135	2148	rVV	759103	1081287	22.92%	1.781%
57	15.763	2151	2155	2159	rVV4	16628	25091	0.53%	0.041%
58	15.810	2159	2163	2170	rVB9	11036	18441	0.39%	0.030%
59	16.169	2219	2224	2230	rBV8	11205	22453	0.48%	0.037%
60	16.310	2244	2248	2252	rVB4	11063	14729	0.31%	0.024%
61	16.398	2256	2263	2268	rBV8	7361	15264	0.32%	0.025%
62	16.686	2309	2312	2320	rVB6	11677	18384	0.39%	0.030%
63	16.827	2329	2336	2342	rBV8	13717	22110	0.47%	0.036%
64	17.186	2391	2397	2400	rBV4	23590	33727	0.72%	0.056%
65	17.280	2404	2413	2418	rBV	1440918	2067223	43.83%	3.405%
66	17.380	2423	2430	2440	rVV2	2775795	4019352	85.21%	6.620%
67	17.480	2440	2447	2451	rVB8	23573	43547	0.92%	0.072%
68	17.668	2477	2479	2485	rVB7	7822	11351	0.24%	0.019%
69	17.792	2496	2500	2504	rBV7	6260	11753	0.25%	0.019%
70	17.880	2511	2515	2519	rBV4	11365	14753	0.31%	0.024%
71	17.968	2526	2530	2535	rVB8	8876	14170	0.30%	0.023%
72	18.068	2540	2547	2553	rBV4	26728	55571	1.18%	0.092%
73	18.127	2553	2557	2562	rBV6	14863	24039	0.51%	0.040%
74	18.192	2563	2568	2579	rBV	451451	650595	13.79%	1.072%
75	18.486	2614	2618	2626	rBV9	20360	43490	0.92%	0.072%
76	18.627	2638	2642	2645	rBV3	20165	22899	0.49%	0.038%

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Misc :
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Instrument : BNA_N
ClientSampleId : C0FJ4

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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77	18.674	2645	2650	2652	rVV5	6404	9777	0.21%	0.016%
78	18.762	2662	2665	2668	rBV2	12294	12451	0.26%	0.021%
79	18.992	2700	2704	2709	rBV4	13737	17105	0.36%	0.028%
80	19.080	2716	2719	2723	rVB5	12591	19132	0.41%	0.032%
81	19.239	2739	2746	2751	rBV4	43368	83615	1.77%	0.138%
82	19.327	2754	2761	2762	rBV4	43383	86921	1.84%	0.143%
83	19.474	2782	2786	2793	rBV	145832	192684	4.09%	0.317%
84	19.621	2807	2811	2814	rBV2	24137	28847	0.61%	0.048%
85	19.674	2814	2820	2829	rBV	3501988	4716793	100.00%	7.769%
86	19.915	2858	2861	2862	rBV3	15553	16013	0.34%	0.026%
87	20.209	2908	2911	2914	rBV4	15669	17136	0.36%	0.028%
88	20.245	2914	2917	2921	rVB	35532	39104	0.83%	0.064%
89	20.621	2979	2981	2987	rVB3	25250	28763	0.61%	0.047%
90	20.745	2999	3002	3005	rVB	37273	36915	0.78%	0.061%
91	21.204	3076	3080	3087	rBV2	430674	602145	12.77%	0.992%
92	21.474	3121	3126	3141	rBV	1522440	2020802	42.84%	3.328%
93	21.656	3154	3157	3163	rVB2	71224	84017	1.78%	0.138%
94	22.121	3232	3236	3244	rBV2	161569	265080	5.62%	0.437%
95	23.174	3410	3415	3419	rBV	312779	515160	10.92%	0.848%
96	23.221	3419	3423	3434	rVB2	161571	296811	6.29%	0.489%
97	23.698	3496	3504	3518	rBV2	2228537	4475199	94.88%	7.371%
98	23.850	3524	3530	3539	rVB2	999085	2053716	43.54%	3.383%
99	24.533	3640	3646	3653	rBV	294990	623017	13.21%	1.026%
100	24.615	3655	3660	3675	rVB2	214866	484597	10.27%	0.798%

Sum of corrected areas: 60714739

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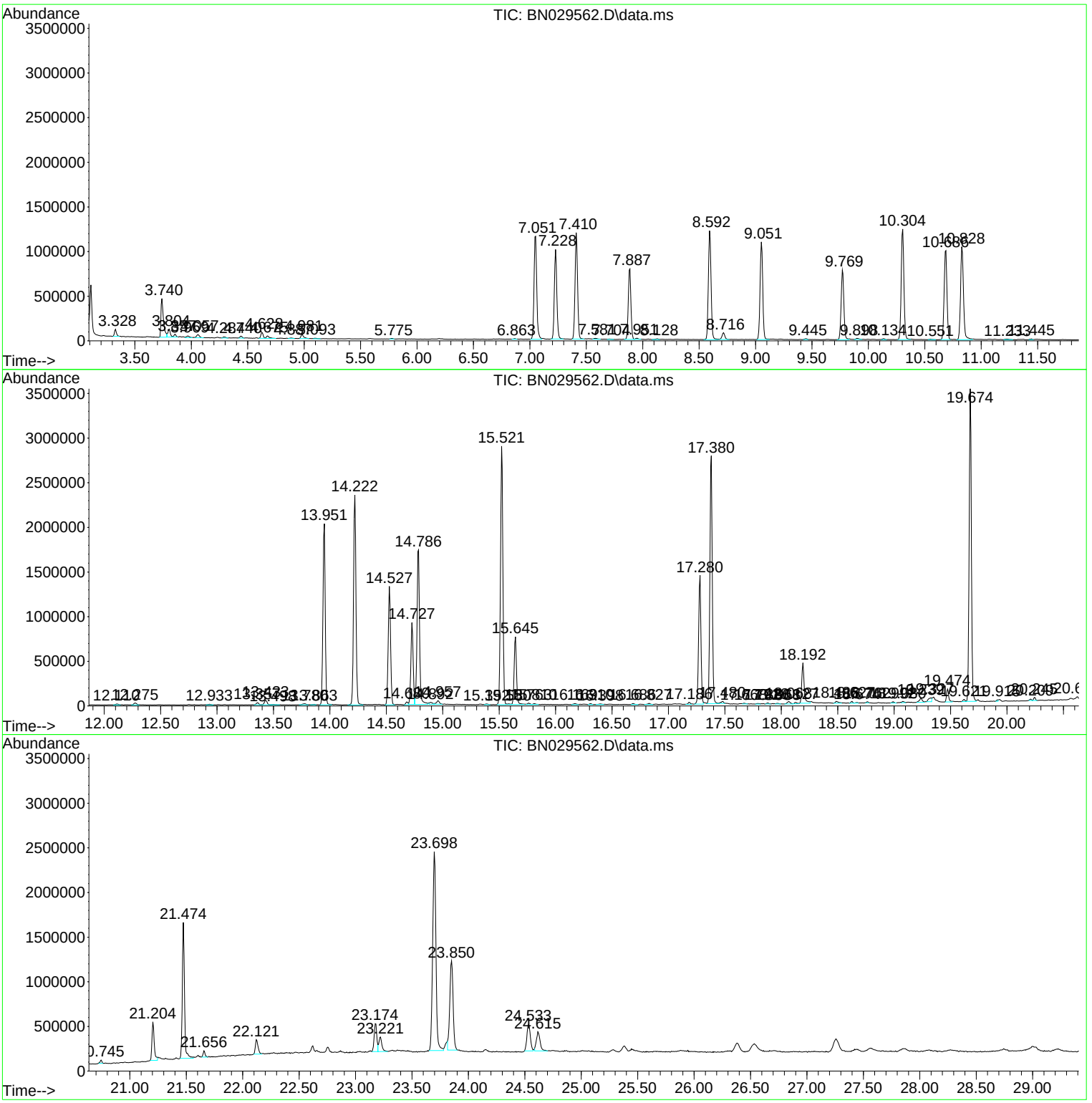
Instrument :
BNA_N
ClientSampleId :
C0FJ4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

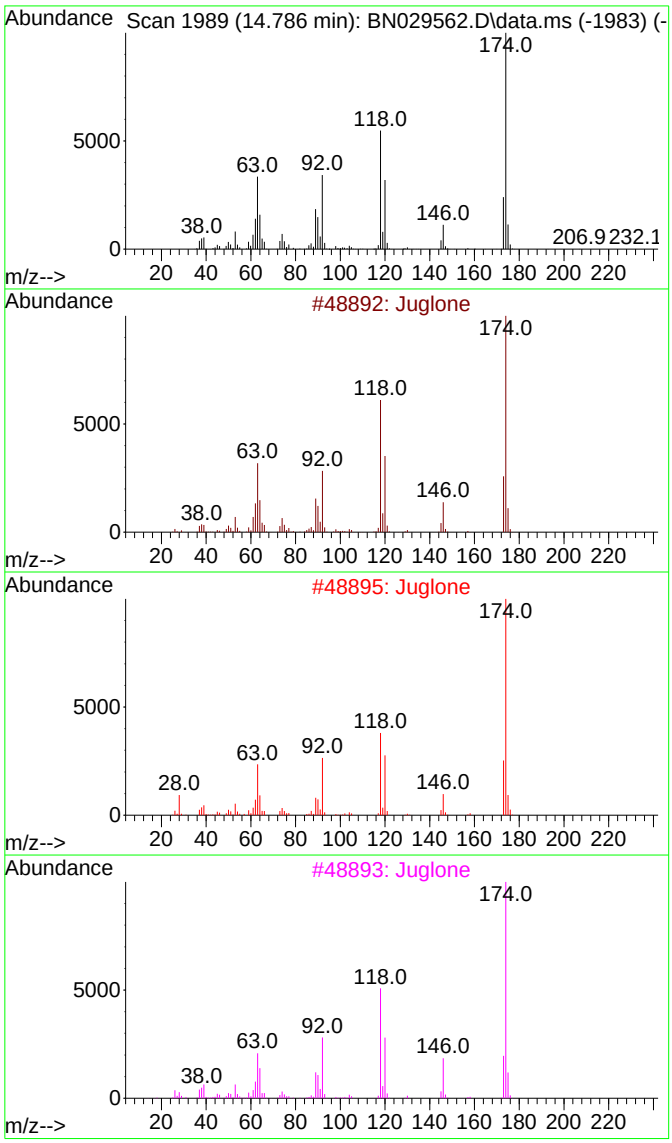
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

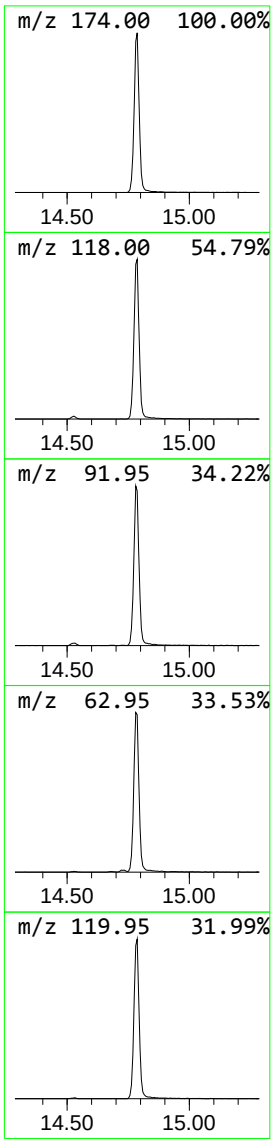
****

Peak Number 1 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	27.85 ng/ul	2690110	Acenaphthene-d10	14.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone	174	C10H6O3	000481-39-0	99
2	Juglone	174	C10H6O3	000481-39-0	96
3	Juglone	174	C10H6O3	000481-39-0	94
4	Juglone	174	C10H6O3	000481-39-0	64
5	1-Methyl-5-(4-methylphenyl)tetra...	174	C9H10N4	068826-33-5	49





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Instrument :
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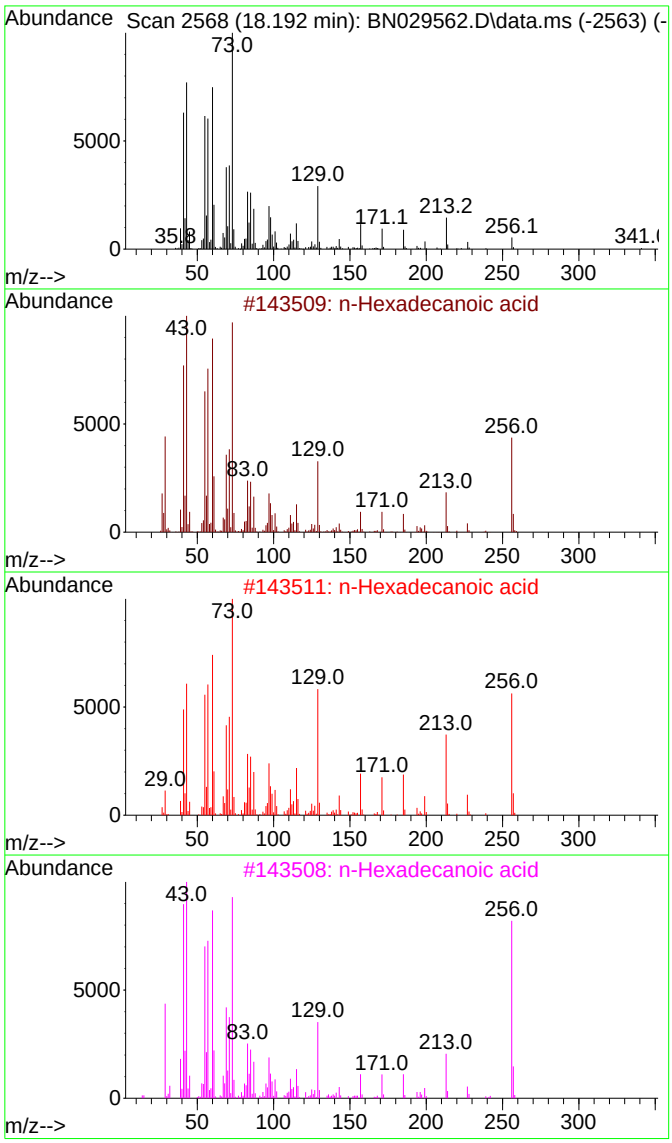
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

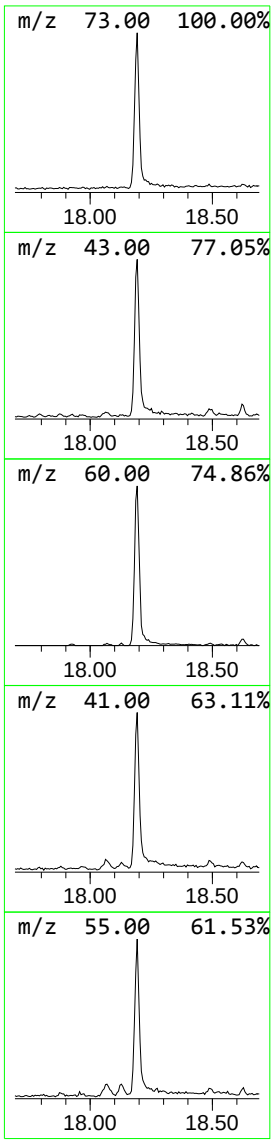
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	6.29 ng/ul	650595	Phenanthrene-d10	17.280

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	95
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81





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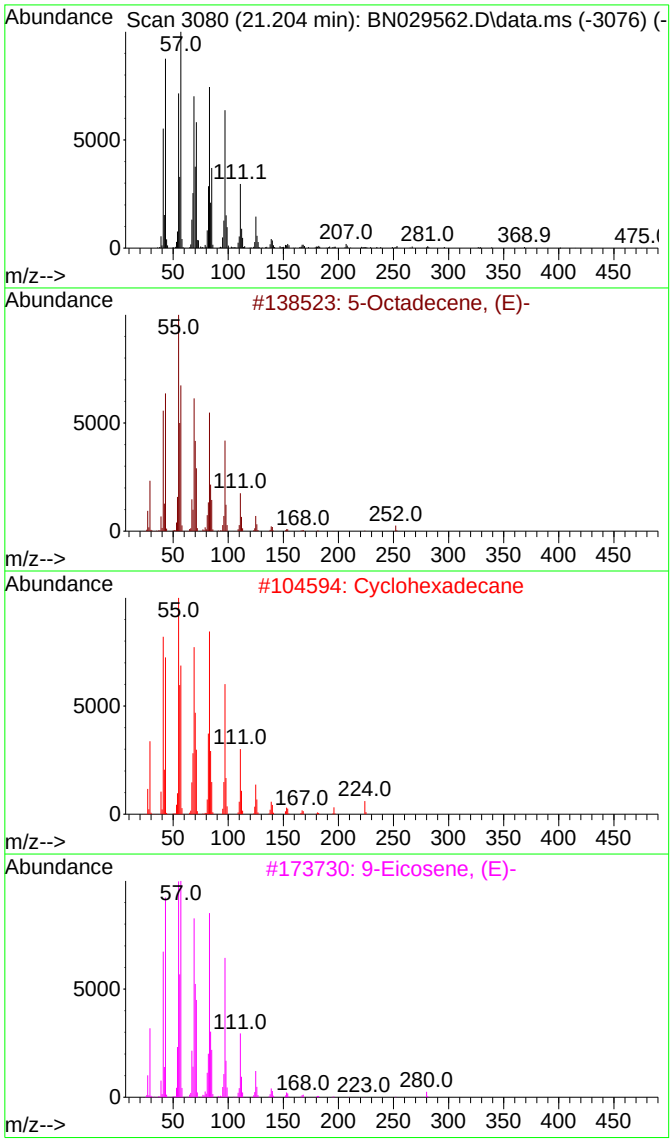
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

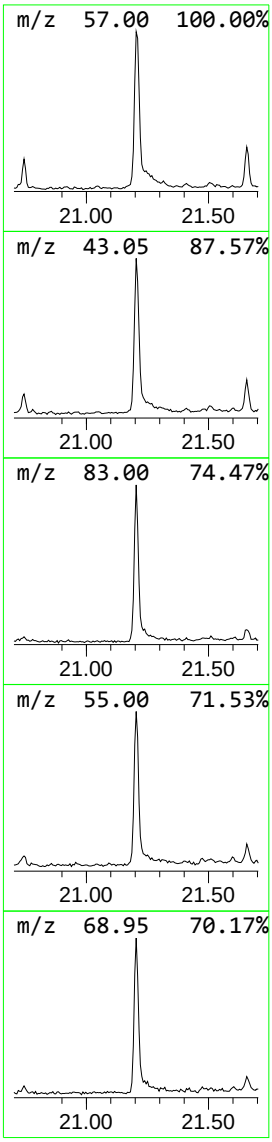
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.203	5.96 ng/ul	602145	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	96
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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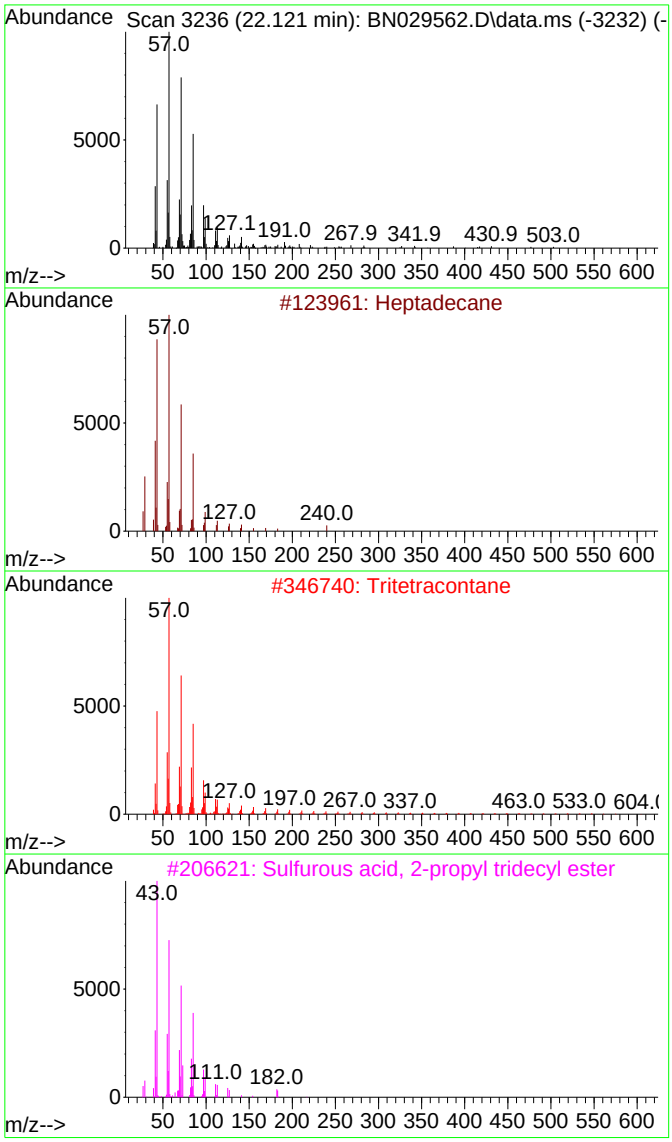
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

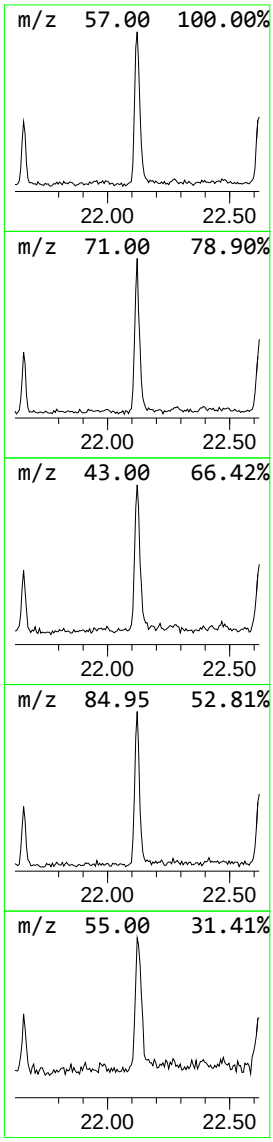
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.121	2.62 ng/ul	265080	Chrysene-d12	21.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Tritetracontane	605	C43H88	007098-21-7	91
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
4	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
5	Nonadecane	268	C19H40	000629-92-5	83





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Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0FJ4

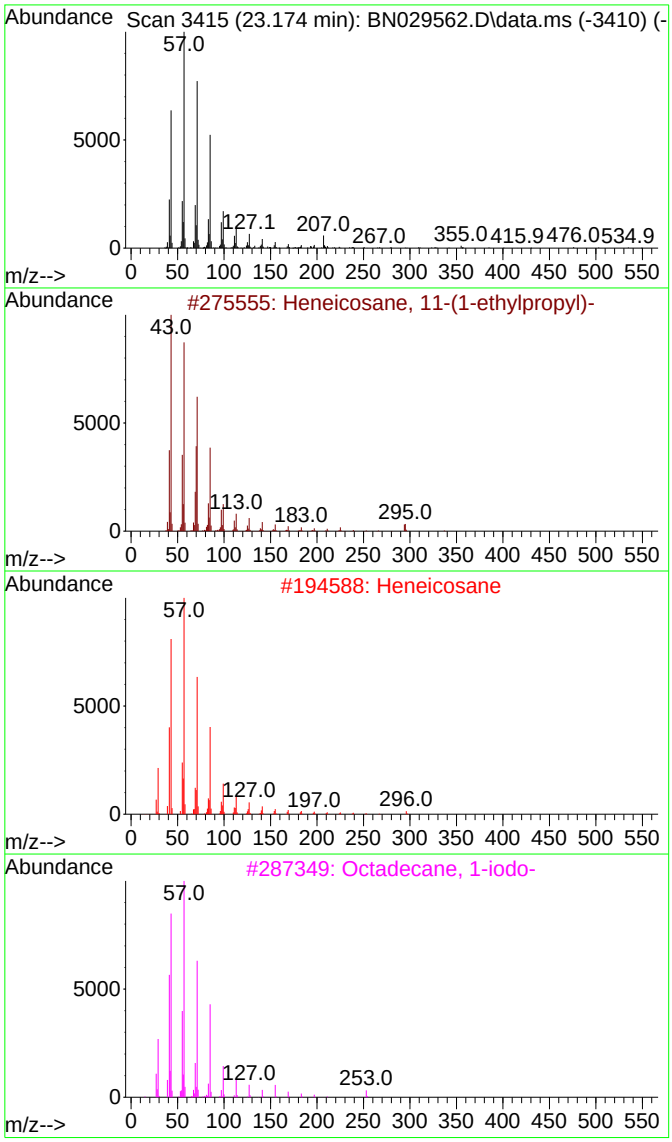
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

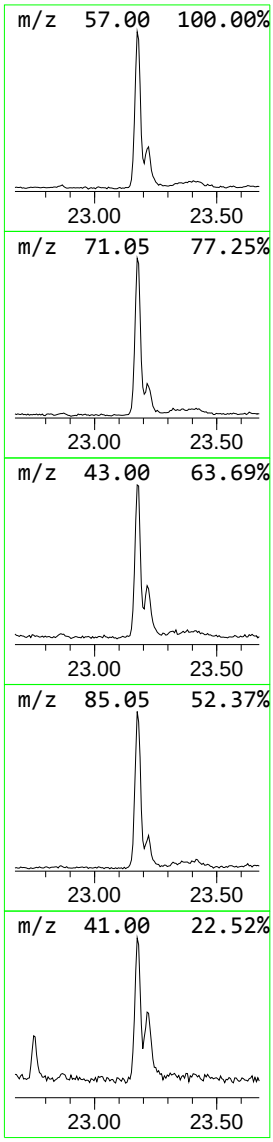
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.174	5.02 ng/ul	515160	Perylene-d12	23.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Hexadecane	226	C16H34	000544-76-3	80





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Data File : BN029562.D
Acq On : 08 Feb 2024 01:17
Operator : MA/JU
Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ4

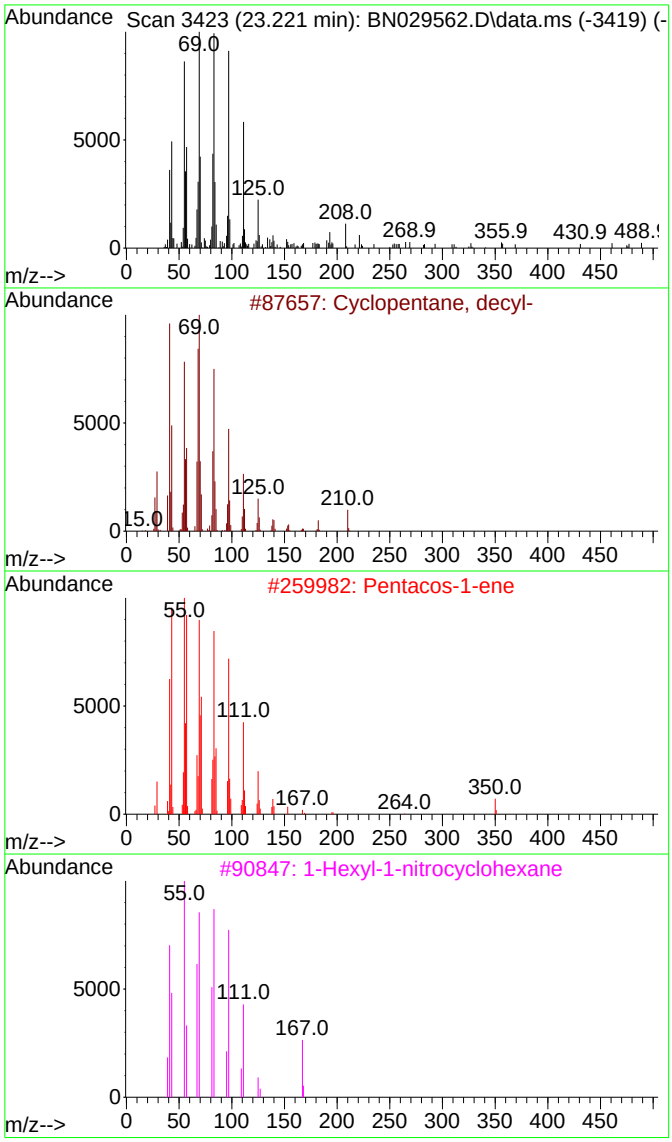
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

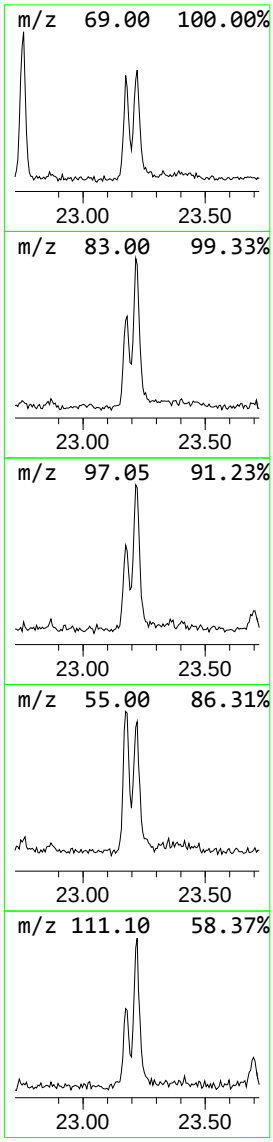
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic23.221 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.221	2.89 ng/ul	296811	Perylene-d12	23.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, decyl-	210	C15H30	001795-21-7	64
2	Pentacos-1-ene	350	C25H50	016980-85-1	64
3	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	53
4	1,2-Dodecanediol	202	C12H26O2	001119-87-5	50
5	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029562.D
Acq On : 08 Feb 2024 01:17
Operator : MA/JU
Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ4

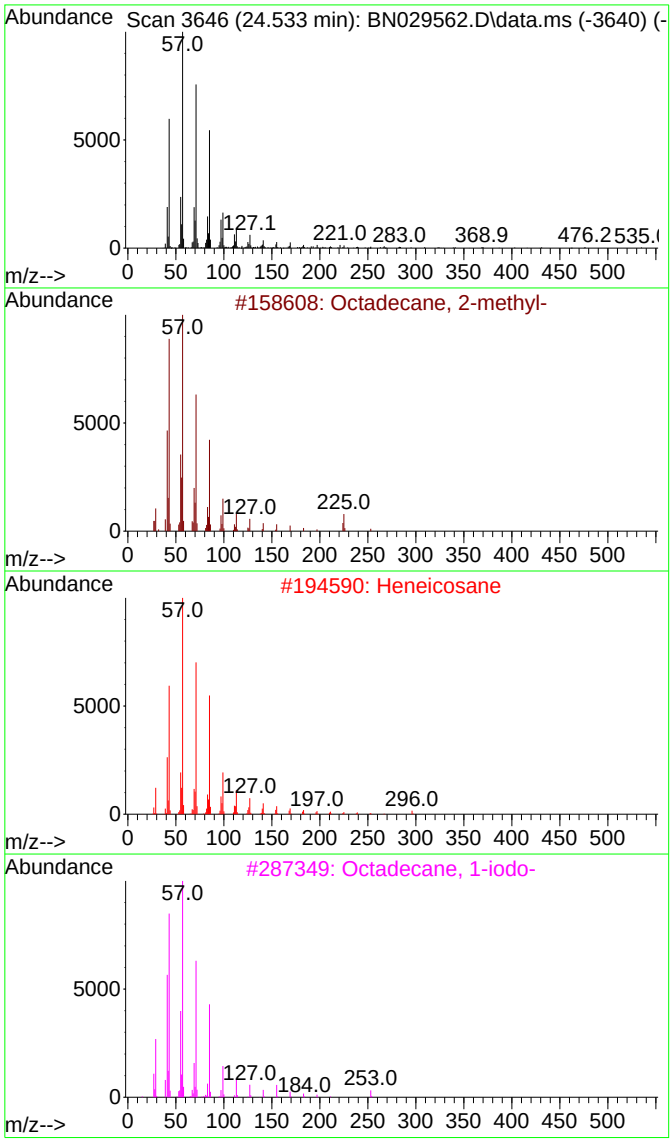
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

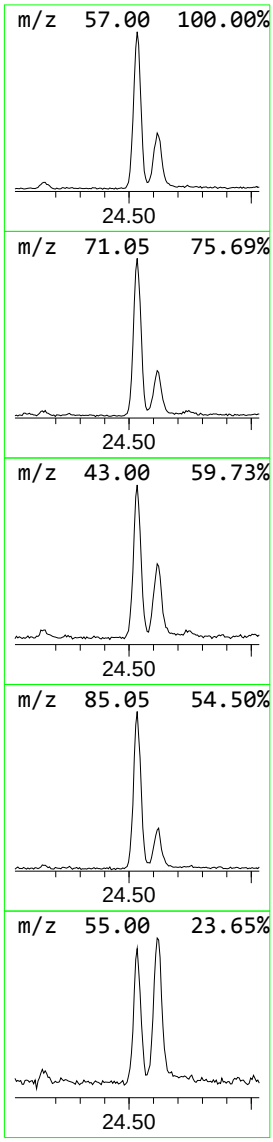
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	6.07 ng/ul	623017	Perylene-d12	23.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029562.D
Acq On : 08 Feb 2024 01:17
Operator : MA/JU
Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ4

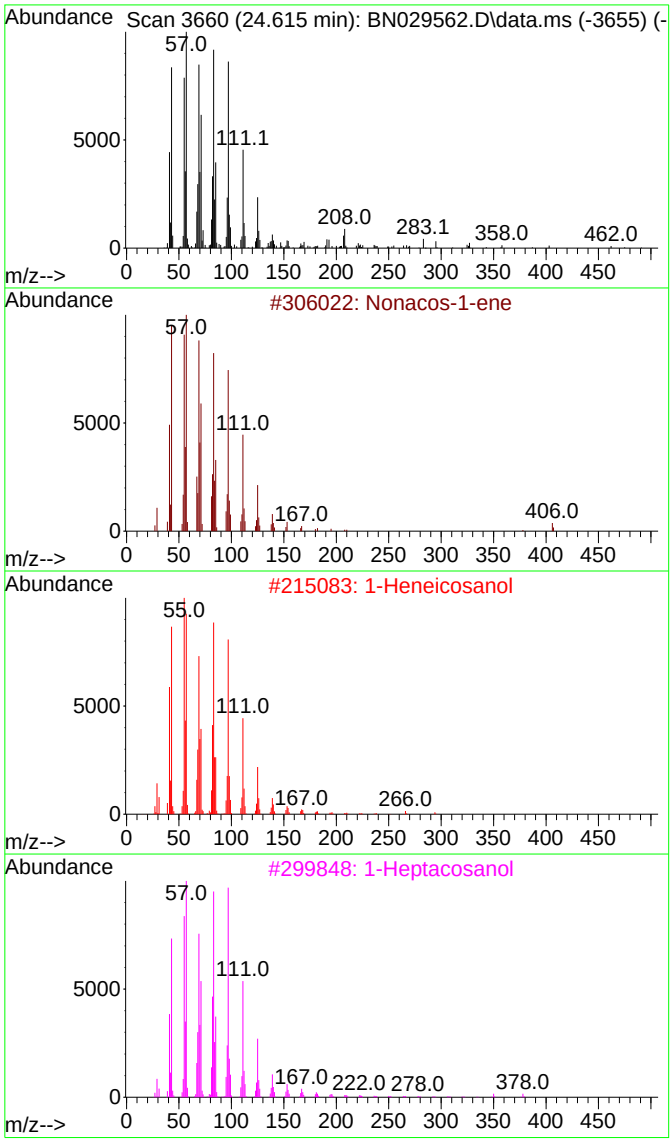
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

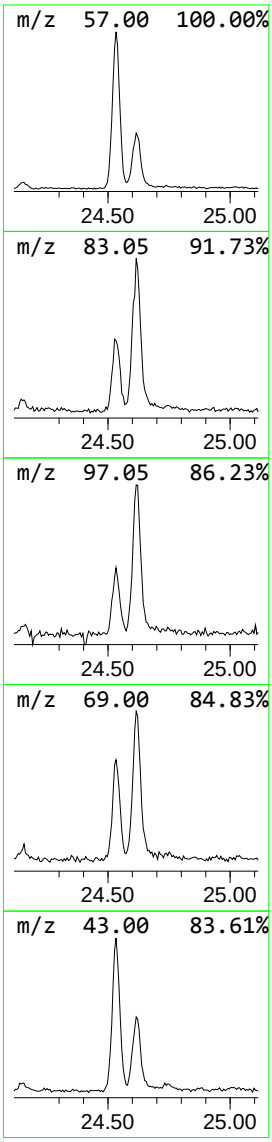
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.615	4.72 ng/ul	484597	Perylene-d12	23.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Triacontan-15-ol	438	C30H62O	031849-26-0	91
5	1-Tetracosene	336	C24H48	010192-32-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029562.D
Acq On : 08 Feb 2024 01:17
Operator : MA/JU
Sample : P1303-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.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
Juglone	14.786	27.9	ng/ul	2690110	3	14.527	1931680	20.0
n-Hexadecanoic ...	18.192	6.3	ng/ul	650595	4	17.280	2067220	20.0
(DEL) Alkane: S...	21.203	6.0	ng/ul	602145	5	21.474	2020800	20.0
(DEL) Alkane: S...	22.121	2.6	ng/ul	265080	5	21.474	2020800	20.0
(DEL) Alkane: S...	23.174	5.0	ng/ul	515160	6	23.850	2053720	20.0
(DEL) Alkane: C...	23.221	2.9	ng/ul	296811	6	23.850	2053720	20.0
(DEL) Alkane: S...	24.533	6.1	ng/ul	623017	6	23.850	2053720	20.0
(DEL) Alkane: S...	24.615	4.7	ng/ul	484597	6	23.850	2053720	20.0