LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041220.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	285	292	299	rVB	71991	108287	1.67%	0.241%
2	5.369	364	371	385	rBV	2647728	3720016	57.21%	8.268%
3	6.981	637	645	660	rBV	2514186	3905117	60.05%	8.679%
4	7.798	777	784	792	rBV	800450	1256914	19.33%	2.794%
5	8.975	975	984	998	rBV	1474664	2432321	37.40%	5.406%
6	10.604	1249	1261	1268	rBV	1044166	1678266	25.81%	3.730%
7	13.080	1674	1682	1692	rBV	3838590	5342208	82.15%	11.873%
8	13.927	1821	1826	1838	rVB	216400	328112	5.05%	0.729%
9	14.186	1864	1870	1879	rVB	33929	70722	1.09%	0.157%
10	14.463	1905	1917	1923	rBV	1411236	2159572	33.21%	4.800%
11	14.886	1979	1989	1997	rBV3	32216	89588	1.38%	0.199%
12	15.963	2163	2172	2180	rBV	2808992	3876332	59.61%	8.615%
13	16.180	2203	2209	2218	rBV5	23470	68695	1.06%	0.153%
14	17.121	2365	2369	2376	rBV5	35747	73716	1.13%	0.164%
15	17.221	2377	2386	2391	rBV	1588468	2238561	34.42%	4.975%
16	17.262	2391	2393	2398	rVB	155893	184572	2.84%	0.410%
17	17.357	2404	2409	2413	rBV	49259	70832	1.09%	0.157%
18	18.004	2514	2519	2525	rBV4	58377	128333	1.97%	0.285%
19	18.062	2525	2529	2533	rBV	91127	130953	2.01%	0.291%
20	18.121	2534	2539	2550	rVV	1172131	1836788	28.25%	4.082%
21	18.298	2565	2569	2573	rBV3	49240	78087	1.20%	0.174%
22	18.421	2585	2590	2598	rBV5	42890	102644	1.58%	0.228%
23	19.027	2689	2693	2698	rBV2	41347	82330	1.27%	0.183%
24	19.239	2726	2729	2731	rBV2	89976	106087	1.63%	0.236%
25	19.286	2733	2737	2747	rVB	516563	799340	12.29%	1.777%
26	19.404	2753	2757	2765	rBV2	480347	751336	11.55%	1.670%
27	19.474	2766	2769	2776	rVB	267634	350308	5.39%	0.779%
28	19.627	2791	2795	2796	rBV2	75731	99501	1.53%	0.221%
29	19.651	2796	2799	2808	rVB	394840	569176	8.75%	1.265%
30	19.862	2829	2835	2840	rBV	5187400	6502861	100.00%	14.453%
31	20.274	2902	2905	2909	rVB	398353	410721	6.32%	0.913%
32	21.133	3048	3051	3060	rVB3	395568	578065	8.89%	1.285%
33	21.333	3083	3085	3090	rVB	178914	164633	2.53%	0.366%
34	21.427	3095	3101	3105	rBV	1835524	2617396	40.25%	5.817%
35	23.797	3499	3504	3510	rVB	1175858	2080703	32.00%	4.624%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

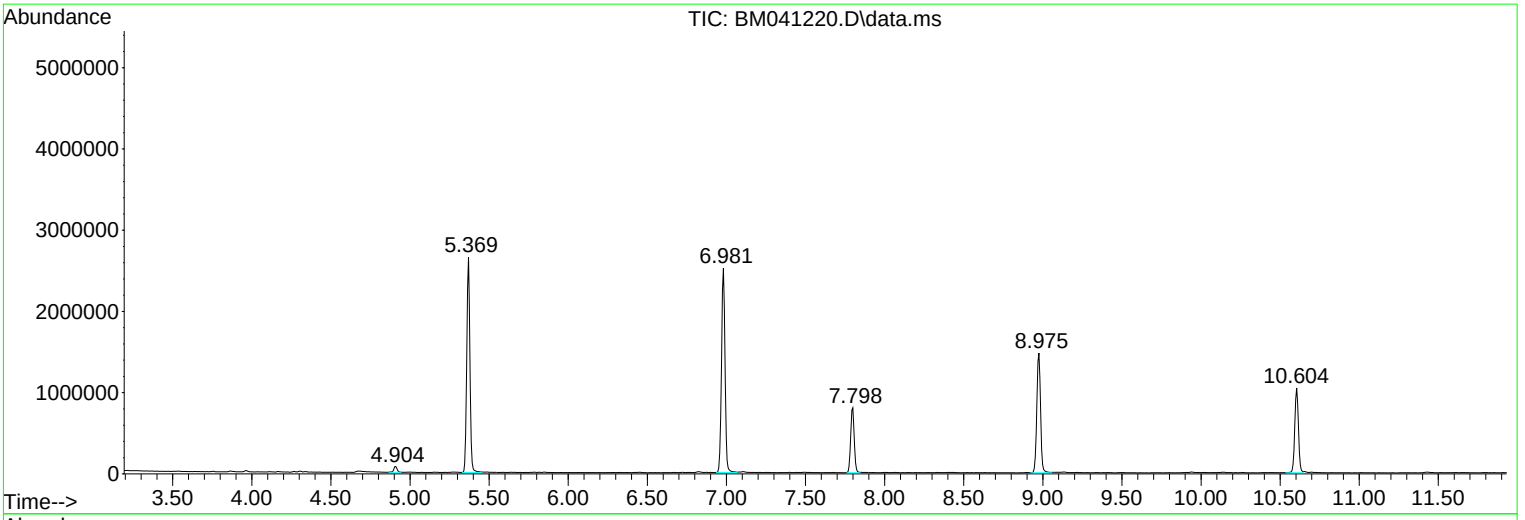
Sum of corrected areas: 44993093

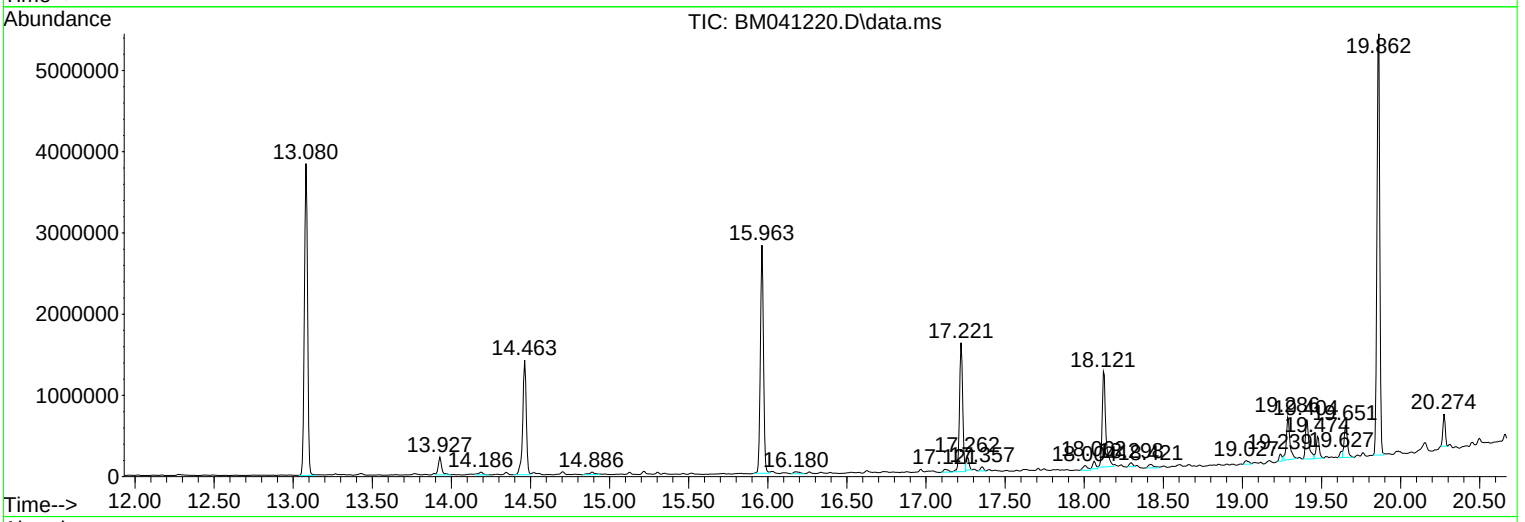
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

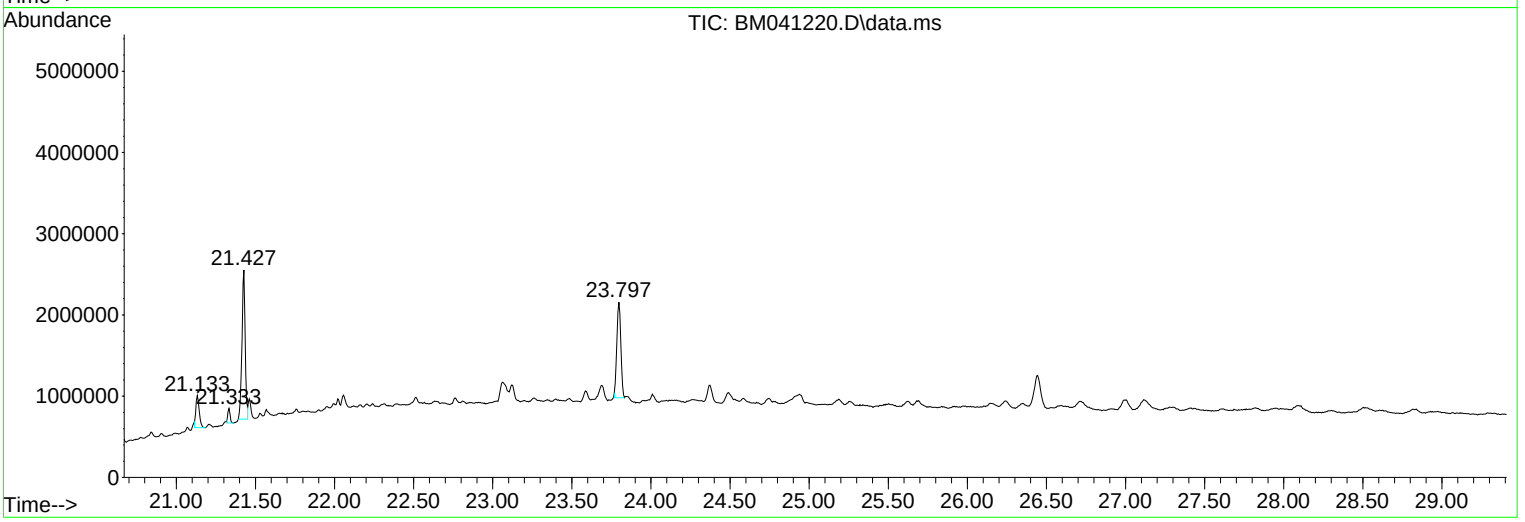
Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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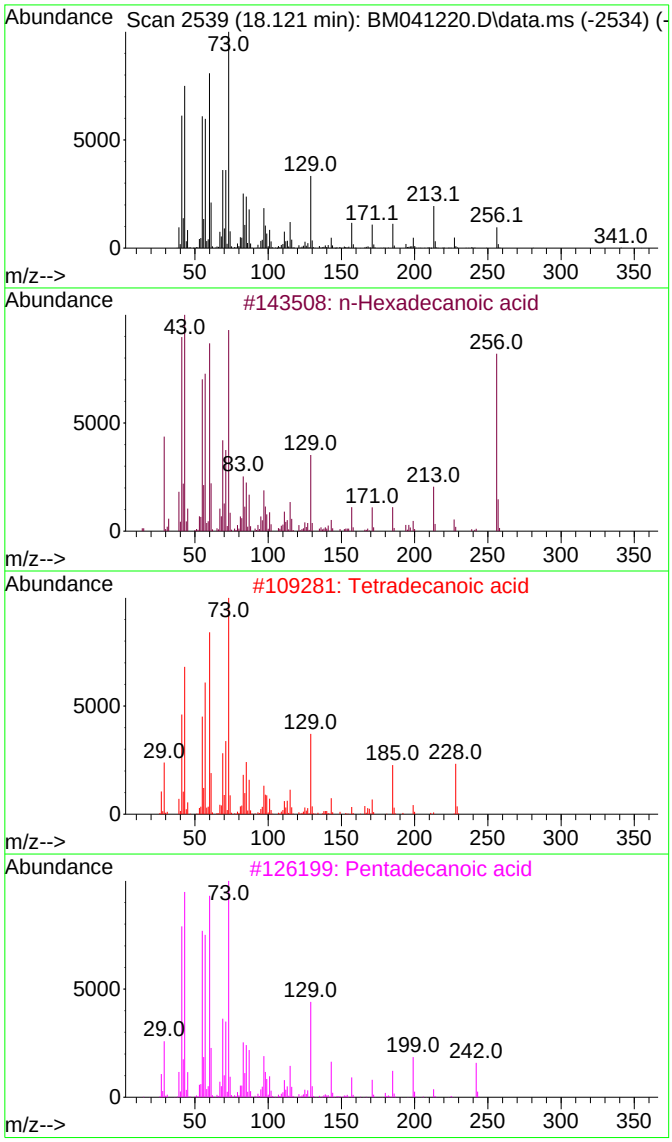
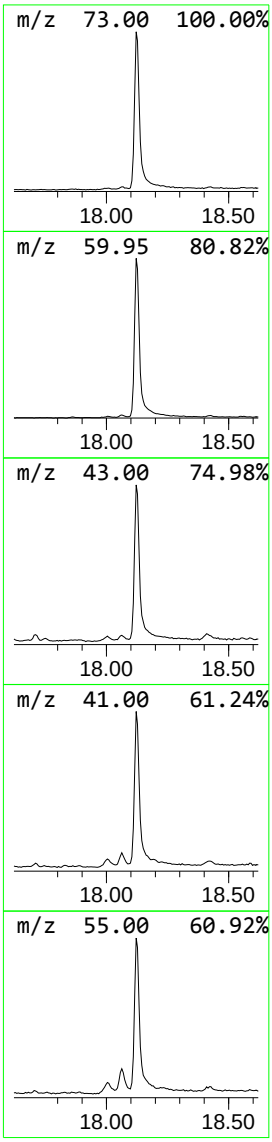
Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	16.41 ng	1836790	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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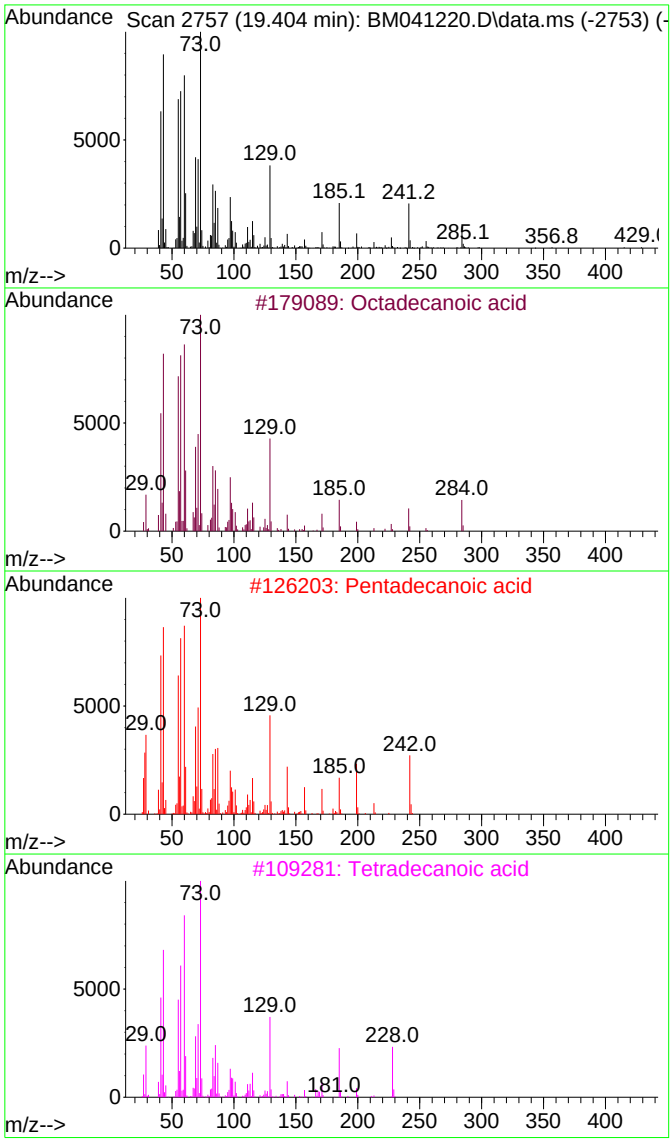
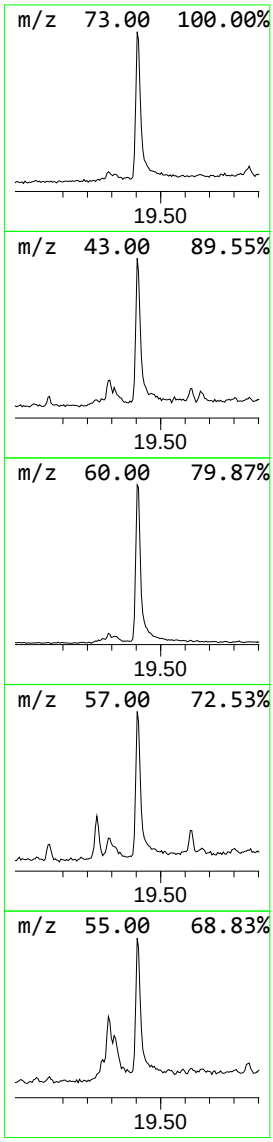
Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	5.74 ng	751336	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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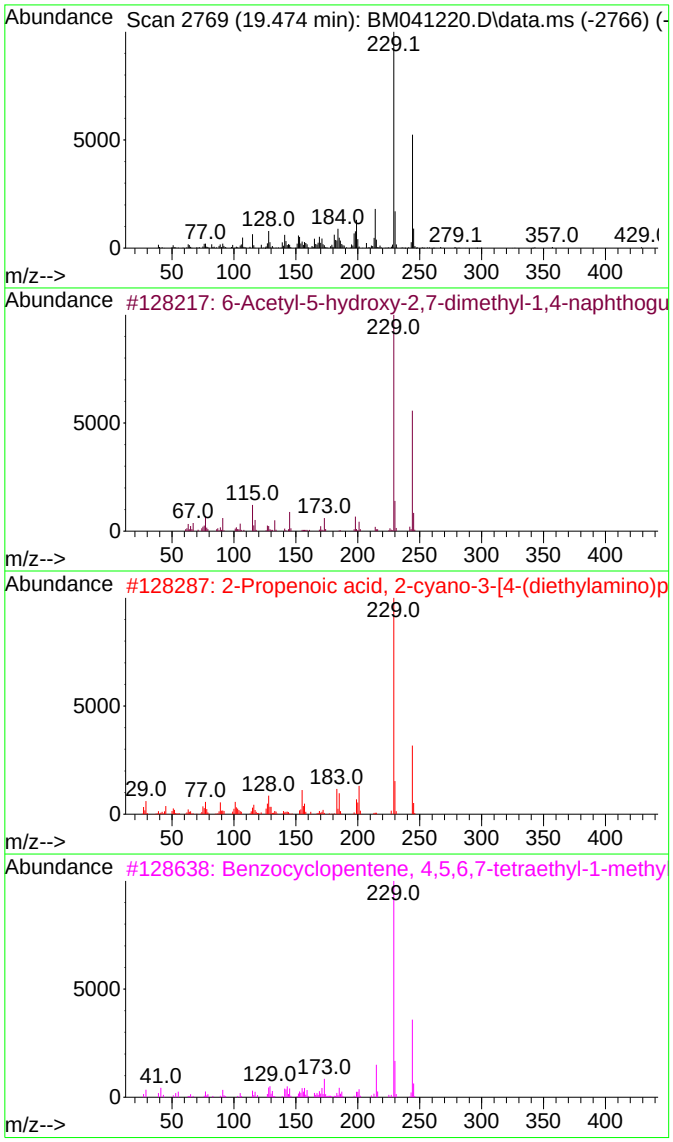
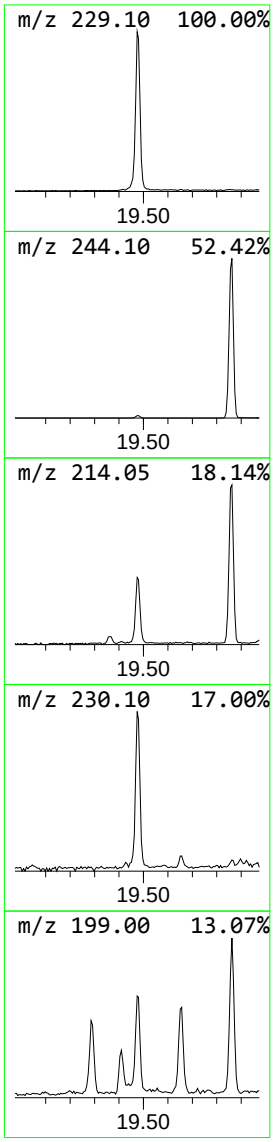
Peak Number 3 6-Acetyl-5-hydroxy-2,7-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	2.68 ng	350308	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Acetyl-5-hydroxy-2,7-dimethyl-...	244	C14H12O4	001086-07-3	74
2	2-Propenoic acid, 2-cyano-3-[4-(...	244	C14H16N2O2	1000115-72-8	74
3	Benzocyclopentene, 4,5,6,7-tetra...	244	C18H28	1000156-41-4	64
4	1,5-Diacetyl-2,6-naphthalenediol	244	C14H12O4	038790-70-4	64
5	Ethanone, 1-(2,3-dihydro-1,1,2,3...	244	C17H24O	015323-35-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
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Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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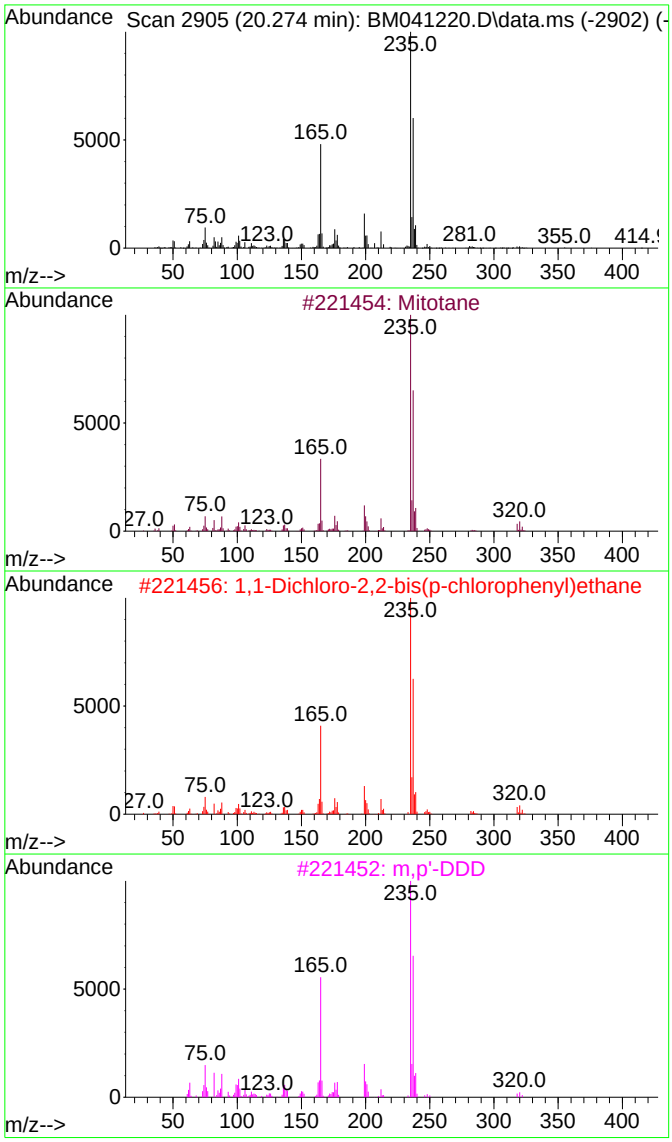
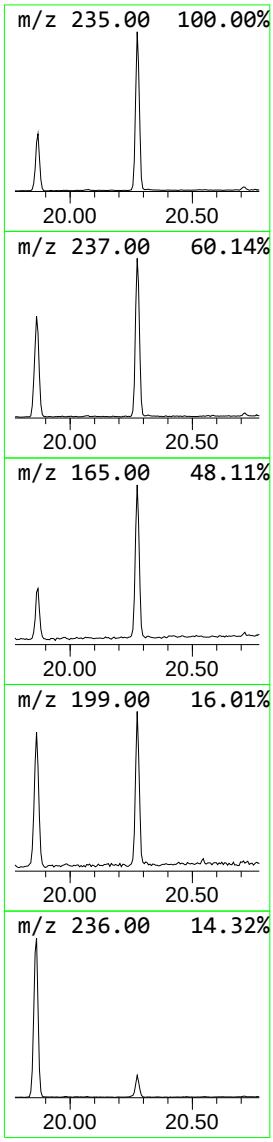
Peak Number 4 Mitotane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.274	3.14 ng	410721	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mitotane	318	C14H10Cl4	000053-19-0	97
2	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	95
3	m,p'-DDD	318	C14H10Cl4	004329-12-8	90
4	2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	90
5	1-Chloro-2,2-Bis(p-chlorophenyl)...	284	C14H11Cl3	002642-80-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041220.D
Acq On : 01 Aug 2023 12:12
Operator : MA/JU
Sample : 03769-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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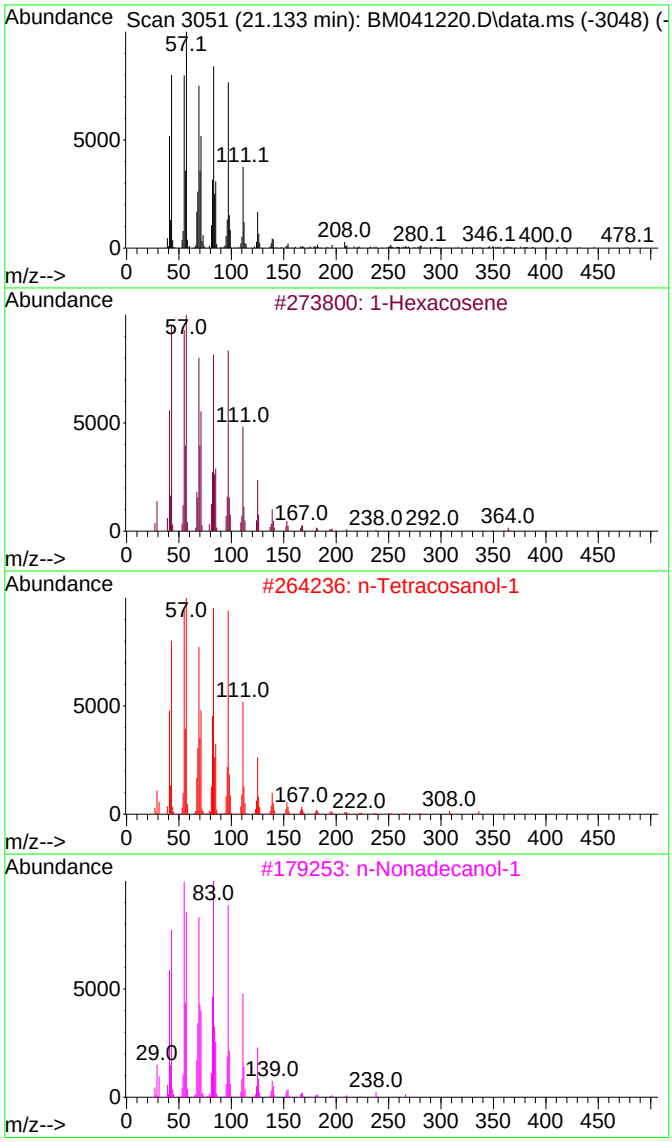
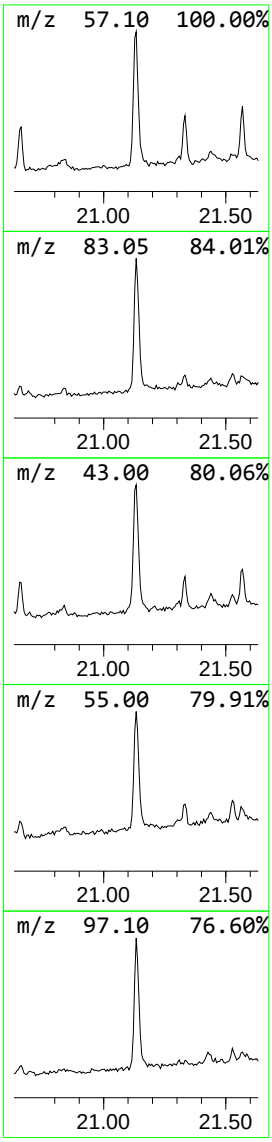
Peak Number 5 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	4.42 ng	578065	Chrysene-d12	21.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
n-Hexadecanoic ...	18.121	16.4	ng	1836790	4	17.221	2238560	20.0
Octadecanoic acid	19.404	5.7	ng	751336	5	21.427	2617400	20.0
6-Acetyl-5-hydr...	19.474	2.7	ng	350308	5	21.427	2617400	20.0
Mitotane	20.274	3.1	ng	410721	5	21.427	2617400	20.0
1-Hexacosene	21.133	4.4	ng	578065	5	21.427	2617400	20.0