LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	321	328	334	rBV2	44284	73676	1.26%	0.161%
2	5.475	400	406	420	rBV	1944465	2926652	49.92%	6.407%
3	7.069	667	677	690	rBV	1852808	2973649	50.73%	6.510%
4	7.898	808	818	825	rBV	487938	784586	13.38%	1.718%
5	9.057	1007	1015	1026	rBV	1167302	1946052	33.20%	4.260%
6	10.698	1286	1294	1300	rBV	612837	1035505	17.66%	2.267%
7	13.163	1705	1713	1732	rBV	2817228	4292287	73.22%	9.396%
8	14.533	1937	1946	1954	rBV	832261	1265981	21.60%	2.771%
9	16.021	2192	2199	2211	rBV	2038219	3055049	52.11%	6.688%
10	16.686	2306	2312	2317	rBV6	42530	71074	1.21%	0.156%
11	17.180	2392	2396	2400	rBV	54472	73930	1.26%	0.162%
12	17.280	2404	2413	2417	rBV	1028427	1530814	26.11%	3.351%
13	17.321	2417	2420	2426	rVB	302075	477143	8.14%	1.045%
14	17.410	2432	2435	2440	rVB	74083	102584	1.75%	0.225%
15	18.062	2541	2546	2552	rBV2	59649	107681	1.84%	0.236%
16	18.127	2552	2557	2562	rBV	565563	832570	14.20%	1.823%
17	18.186	2562	2567	2581	rVB	1162802	1661515	28.34%	3.637%
18	18.351	2591	2595	2599	rBV2	54218	84438	1.44%	0.185%
19	18.480	2613	2617	2621	rBV3	51754	73350	1.25%	0.161%
20	18.898	2685	2688	2693	rVB3	58100	83808	1.43%	0.183%
21	19.145	2727	2730	2737	rVB4	68508	102756	1.75%	0.225%
22	19.209	2738	2741	2749	rVV5	38859	71909	1.23%	0.157%
23	19.339	2755	2763	2766	rBV	989795	1463606	24.97%	3.204%
24	19.462	2779	2784	2793	rBV2	446933	613351	10.46%	1.343%
25	19.698	2815	2824	2833	rBV2	647193	1214713	20.72%	2.659%
26	19.903	2853	2859	2864	rBV	4932438	5862138	100.00%	12.833%
27	20.056	2883	2885	2893	rVB2	76181	110267	1.88%	0.241%
28	20.198	2906	2909	2912	rBV	96040	95557	1.63%	0.209%
29	20.298	2923	2926	2929	rBV	72126	81385	1.39%	0.178%
30	20.451	2948	2952	2956	rBV	194016	257308	4.39%	0.563%
31	20.539	2964	2967	2972	rVB6	108755	166556	2.84%	0.365%
32	20.715	2995	2997	3000	rVB	85376	90235	1.54%	0.198%
33	21.145	3067	3070	3073	rBV	206165	247881	4.23%	0.543%
34	21.180	3073	3076	3083	rVB2	571487	733893	12.52%	1.607%
35	21.462	3117	3124	3128	rBV2	1599696	2695331	45.98%	5.900%
36	21.498	3128	3130	3141	rVB	458057	521341	8.89%	1.141%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.621	3148	3151	3157	rBV	248040	309898	5.29%	0.678%
38	22.086	3226	3230	3231	rBV2	278851	339628	5.79%	0.743%
39	22.580	3311	3314	3324	rVB2	262422	469310	8.01%	1.027%
40	23.127	3401	3407	3411	rBV	842690	1565377	26.70%	3.427%
41	23.180	3412	3416	3433	rVB5	586486	1293854	22.07%	2.832%
42	23.739	3507	3511	3519	rVB2	506110	996401	17.00%	2.181%
43	23.844	3523	3529	3535	rVV2	960445	1837688	31.35%	4.023%
44	24.462	3630	3634	3643	rVB	532575	1087897	18.56%	2.382%

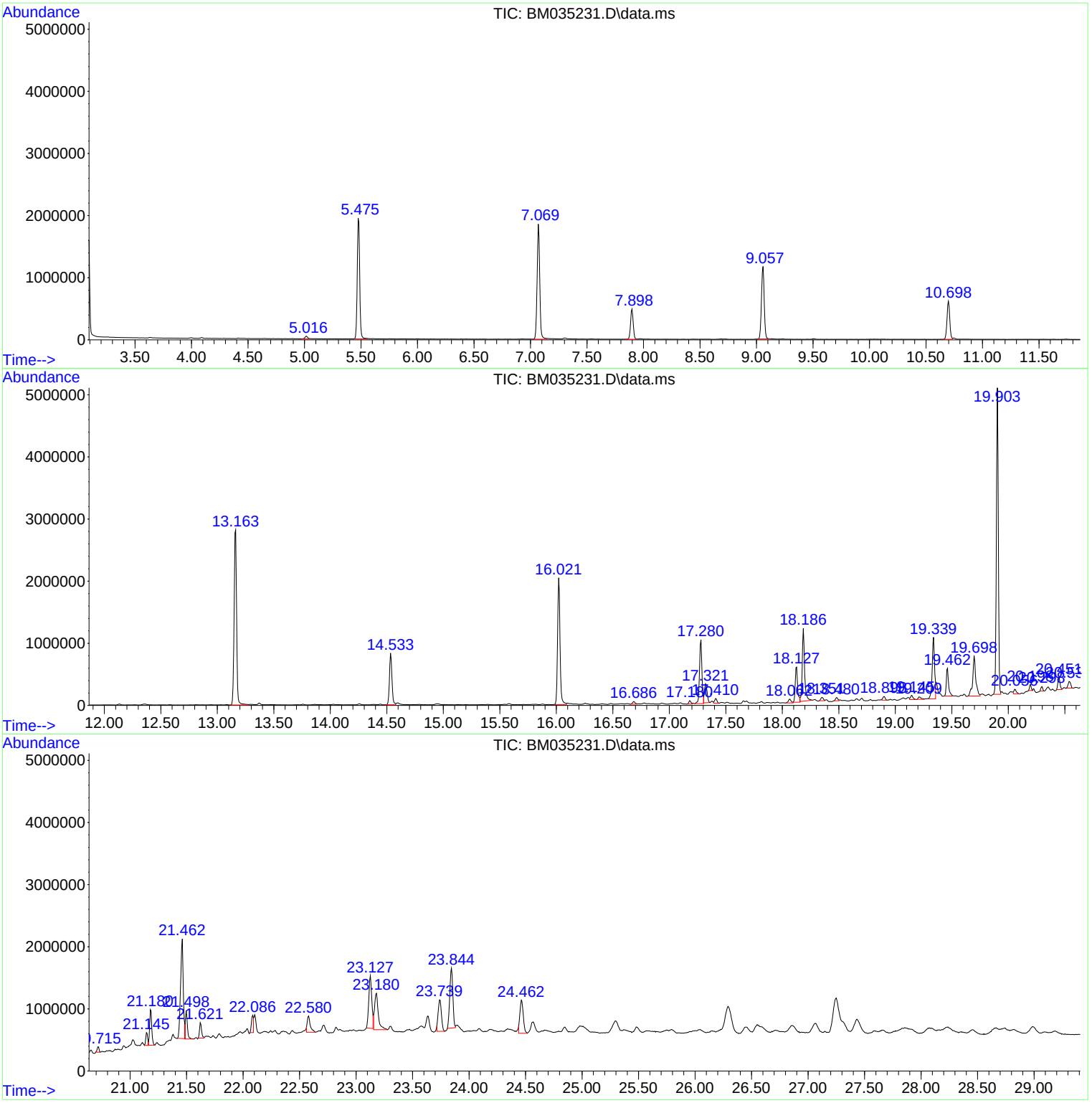
Sum of corrected areas: 45680624

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

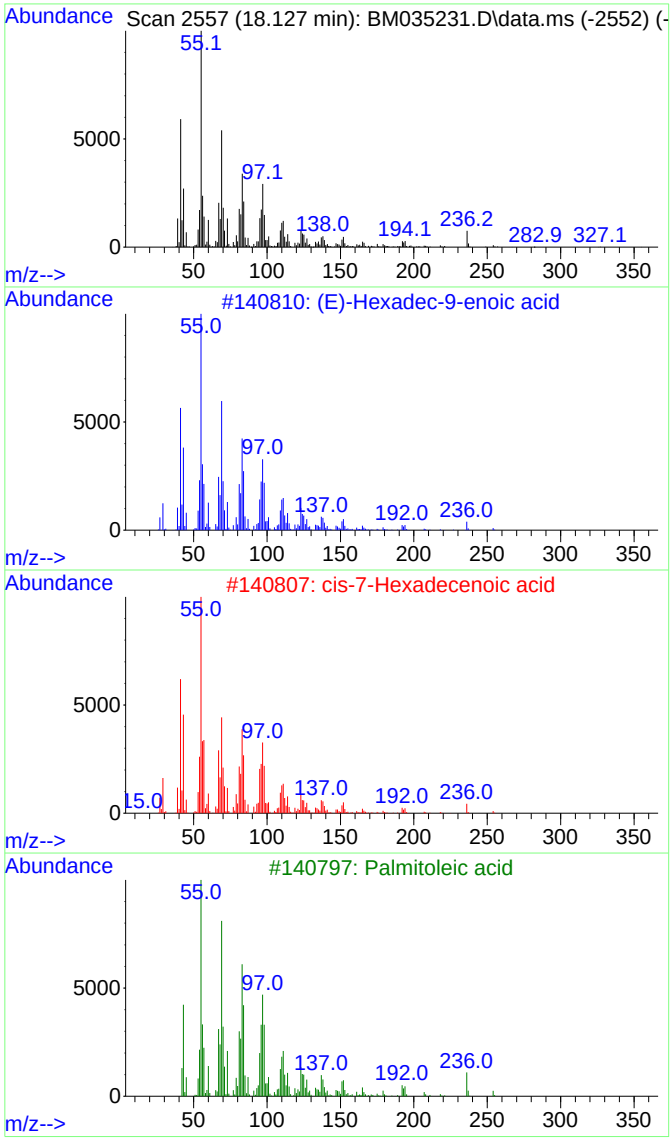
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

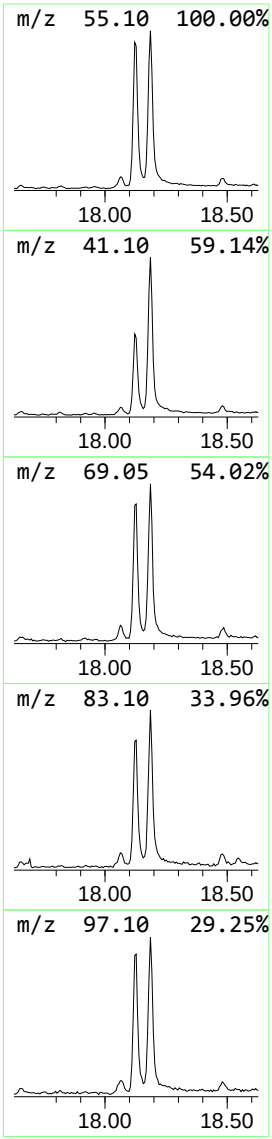
****

Peak Number 1 (E)-Hexadec-9-enoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	10.88 ng	832570	Phenanthrene-d10	17.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
3	Palmitoleic acid	254	C16H30O2	000373-49-9	96
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	94
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

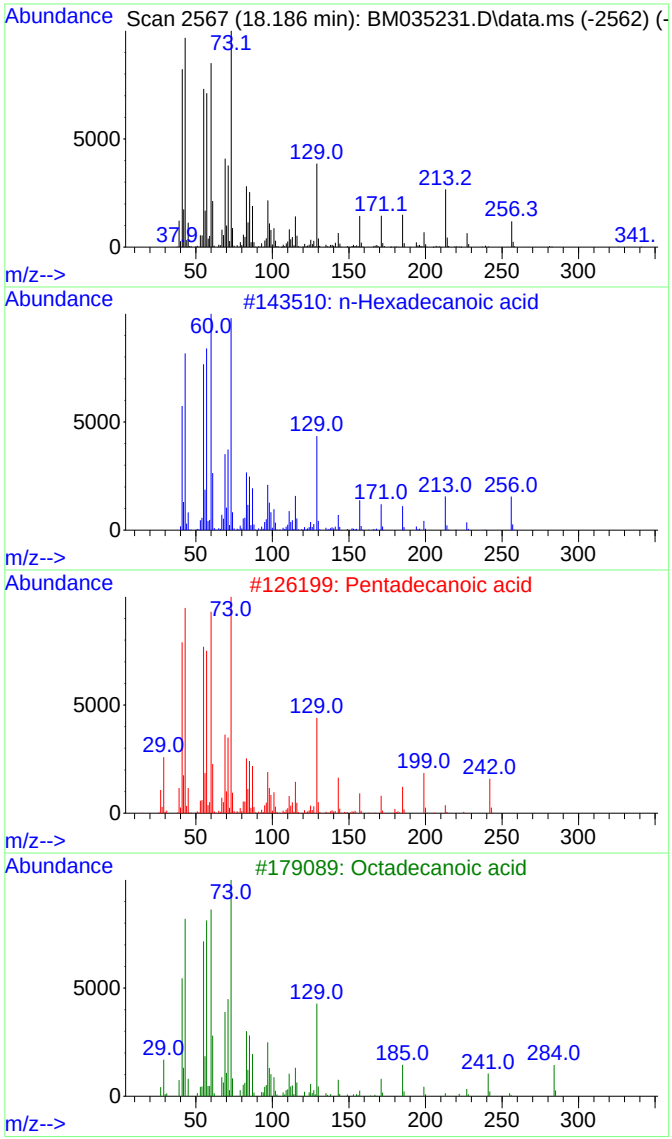
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

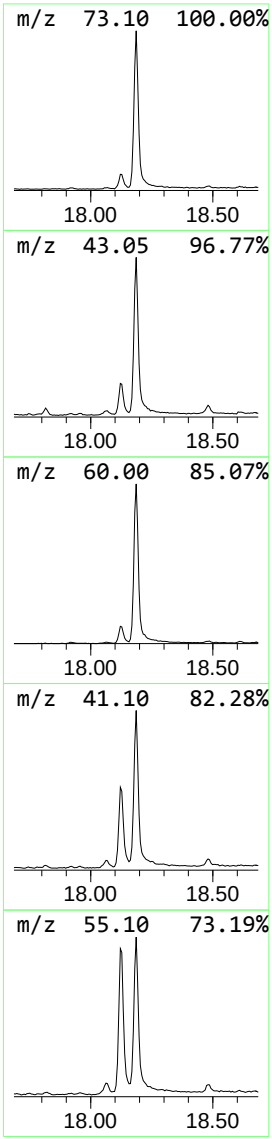
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	21.71 ng	1661520	Phenanthrene-d10	17.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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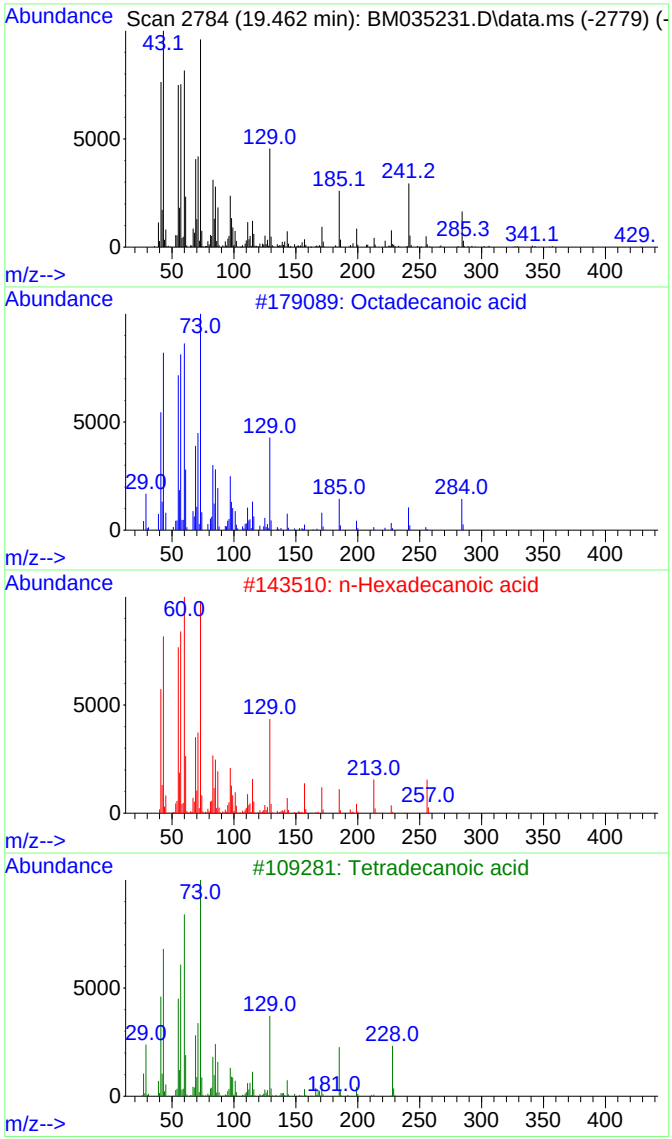
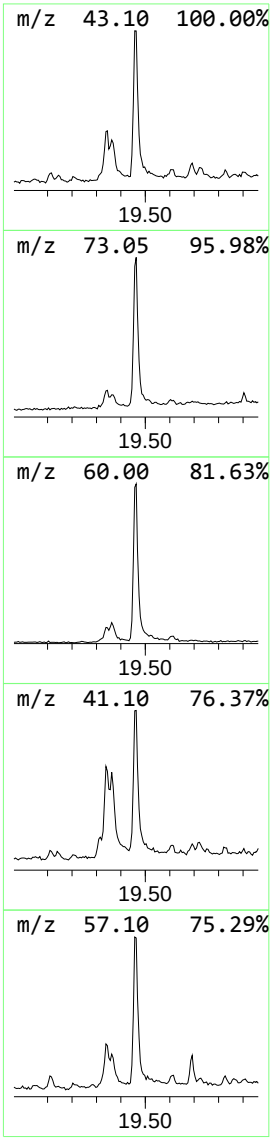
Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	4.55 ng	613351	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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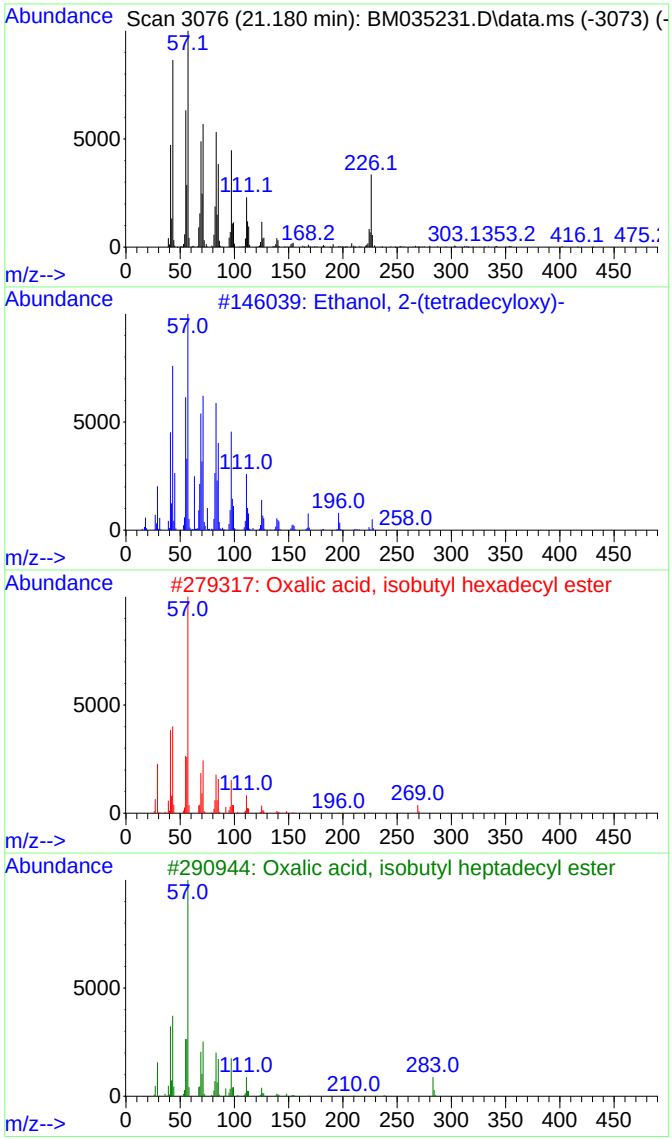
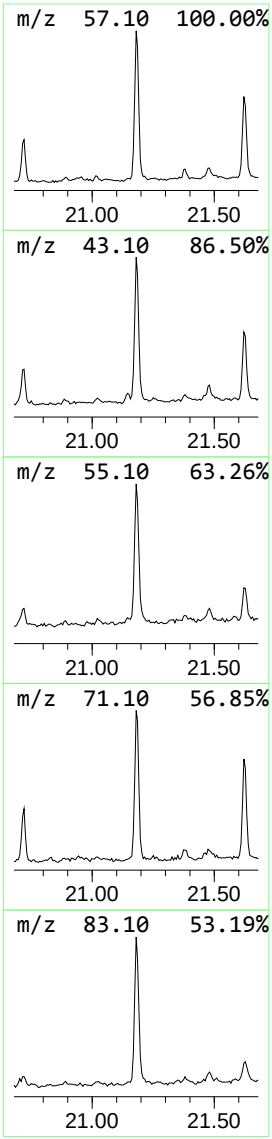
Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	5.45 ng	733893	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	99
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
4	17-Pentatriacontene	491	C35H70	006971-40-0	76
5	Trihexadecyl borate	735	C48H99BO3	002665-11-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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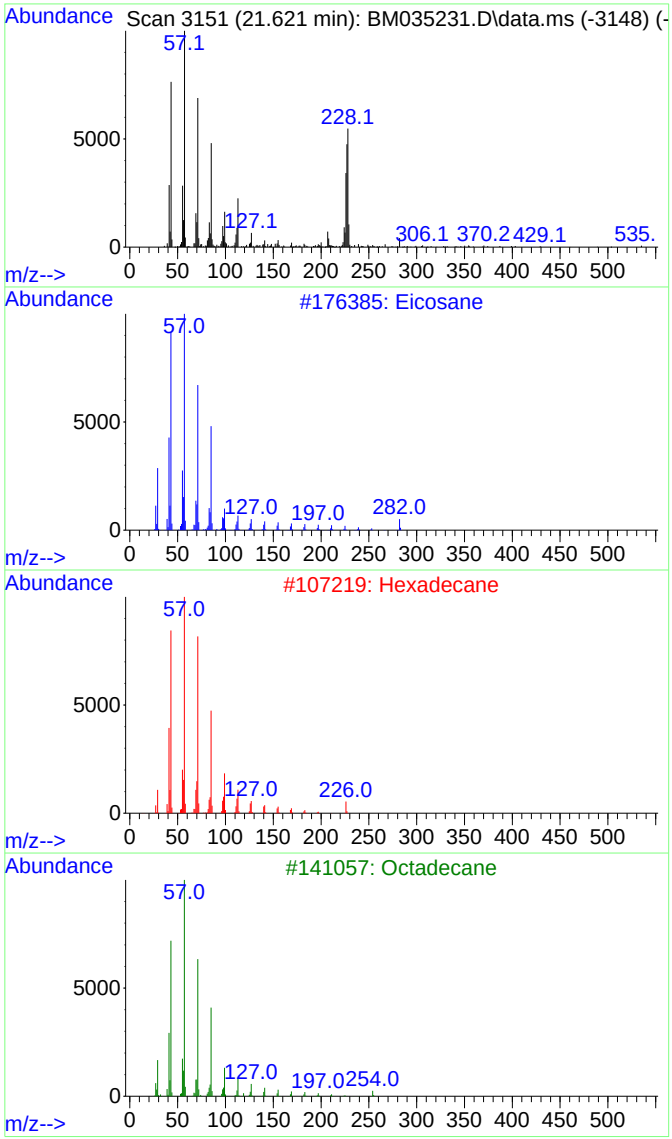
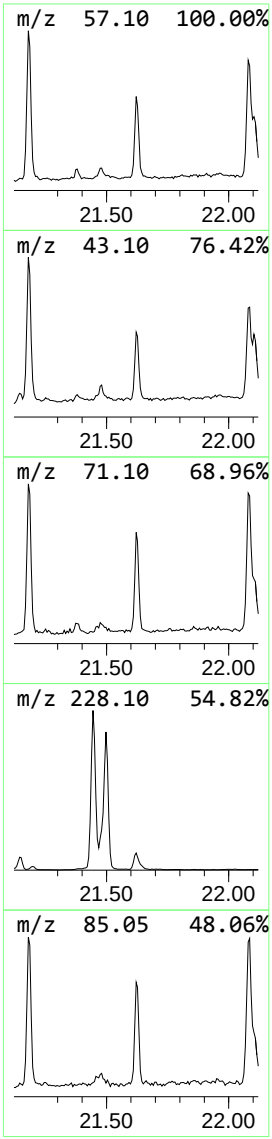
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.621	2.30 ng	309898	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Hexadecane	226	C16H34	000544-76-3	38
3	Octadecane	254	C18H38	000593-45-3	38
4	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	38
5	Octacosane	394	C28H58	000630-02-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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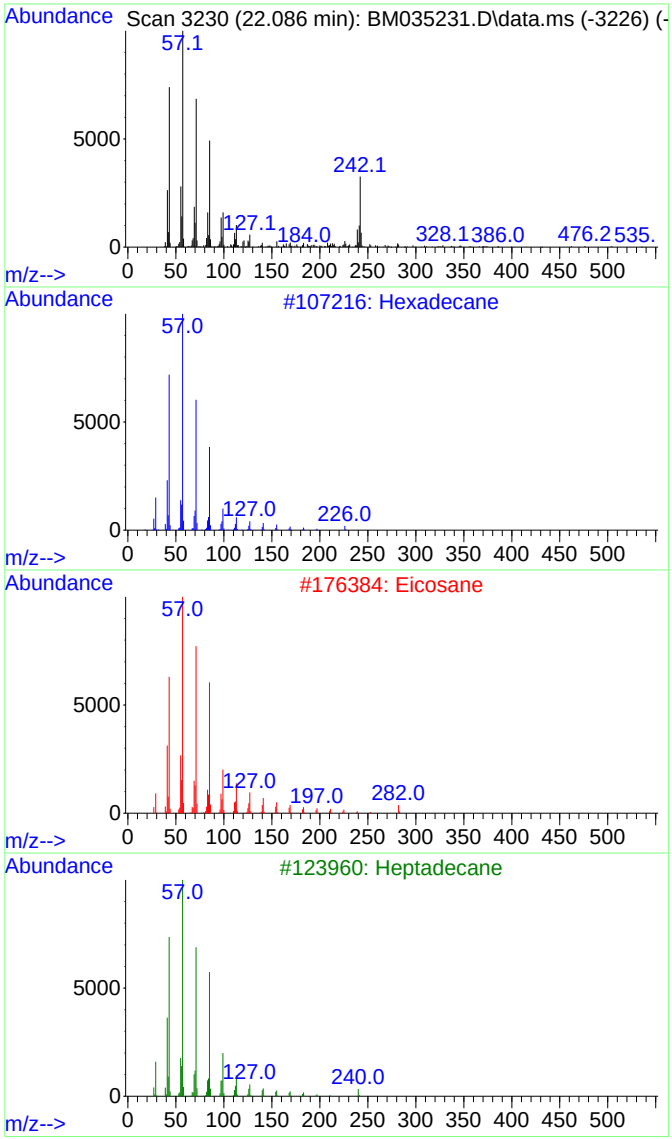
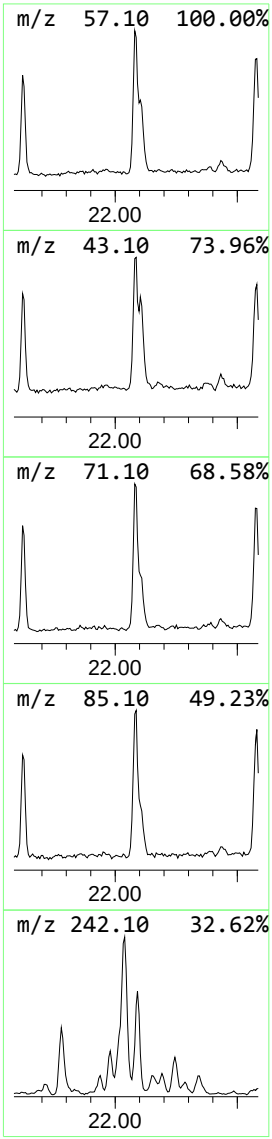
Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.086	2.52 ng	339628	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Eicosane	282	C20H42	000112-95-8	95
3	Heptadecane	240	C17H36	000629-78-7	93
4	Tetracosane	338	C24H50	000646-31-1	89
5	Octacosane	394	C28H58	000630-02-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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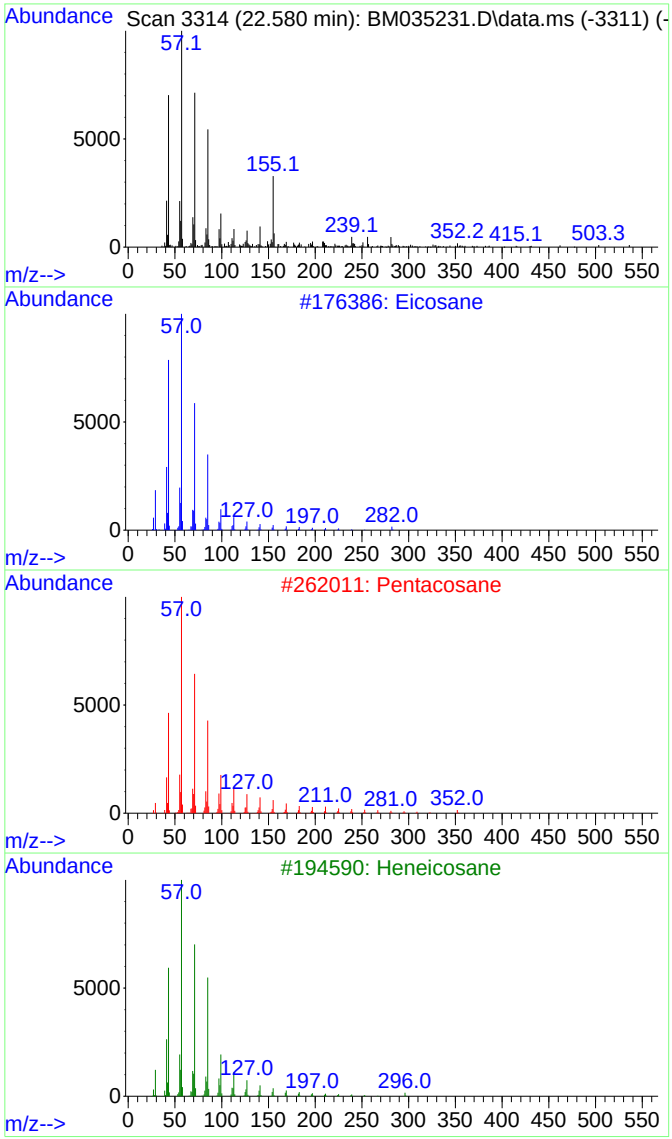
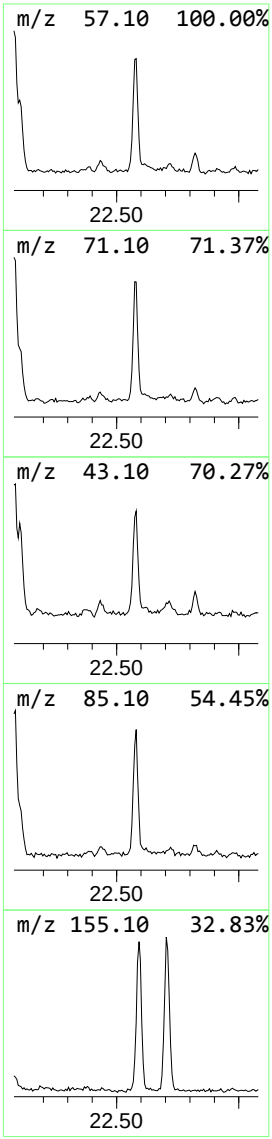
Peak Number 7 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.580	3.48 ng	469310	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentacosane	352	C25H52	000629-99-2	90
3	Heneicosane	296	C21H44	000629-94-7	76
4	Octadecane	254	C18H38	000593-45-3	68
5	Tetracosane	338	C24H50	000646-31-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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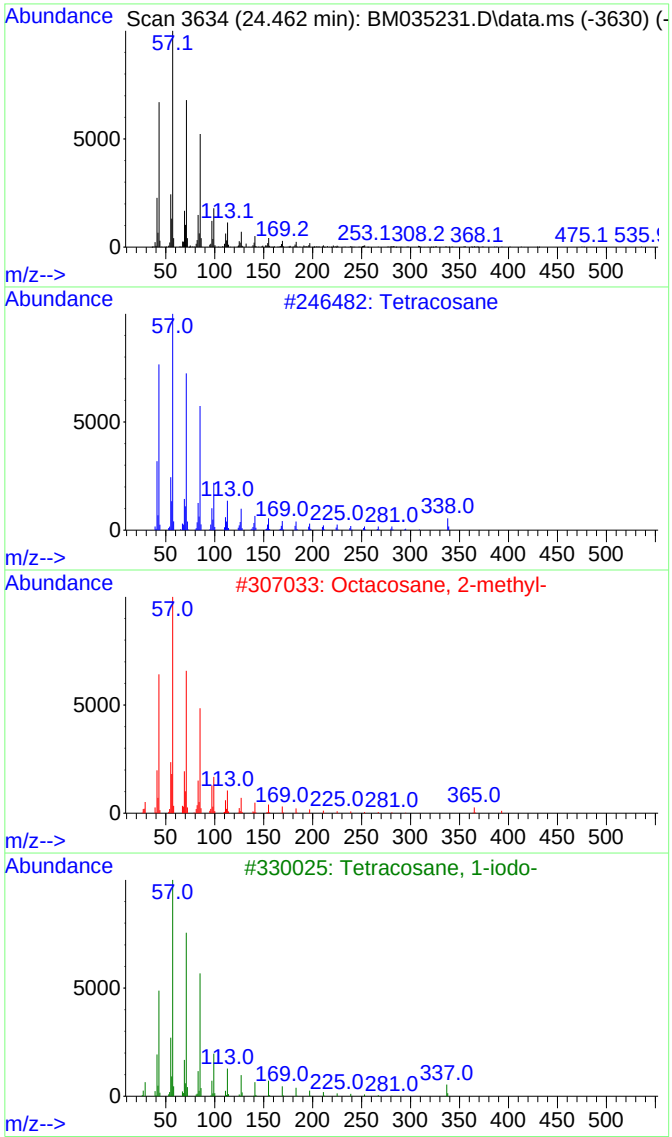
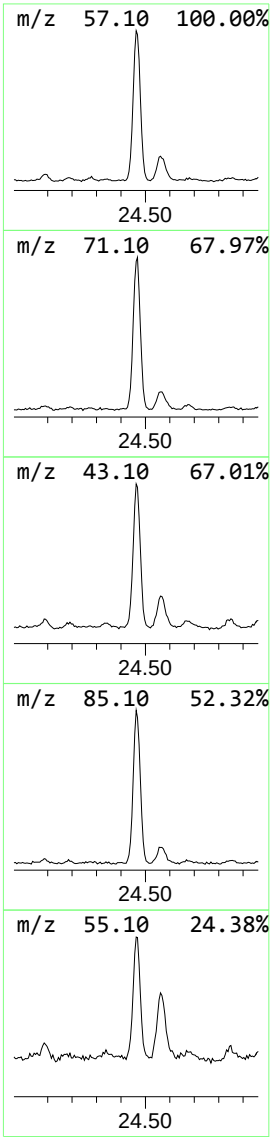
Peak Number 8 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.462	11.84 ng	1087900	Perylene-d12	23.844

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	96
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052422\
Data File : BM035231.D
Acq On : 24 May 2022 22:21
Operator : CG/JU
Sample : N2981-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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
(E)-Hexadec-9-e...	18.127	10.9	ng	832570	4	17.280	1530810	20.0
n-Hexadecanoic ...	18.186	21.7	ng	1661520	4	17.280	1530810	20.0
Octadecanoic acid	19.462	4.5	ng	613351	5	21.462	2695330	20.0
Ethanol, 2-(tet...	21.180	5.5	ng	733893	5	21.462	2695330	20.0
Eicosane	21.621	2.3	ng	309898	5	21.462	2695330	20.0
Hexadecane	22.086	2.5	ng	339628	5	21.462	2695330	20.0
Pentacosane	22.580	3.5	ng	469310	5	21.462	2695330	20.0
Tetracosane	24.462	11.8	ng	1087900	6	23.844	1837690	20.0