LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035177.D
Acq On : 20 May 2022 15:32
Operator : CG/JU
Sample : N2939-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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: BM035177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	400	407	415	rBV	1030949	1479265	14.67%	3.232%
2	7.069	671	677	688	rBV	558424	904362	8.97%	1.976%
3	7.904	813	819	826	rBV	430868	668411	6.63%	1.460%
4	9.063	1009	1016	1025	rBV	1367876	2207366	21.88%	4.823%
5	10.704	1288	1295	1303	rBV	524062	892305	8.85%	1.950%
6	13.169	1706	1714	1727	rBV	3469778	5075974	50.32%	11.091%
7	14.539	1941	1947	1958	rBV	781037	1184920	11.75%	2.589%
8	15.363	2079	2087	2101	rVB	339358	596031	5.91%	1.302%
9	15.915	2175	2181	2190	rVB2	147135	248412	2.46%	0.543%
10	16.027	2194	2200	2218	rVB	2792514	4069685	40.35%	8.892%
11	17.286	2408	2414	2420	rBV	1028236	1404825	13.93%	3.069%
12	18.198	2562	2569	2576	rBV	2396530	3652057	36.21%	7.979%
13	18.256	2576	2579	2597	rVB	232526	474582	4.71%	1.037%
14	19.321	2756	2760	2762	rBV2	131620	185000	1.83%	0.404%
15	19.345	2762	2764	2772	rVB	180772	284622	2.82%	0.622%
16	19.480	2780	2787	2817	rVB	6581357	10086484	100.00%	22.038%
17	19.915	2855	2861	2869	rVB	6605720	8263590	81.93%	18.055%
18	21.192	3074	3078	3084	rBV2	154851	239670	2.38%	0.524%
19	21.392	3109	3112	3119	rVB	151569	162535	1.61%	0.355%
20	21.468	3121	3125	3131	rBV	1368572	1759751	17.45%	3.845%
21	23.856	3525	3531	3541	rVB2	953198	1928807	19.12%	4.214%

Sum of corrected areas: 45768654

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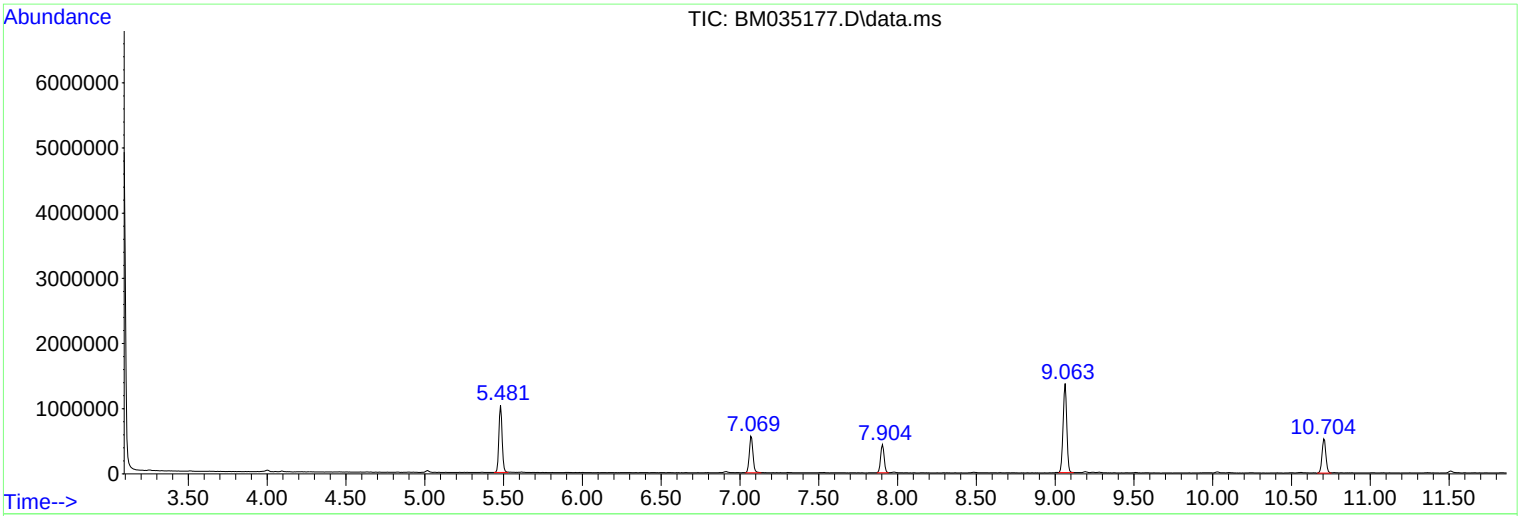
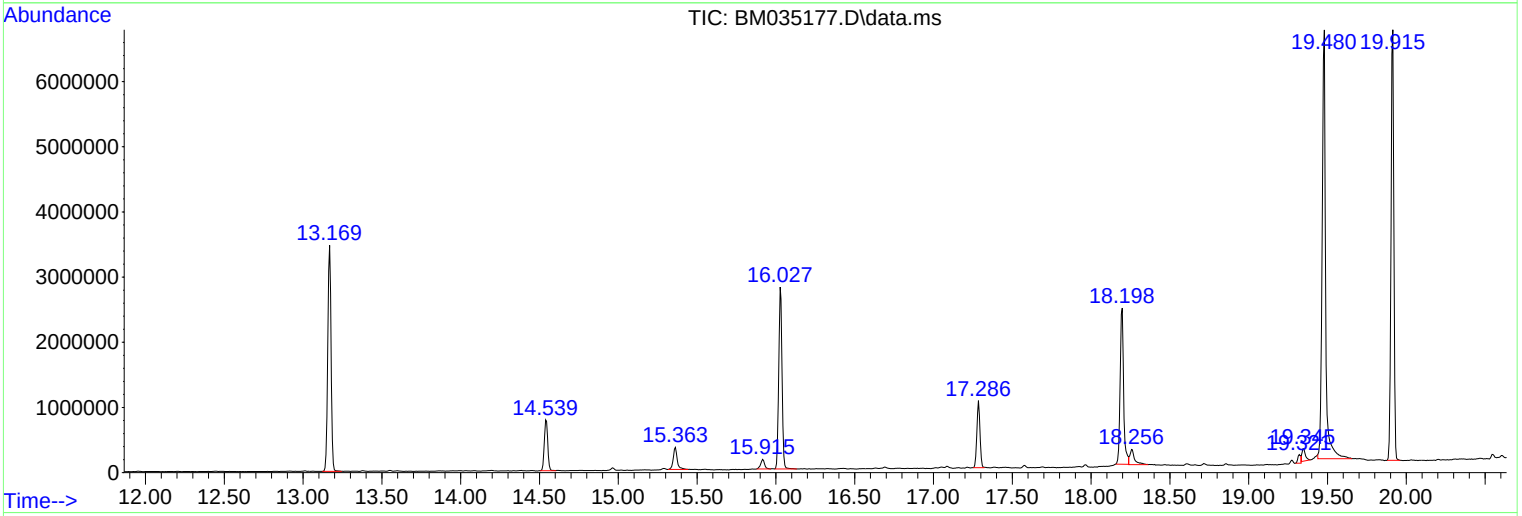
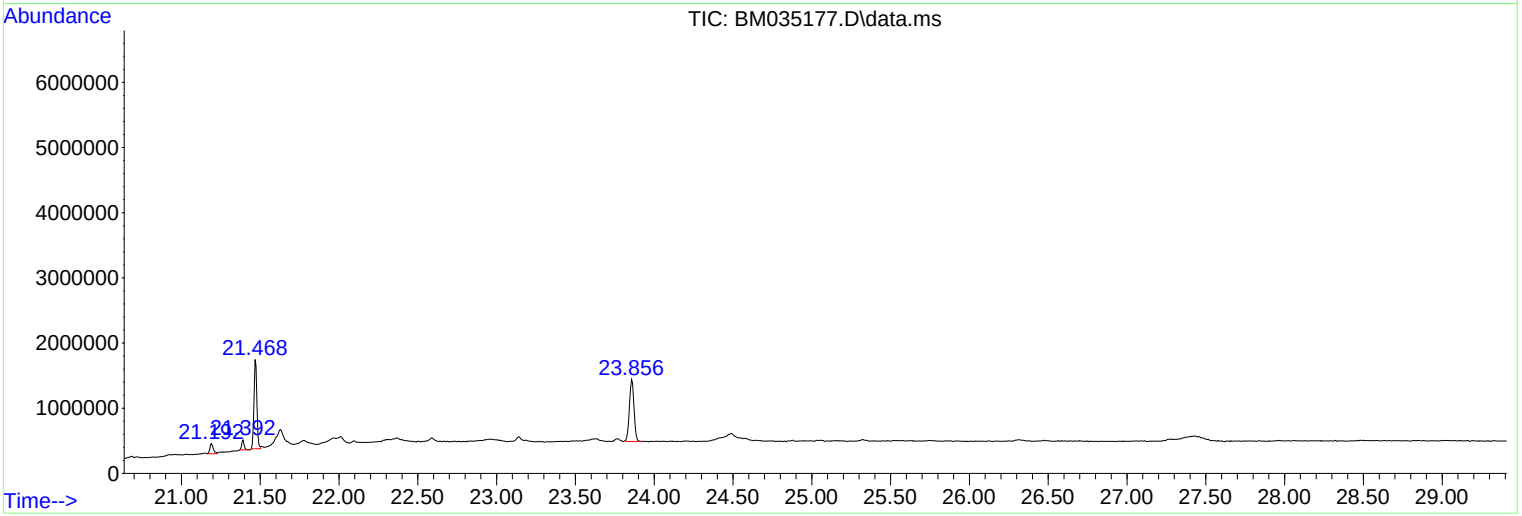
Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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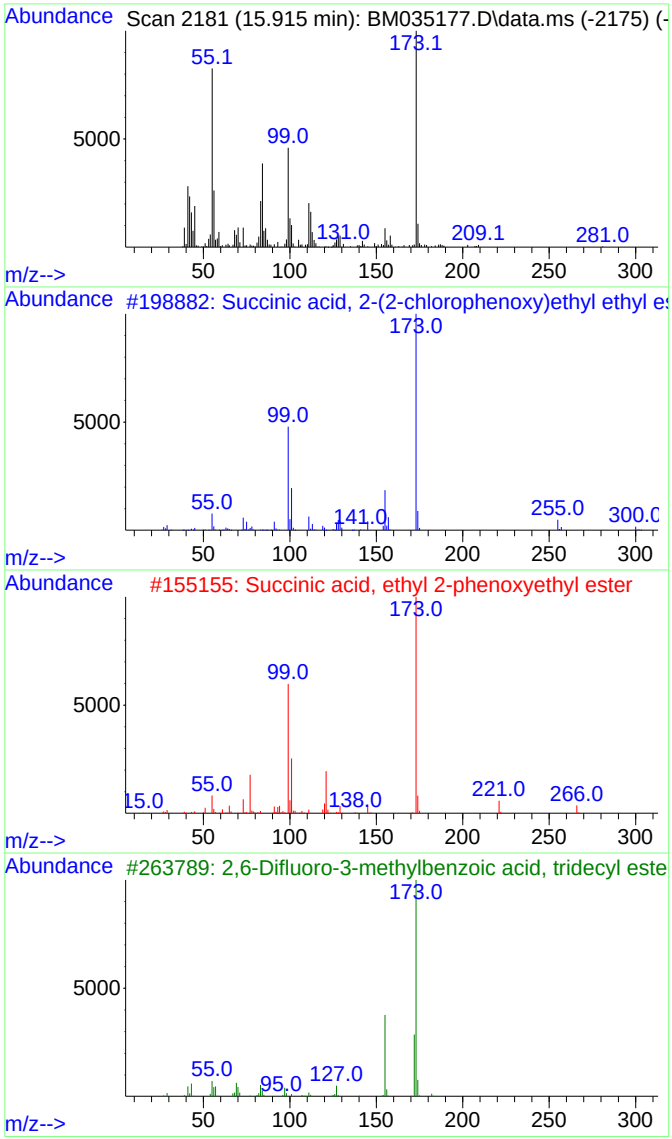
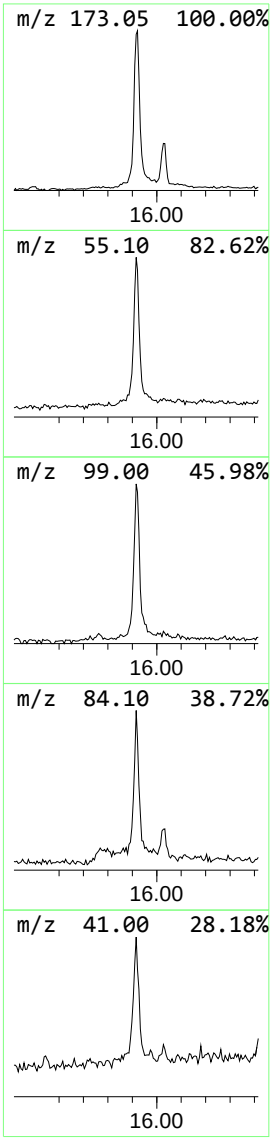
Peak Number 1 unknown15.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.916	3.54 ng	248412	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-(2-chlorophenox...	300	C14H17ClO5	1000381-53-1	38
2	Succinic acid, ethyl 2-phenoxyet...	266	C14H18O5	1000381-19-1	37
3	2,6-Difluoro-3-methylbenzoic aci...	354	C21H32F2O2	1000338-85-0	35
4	ethanone, 1-(2,3-dihydro-4-methy...	173	C6H7NOS2	1010404-67-0	25
5	2,6-Difluoro-3-methylbenzoic aci...	410	C25H40F2O2	1000338-85-4	25





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Operator : CG/JU
Sample : N2939-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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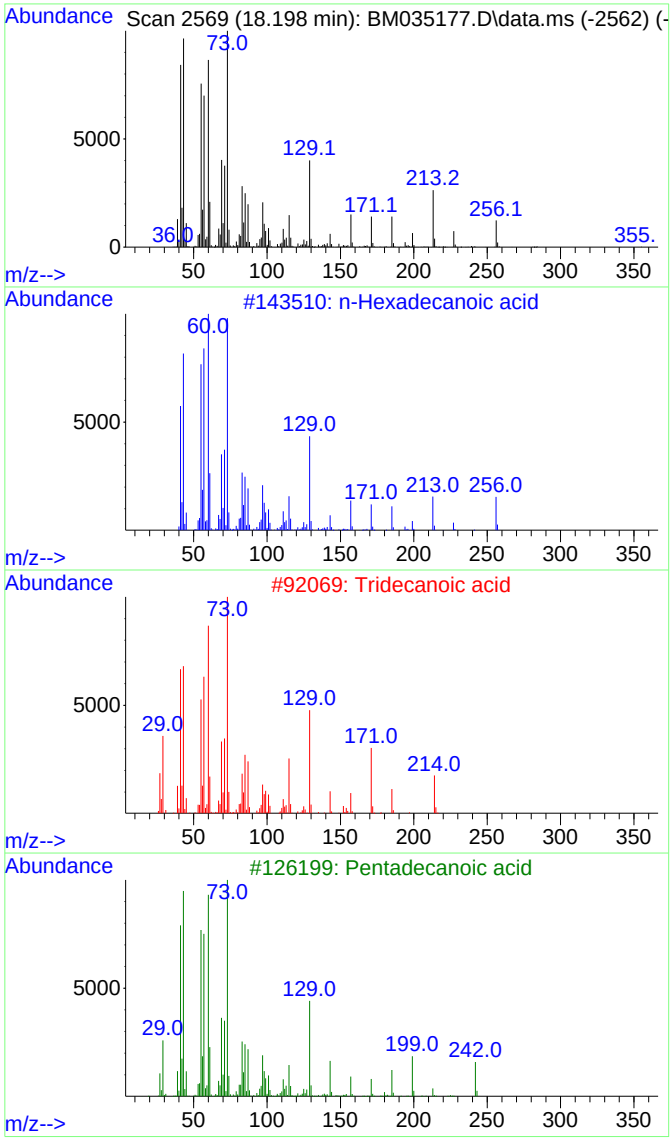
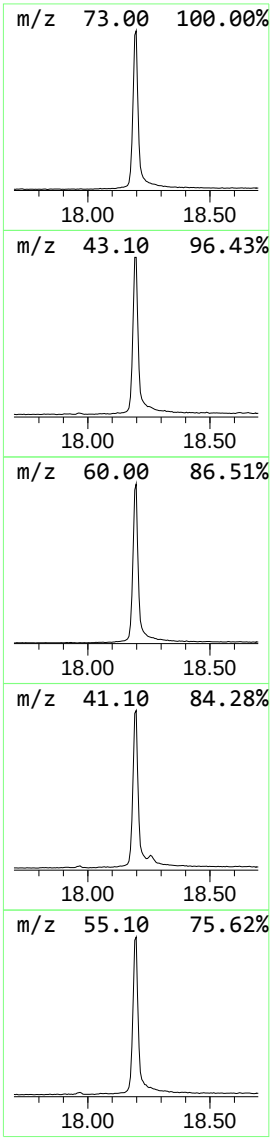
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	51.99 ng	3652060	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035177.D
Acq On : 20 May 2022 15:32
Operator : CG/JU
Sample : N2939-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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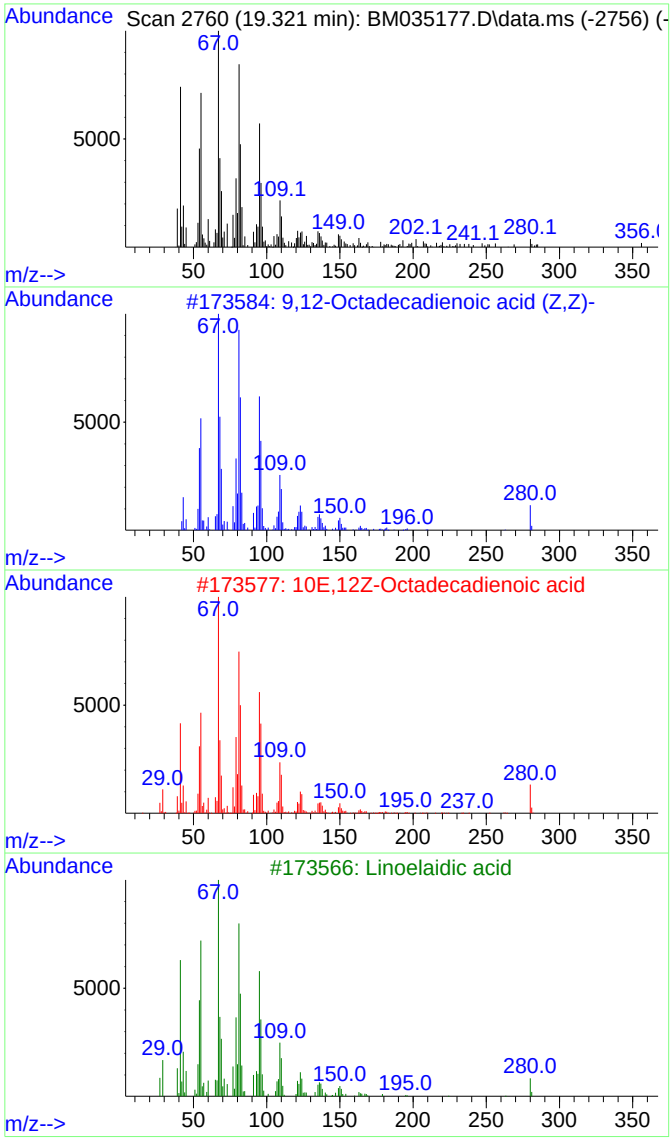
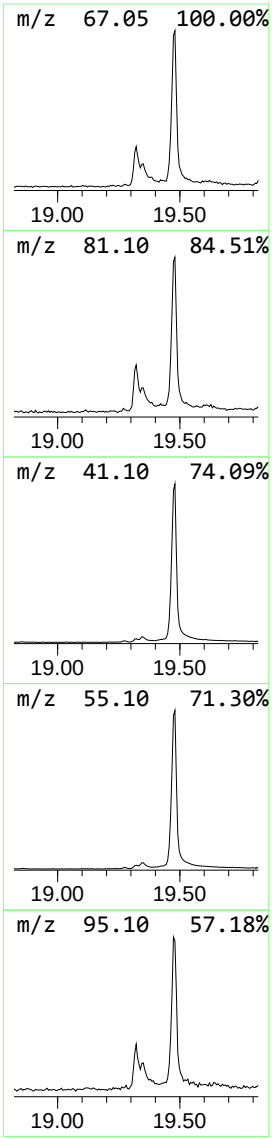
Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	2.63 ng	185000	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	97
3	Linoelaidic acid	280	C18H32O2	000506-21-8	96
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	95
5	E-7-Tetradecenol	212	C14H28O	037011-95-3	89





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Data File : BM035177.D
Acq On : 20 May 2022 15:32
Operator : CG/JU
Sample : N2939-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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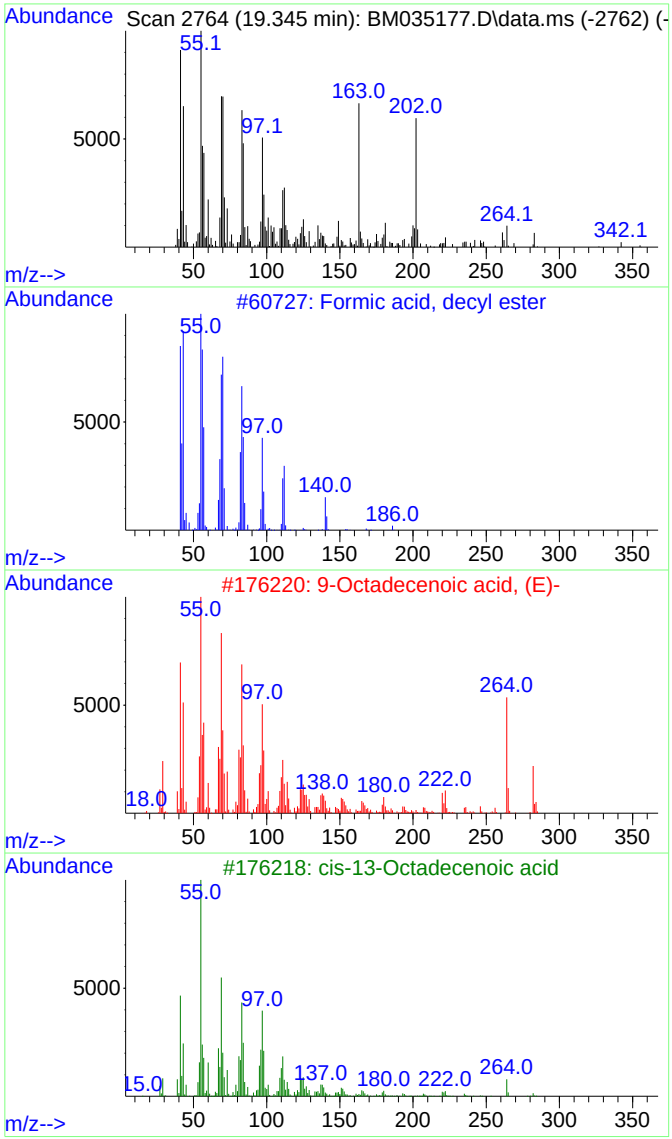
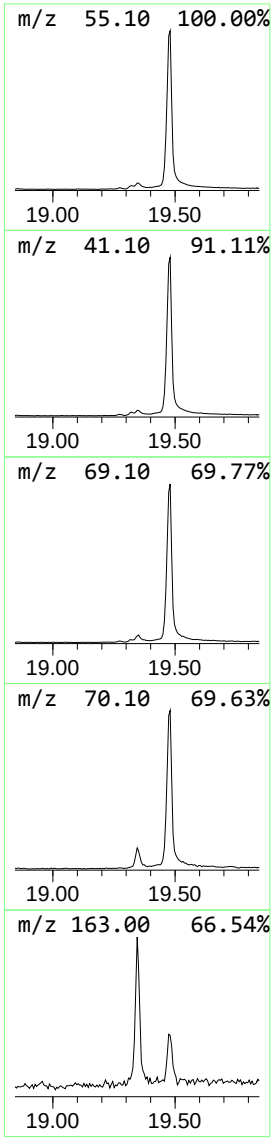
Peak Number 4 Formic acid, decyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	4.05 ng	284622	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, decyl ester	186	C11H22O2	005451-52-5	70
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	70
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	70
4	Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	58
5	Decyl acrylate	212	C13H24O2	002156-96-9	58





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Acq On : 20 May 2022 15:32
Operator : CG/JU
Sample : N2939-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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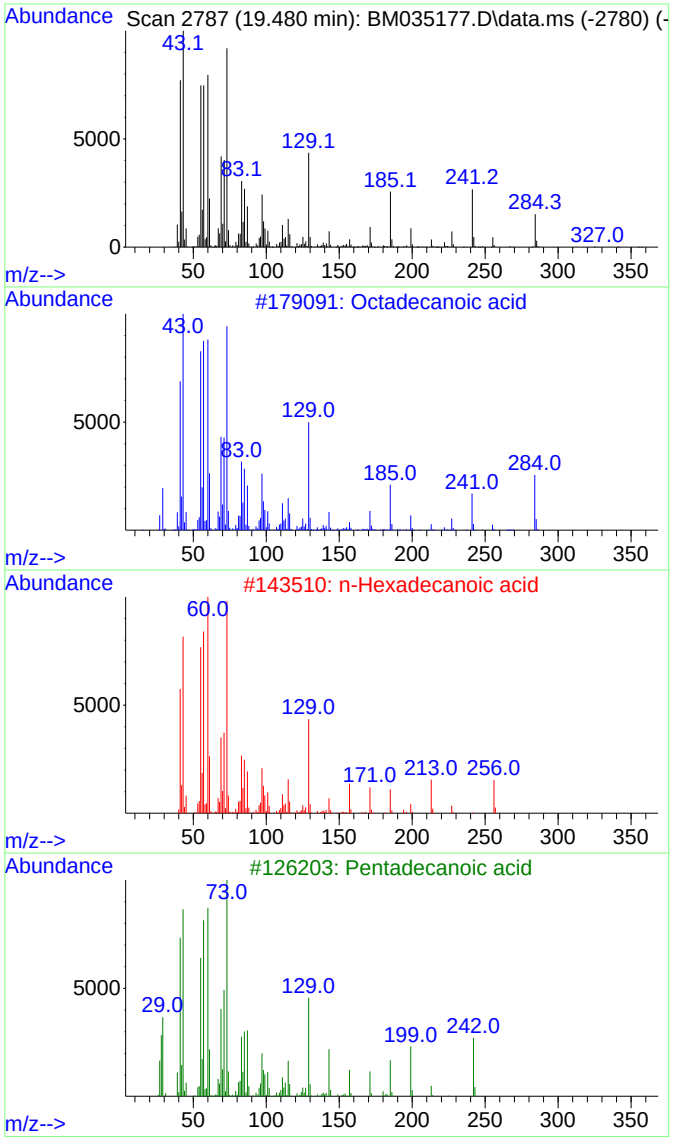
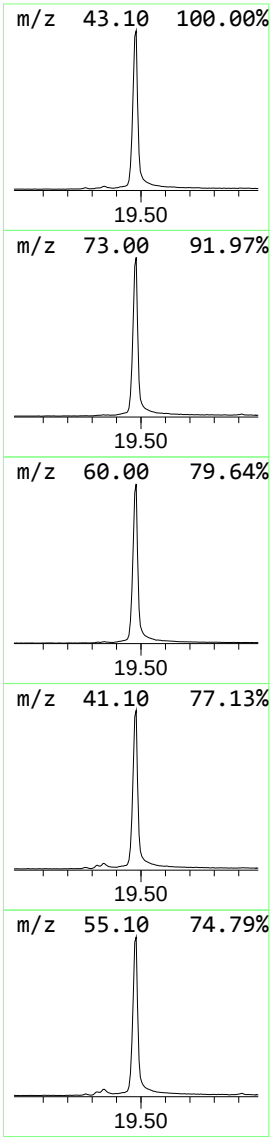
Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	114.64 ng	10086500	Chrysene-d12	21.468

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B1-WATER

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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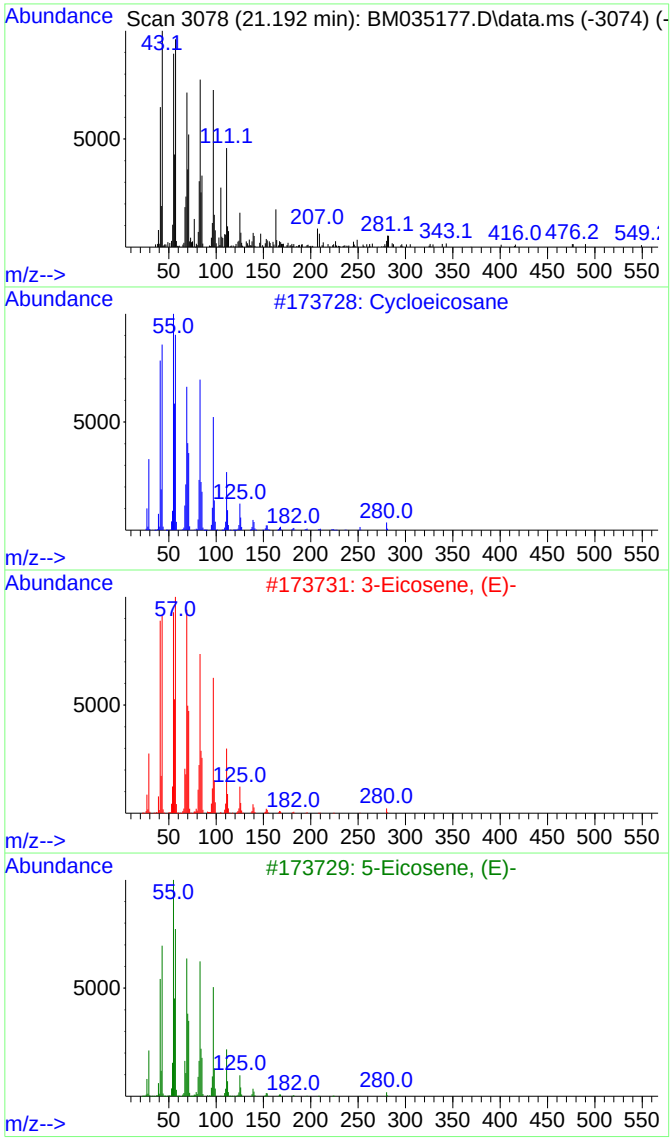
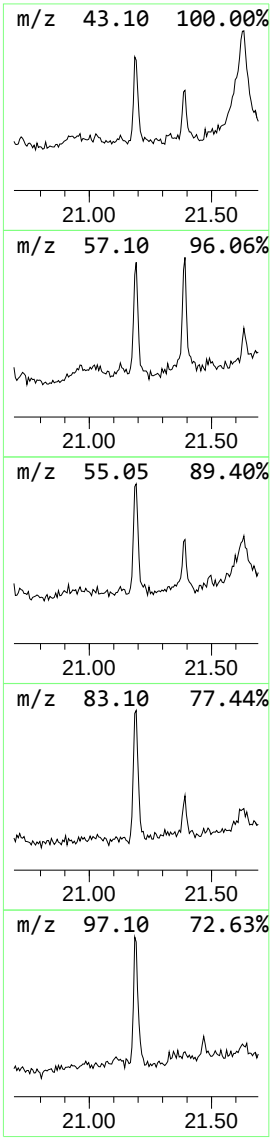
Peak Number 6 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	2.72 ng	239670	Chrysene-d12	21.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	98
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
4	17-Pentatriacontene	491	C35H70	006971-40-0	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Tentatively Identified Compound (LSC) summary

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Instrument :
BNA_M
ClientSampleId :
B1-WATER

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
unknown15.916	15.916	3.5	ng	248412	4	17.286	1404830	20.0
n-Hexadecanoic ...	18.198	52.0	ng	3652060	4	17.286	1404830	20.0
9,12-Octadecadi...	19.321	2.6	ng	185000	4	17.286	1404830	20.0
Formic acid, de...	19.345	4.0	ng	284622	4	17.286	1404830	20.0
Octadecanoic acid	19.480	114.6	ng	10086500	5	21.468	1759750	20.0
Cycloeicosane	21.192	2.7	ng	239670	5	21.468	1759750	20.0