LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : A44E9

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-BM010423.M
Title : SVOA CALIBRATION

Signal : TIC: BM038397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	26	30	36	rVB	26848	31157	1.32%	0.140%
2	3.810	103	106	116	rBV	33232	63676	2.69%	0.286%
3	4.022	138	142	150	rVB2	13001	19029	0.80%	0.085%
4	4.122	155	159	163	rVB2	7228	10998	0.46%	0.049%
5	4.234	175	178	182	rVB4	8955	11261	0.48%	0.051%
6	5.057	315	318	330	rVB4	5439	9803	0.41%	0.044%
7	5.510	392	395	402	rVB4	2027	2987	0.13%	0.013%
8	6.375	540	542	546	rVB4	5600	7170	0.30%	0.032%
9	7.093	663	664	668	rVB4	2516	2704	0.11%	0.012%
10	7.157	670	675	692	rVB	91539	152920	6.46%	0.687%
11	7.322	697	703	714	rBV	309823	490354	20.70%	2.203%
12	7.522	731	737	747	rBV	308820	489188	20.65%	2.197%
13	7.998	811	818	825	rBV	335465	523472	22.10%	2.351%
14	8.057	825	828	834	rVB4	7196	10601	0.45%	0.048%
15	8.710	933	939	948	rBV	211288	345549	14.59%	1.552%
16	9.098	1000	1005	1010	rBV5	2197	3736	0.16%	0.017%
17	9.169	1010	1017	1027	rVV	381720	611584	25.82%	2.747%
18	9.240	1027	1029	1034	rVB4	2168	2434	0.10%	0.011%
19	9.328	1040	1044	1048	rVB4	4401	6269	0.26%	0.028%
20	9.545	1076	1081	1086	rVB5	2837	4276	0.18%	0.019%
21	9.892	1133	1140	1151	rBV	303500	487186	20.57%	2.188%
22	10.428	1225	1231	1241	rBV	387520	647188	27.32%	2.907%
23	10.492	1241	1242	1249	rVB4	2446	2823	0.12%	0.013%
24	10.810	1289	1296	1304	rBV	417465	670219	28.29%	3.011%
25	10.951	1313	1320	1335	rBV	309461	534399	22.56%	2.400%
26	11.551	1417	1422	1426	rBV4	1495	3548	0.15%	0.016%
27	11.622	1428	1434	1443	rVV6	2157	6599	0.28%	0.030%
28	12.104	1510	1516	1524	rVV4	5713	10849	0.46%	0.049%
29	12.392	1559	1565	1572	rBV	5367	7863	0.33%	0.035%
30	12.910	1647	1653	1657	rBV3	8792	11639	0.49%	0.052%
31	12.980	1663	1665	1669	rBV5	2083	2576	0.11%	0.012%
32	13.233	1703	1708	1712	rBV2	4491	6956	0.29%	0.031%
33	13.516	1751	1756	1762	rVB3	5194	7029	0.30%	0.032%
34	14.039	1838	1845	1855	rBV	781361	1006787	42.50%	4.522%
35	14.327	1887	1894	1904	rBV	774313	1105608	46.67%	4.966%
36	14.627	1939	1945	1953	rBV	588745	849764	35.87%	3.817%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_M
ClientSampleId :
A44E9

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-BM010423.M
Title : SVOA CALIBRATION

37	14.704	1953	1958	1964	rVB	10512	14064	0.59%	0.063%
38	14.839	1975	1981	1994	rBV	42251	86077	3.63%	0.387%
39	15.033	2010	2014	2020	rBV3	15230	21634	0.91%	0.097%
40	15.298	2054	2059	2064	rBV	15856	22628	0.96%	0.102%
41	15.410	2073	2078	2079	rBV3	3308	3846	0.16%	0.017%
42	15.616	2107	2113	2120	rBV	1027862	1415658	59.76%	6.359%
43	15.739	2129	2134	2150	rVB	408711	553672	23.37%	2.487%
44	15.851	2150	2153	2157	rBV2	2629	3546	0.15%	0.016%
45	15.980	2168	2175	2178	rBV7	3507	6061	0.26%	0.027%
46	16.757	2302	2307	2309	rBV2	4132	5235	0.22%	0.024%
47	16.951	2338	2340	2345	rVB4	3598	4240	0.18%	0.019%
48	17.368	2406	2411	2422	rBV	713072	942635	39.79%	4.234%
49	17.468	2422	2428	2436	rBV	1266929	1675890	70.75%	7.528%
50	17.633	2450	2456	2461	rBV3	9971	15831	0.67%	0.071%
51	17.686	2461	2465	2469	rVB2	15675	18199	0.77%	0.082%
52	17.880	2496	2498	2502	rVB4	3262	2930	0.12%	0.013%
53	18.027	2518	2523	2530	rBV	210162	244608	10.33%	1.099%
54	18.245	2556	2560	2567	rBV3	40700	56158	2.37%	0.252%
55	18.327	2570	2574	2576	rVV	9456	11744	0.50%	0.053%
56	18.351	2576	2578	2583	rVB5	6762	9523	0.40%	0.043%
57	18.662	2629	2631	2634	rBV4	2166	2568	0.11%	0.012%
58	18.833	2655	2660	2667	rVB9	7841	15642	0.66%	0.070%
59	18.892	2667	2670	2671	rBV3	2757	2920	0.12%	0.013%
60	18.951	2676	2680	2683	rBV	29786	32646	1.38%	0.147%
61	18.992	2683	2687	2692	rVV	59510	65701	2.77%	0.295%
62	19.321	2739	2743	2749	rVB4	15058	20238	0.85%	0.091%
63	19.392	2751	2755	2757	rBV	13773	18345	0.77%	0.082%
64	19.515	2772	2776	2786	rBV	56954	90709	3.83%	0.407%
65	19.662	2798	2801	2806	rVB4	11419	13307	0.56%	0.060%
66	19.756	2811	2817	2827	rBV	1703461	2080133	87.81%	9.344%
67	20.068	2865	2870	2873	rBV	299725	322629	13.62%	1.449%
68	20.104	2873	2876	2882	rVB	649708	678047	28.62%	3.046%
69	20.656	2968	2970	2973	rVB3	13031	11693	0.49%	0.053%
70	20.727	2976	2982	2986	rBV	107724	136751	5.77%	0.614%
71	21.039	3031	3035	3037	rBV	121846	127549	5.38%	0.573%
72	21.074	3037	3041	3045	rVB	240037	263352	11.12%	1.183%
73	21.539	3115	3120	3128	rBV	881306	1132691	47.82%	5.088%
74	21.927	3183	3186	3189	rBV	66660	77488	3.27%	0.348%
75	21.962	3189	3192	3197	rVB	133107	148179	6.26%	0.666%
76	22.974	3361	3364	3369	rVB	100312	124408	5.25%	0.559%

LSC Area Percent Report

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Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

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-BM010423.M
Title : SVOA CALIBRATION

77	23.815	3500	3507	3518	rBV	1263110	2368868	100.00%	10.641%
78	23.968	3527	3533	3543	rVB2	630695	1254174	52.94%	5.634%

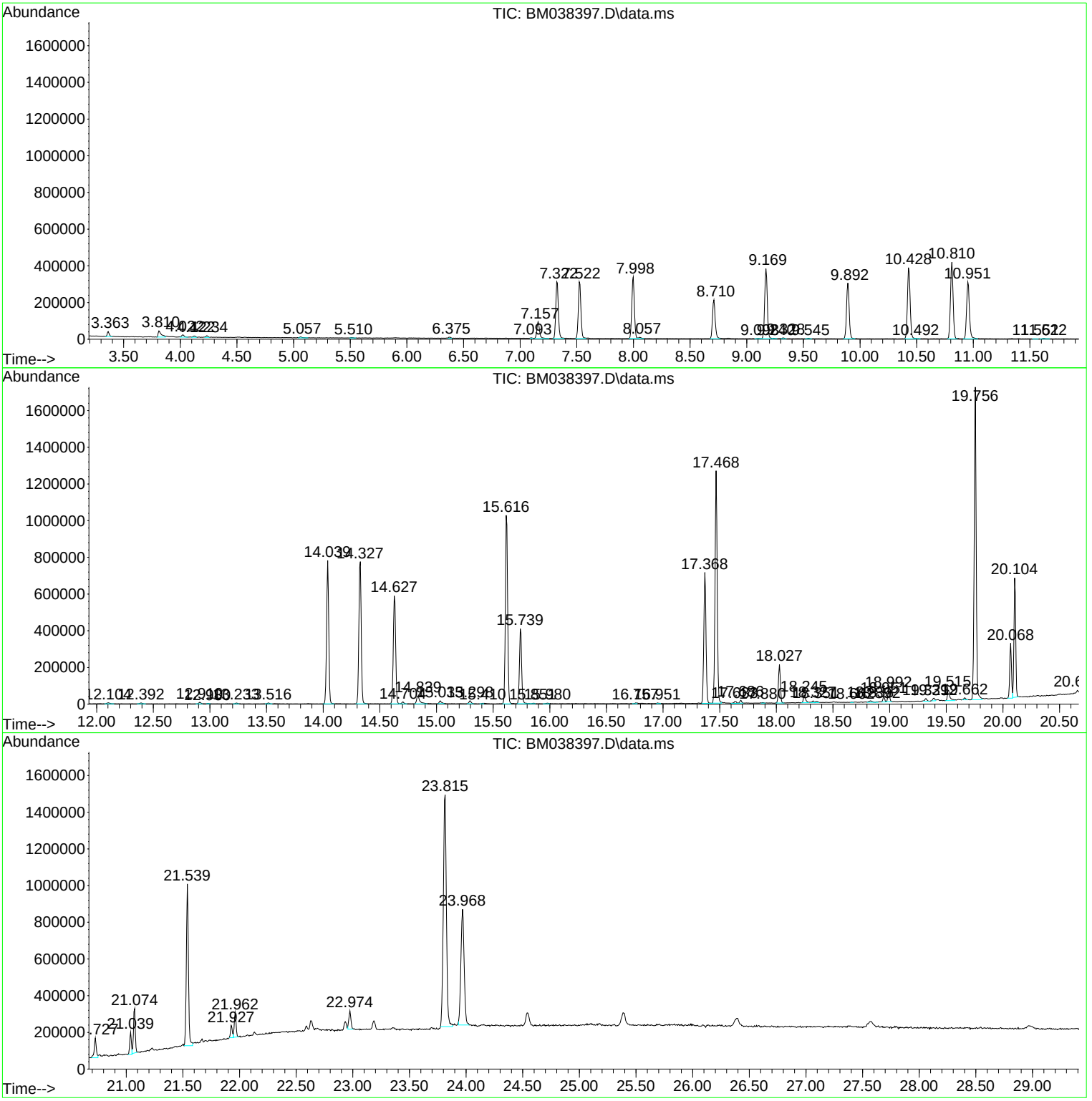
Sum of corrected areas: 22262418

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
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Instrument :
BNA_M
ClientSampleId :
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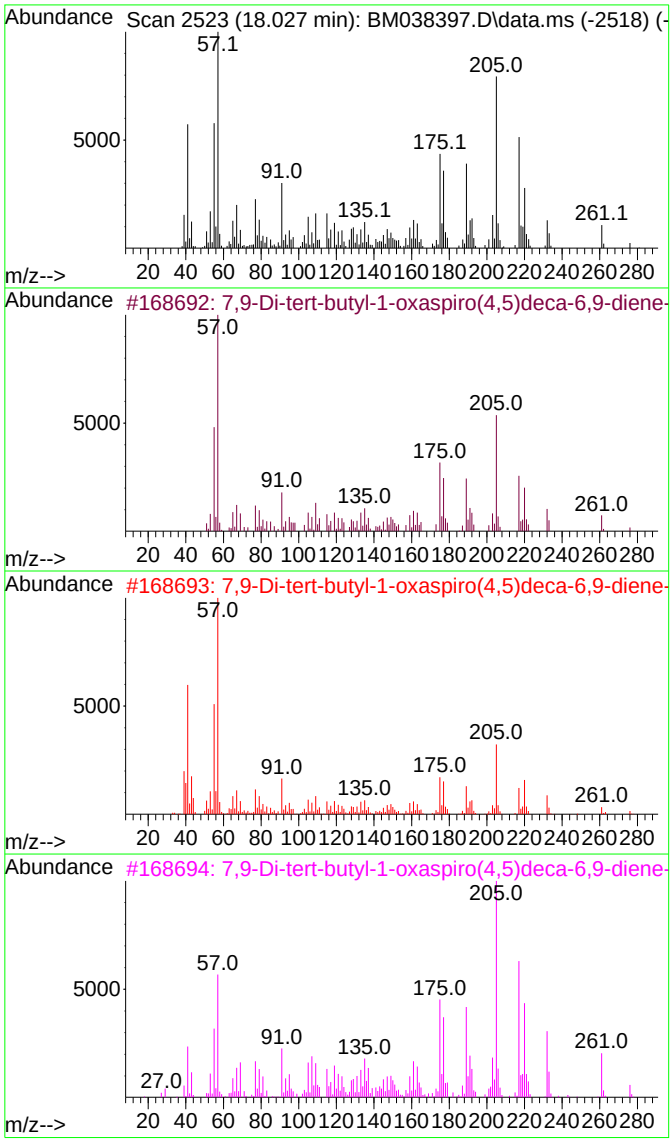
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

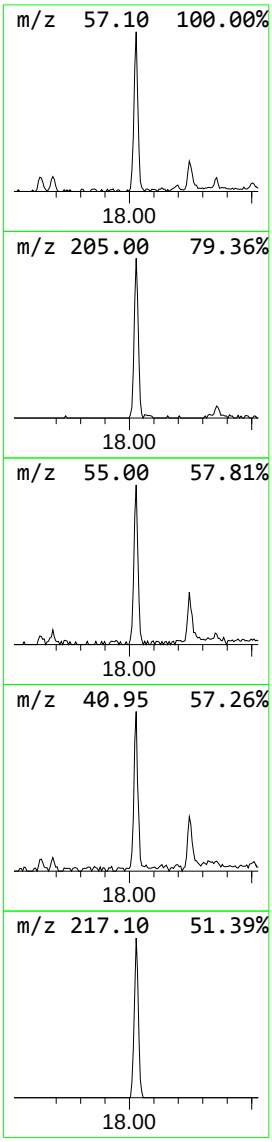
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.027	5.19 ng/ul	244608	Phenanthrene-d10	17.368

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	90
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	46
4	(Z)-((2-Benzylideneheptyl)oxy)tr...	276	C17H28OSi	1000495-65-9	38
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

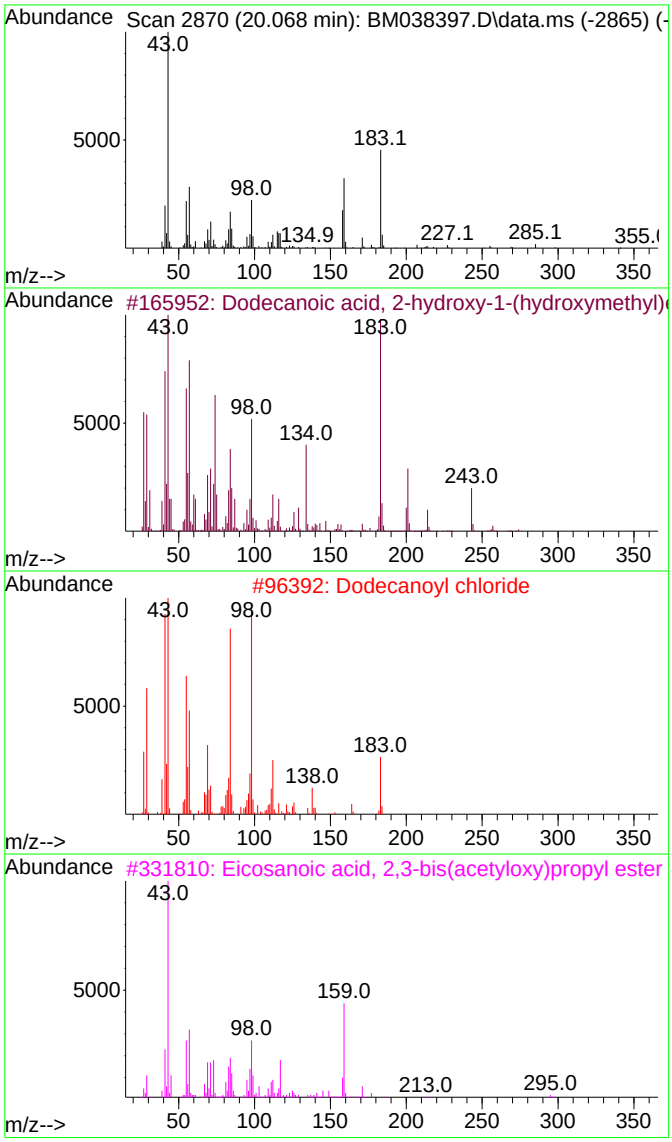
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

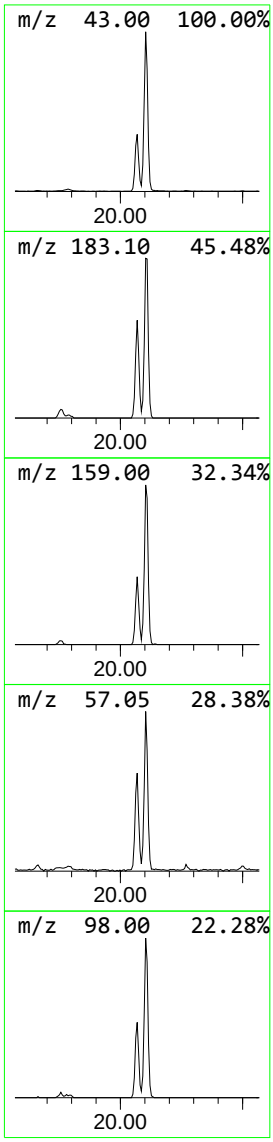
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dodecanoic acid, 2-hydroxy-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.068	5.70 ng/ul	322629	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	53
2	Dodecanoyl chloride	218	C12H23ClO	000112-16-3	17
3	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	16
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	14
5	1-Pentanamine, N-(1-methylethyl)...	158	C8H18N2O	028023-77-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
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Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

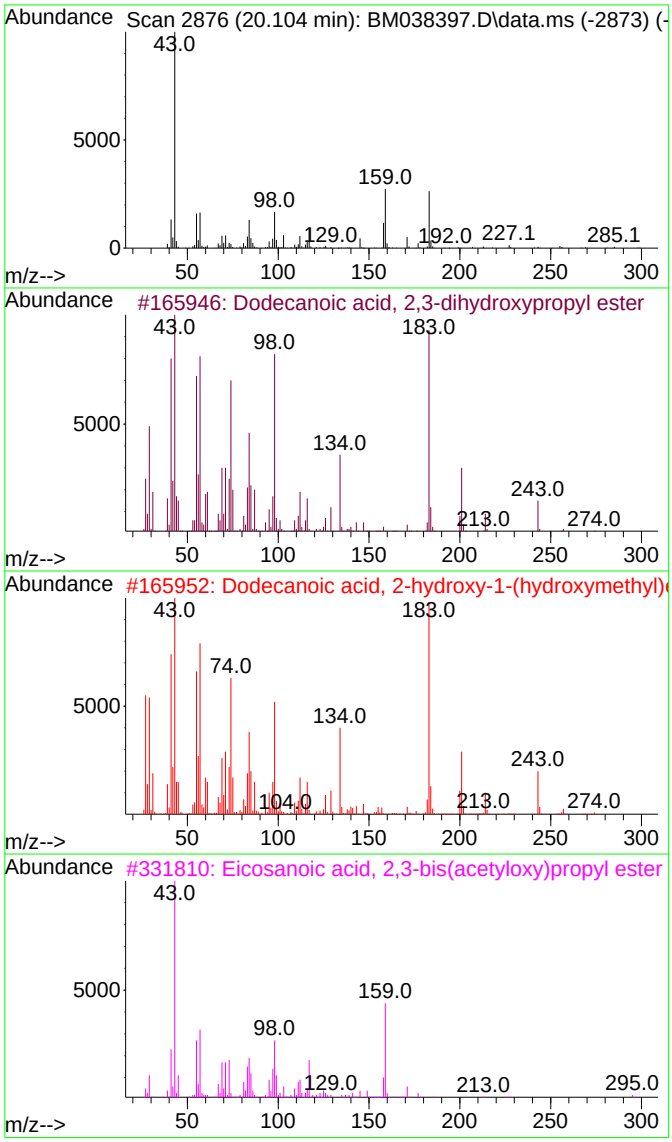
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

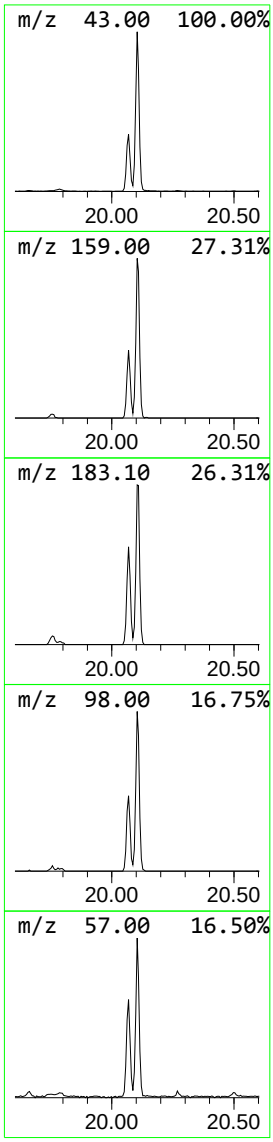
****

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.104	11.97 ng/ul	678047	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	38
2	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	32
3	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	32
4	Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12
5	9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	10





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Instrument :
BNA_M
ClientSampleId :
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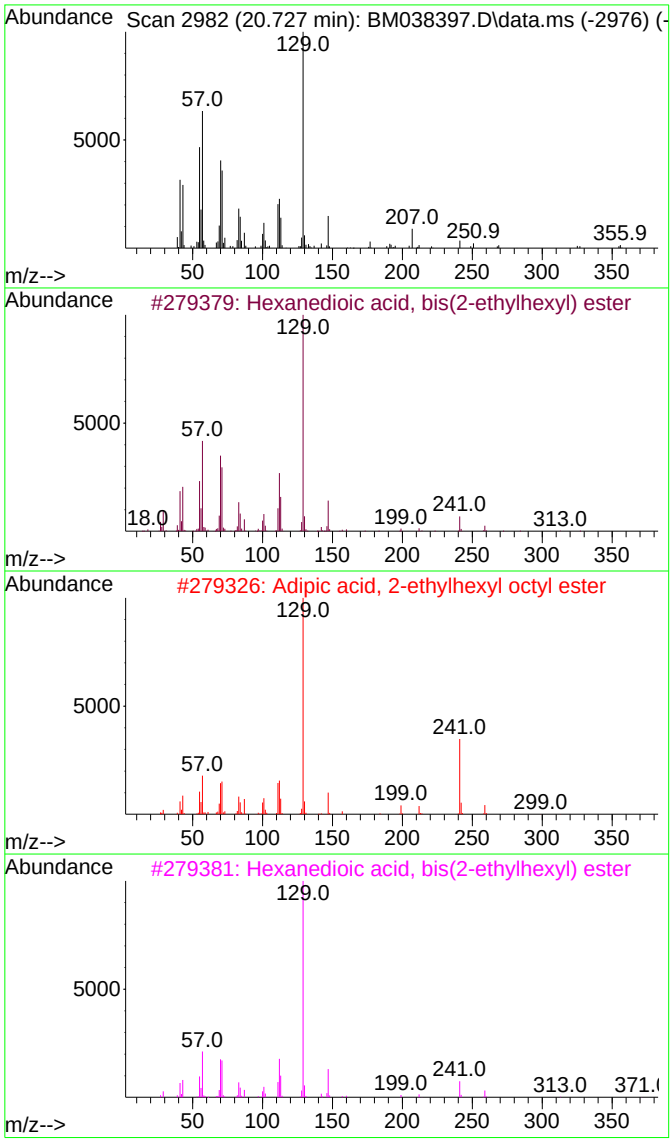
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

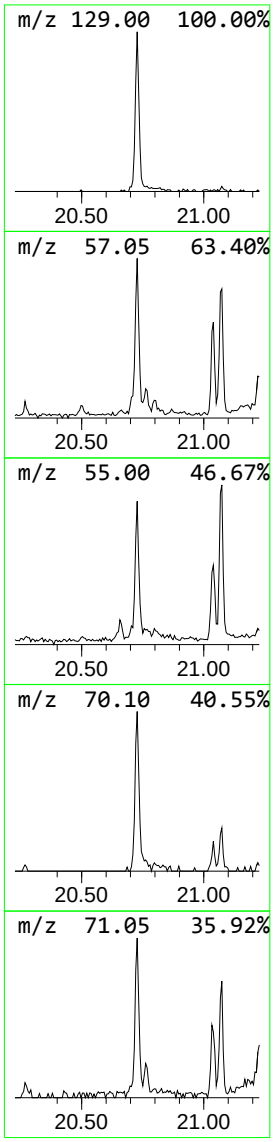
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.727	2.41 ng/ul	136751	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	83
5	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	72





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Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

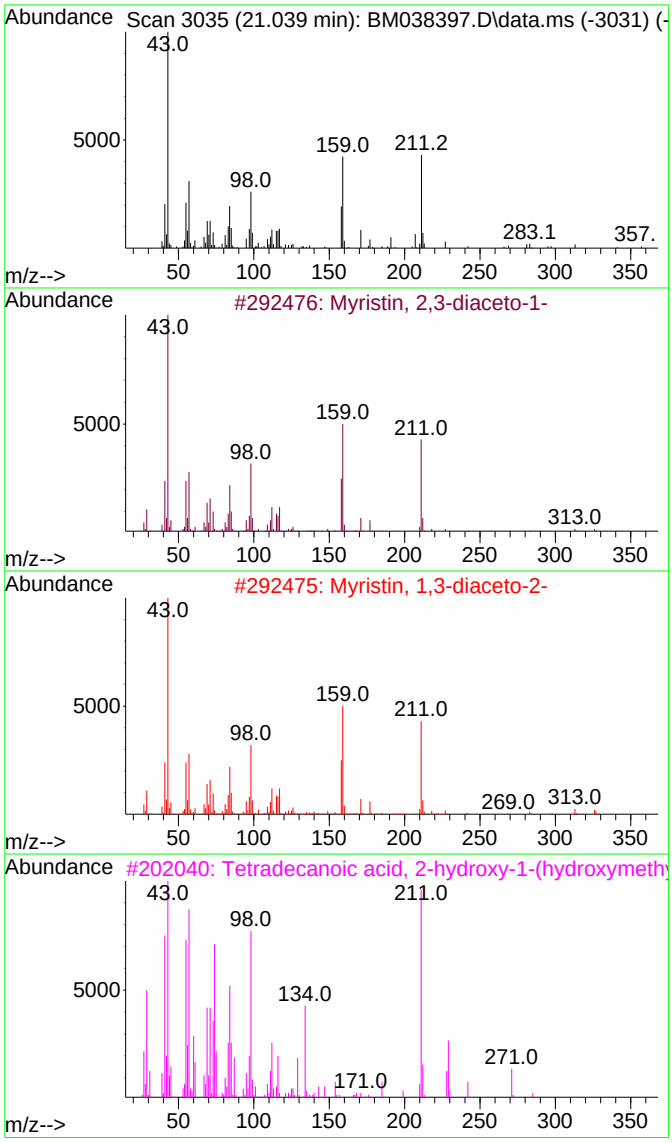
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

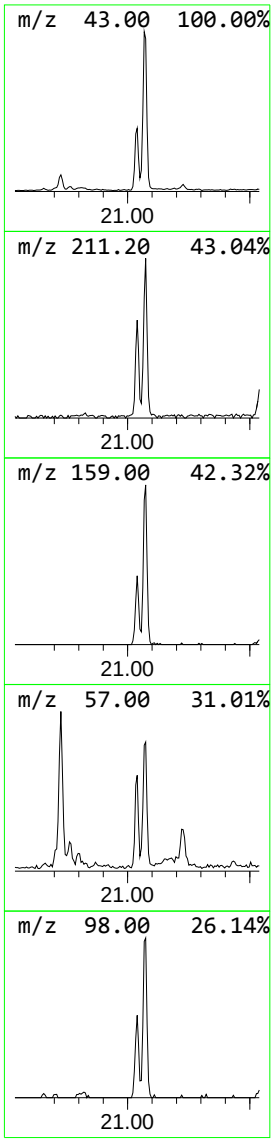
****

Peak Number 5 Myristin, 2,3-diaceto-1- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	2.25 ng/ul	127549	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	95
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	81
3	Tetradecanoic acid, 2-hydroxy-1-...	302	C17H34O4	003443-83-2	43
4	Tetradecanoic acid, 2,3-dihydrox...	302	C17H34O4	000589-68-4	35
5	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

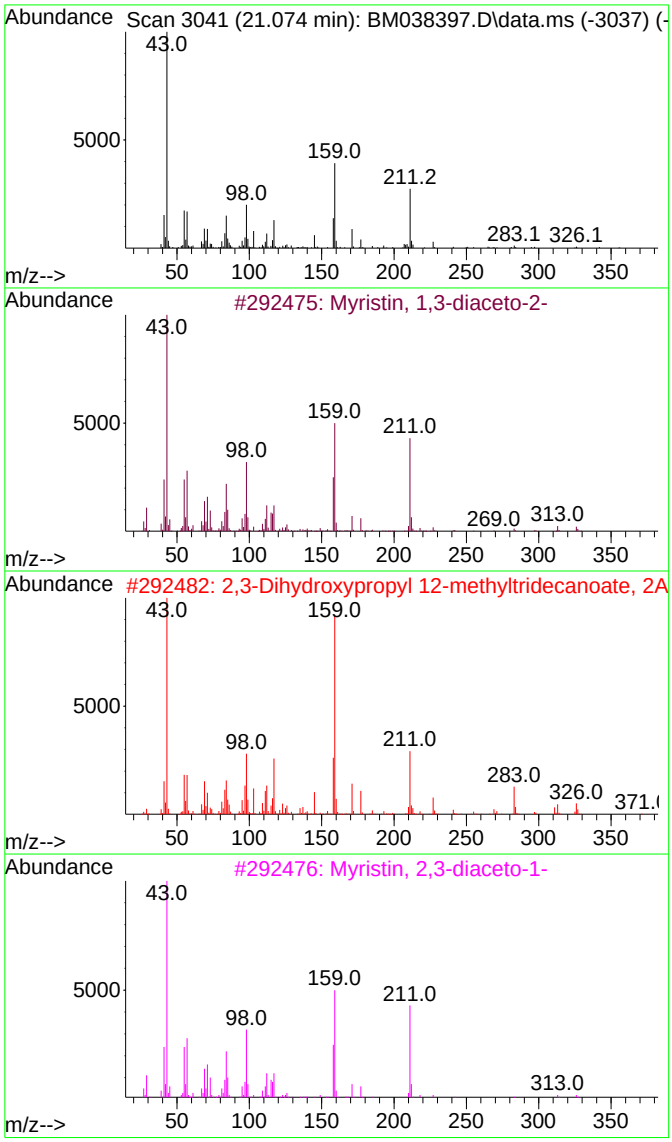
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

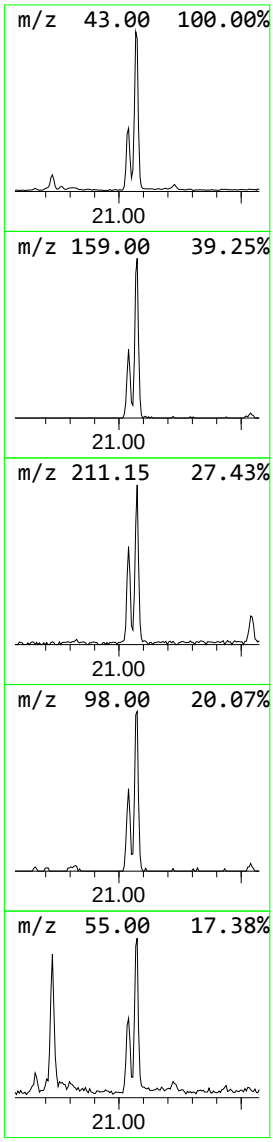
****

Peak Number 6 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	4.65 ng/ul	263352	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	45
2	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	43
3	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	38
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10
5	1,3-Dioxolane-4-methanol, 2,2-di...	174	C8H14O4	014739-11-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.M
Quant Title : SVOA CALIBRATION

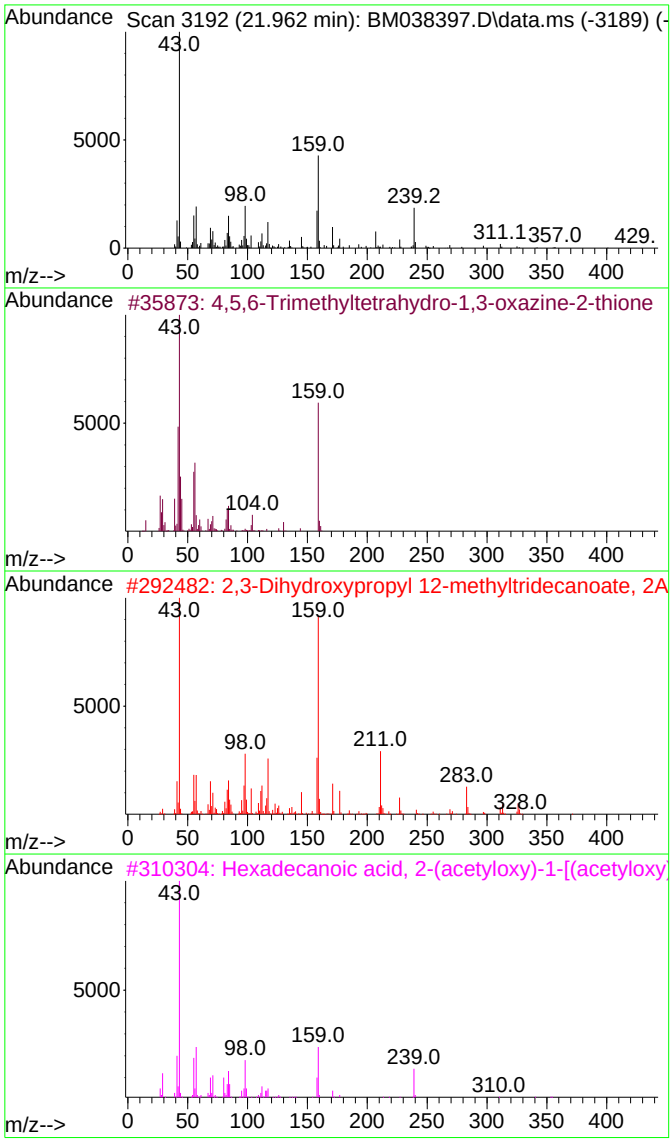
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

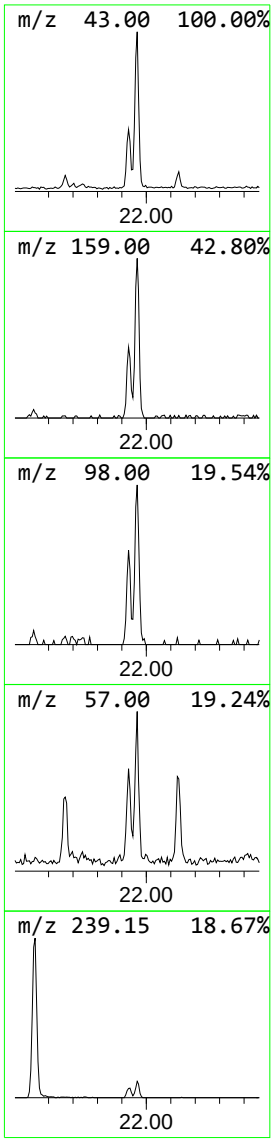
****

Peak Number 7 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.962	2.62 ng/ul	148179	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	27
2	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	25
3	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	22
4	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	16
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010623\
Data File : BM038397.D
Acq On : 06 Jan 2023 21:49
Operator : CG/JU
Sample : 01035-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A44E9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM010423.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
7,9-Di-tert-but...	18.027	5.2	ng/ul	244608	4	17.368	942635	20.0
Dodecanoic acid...	20.068	5.7	ng/ul	322629	5	21.539	1132690	20.0
unknown-01	20.104	12.0	ng/ul	678047	5	21.539	1132690	20.0
Hexanedioic aci...	20.727	2.4	ng/ul	136751	5	21.539	1132690	20.0
Myristin, 2,3-d...	21.039	2.3	ng/ul	127549	5	21.539	1132690	20.0
unknown-02	21.074	4.7	ng/ul	263352	5	21.539	1132690	20.0
unknown-03	21.962	2.6	ng/ul	148179	5	21.539	1132690	20.0