

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081524\
 Data File : BM047210.D
 Acq On : 15 Aug 2024 11:31
 Operator : RC/JU
 Sample : PB162717BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB162717BL

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.575	282	287	294	rBV	271455	355233	3.08%	0.589%
2	5.022	356	363	380	rBV	4469178	6185468	53.69%	10.259%
3	6.581	620	628	642	rBV	4032556	6251734	54.27%	10.369%
4	7.363	755	761	771	rBV	1008649	1553588	13.49%	2.577%
5	8.510	947	956	967	rBV	2610804	4222030	36.65%	7.002%
6	10.122	1223	1230	1241	rBV	1193936	1990330	17.28%	3.301%
7	12.633	1649	1657	1666	rBV	6169094	9086497	78.87%	15.070%
8	14.021	1886	1893	1903	rBV	1716506	2533996	22.00%	4.203%
9	15.533	2143	2150	2165	rBV	4619018	6813980	59.15%	11.301%
10	16.786	2356	2363	2376	rBV	2048820	2806136	24.36%	4.654%
11	17.721	2517	2522	2531	rBV2	192525	365825	3.18%	0.607%
12	19.021	2739	2743	2759	rBV	143747	347832	3.02%	0.577%
13	19.451	2811	2816	2822	rBV	8819133	11520732	100.00%	19.107%
14	21.021	3078	3083	3091	rBV	2215690	2938845	25.51%	4.874%
15	23.715	3534	3541	3555	rVB	1414558	3322361	28.84%	5.510%

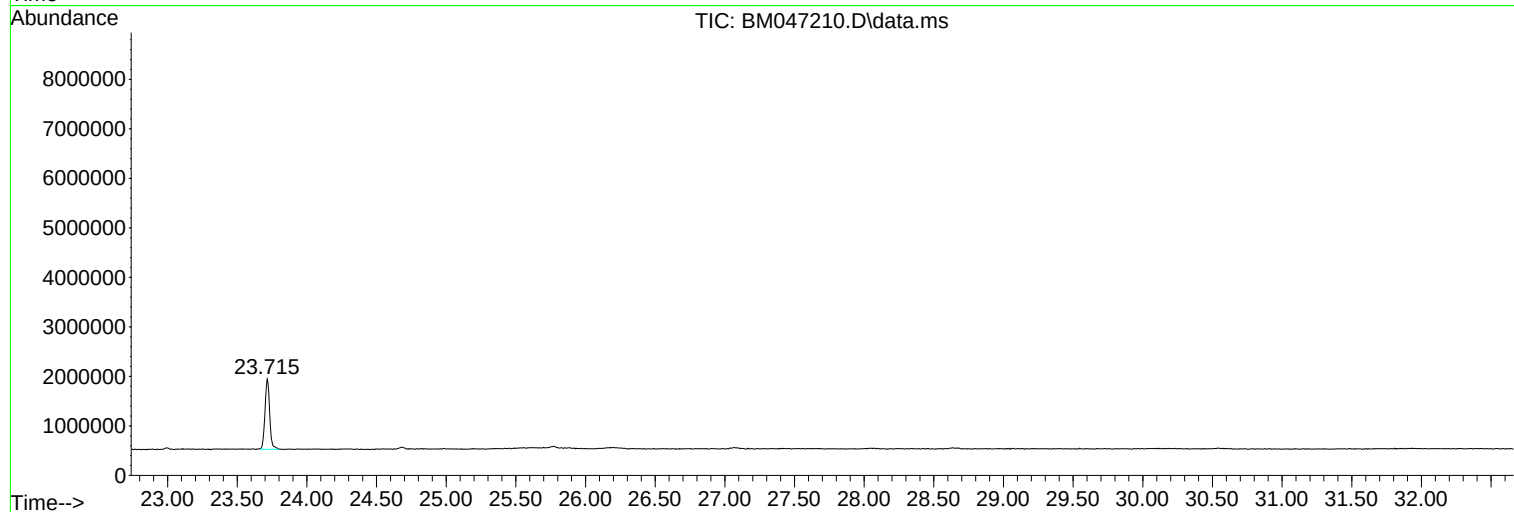
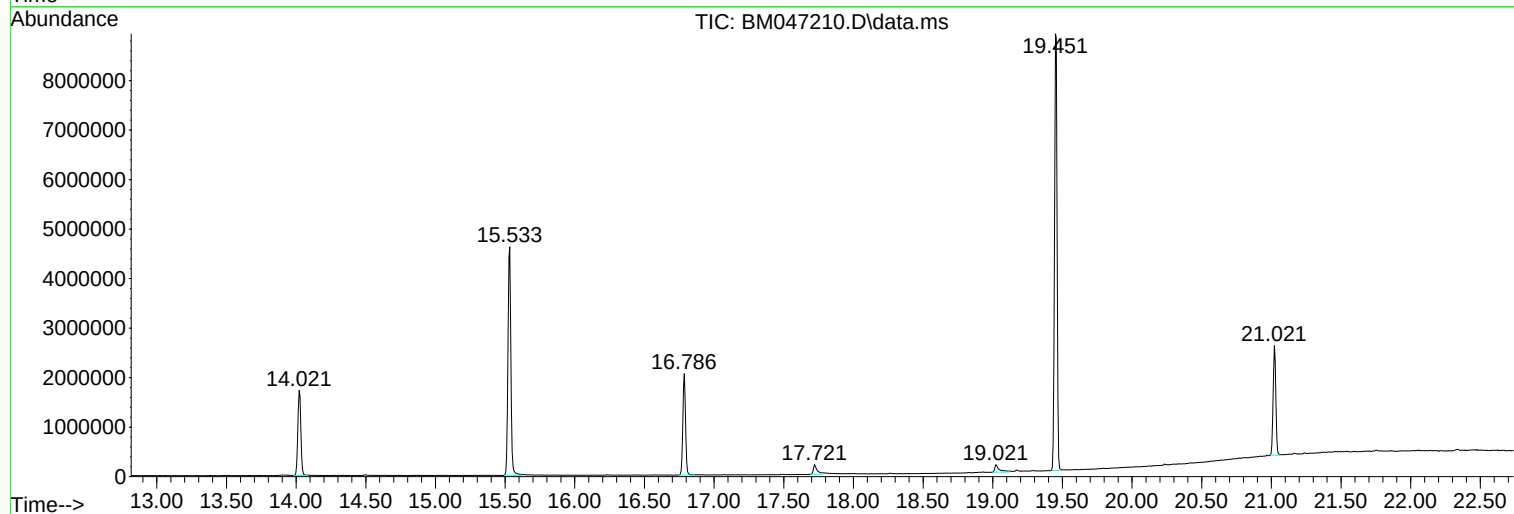
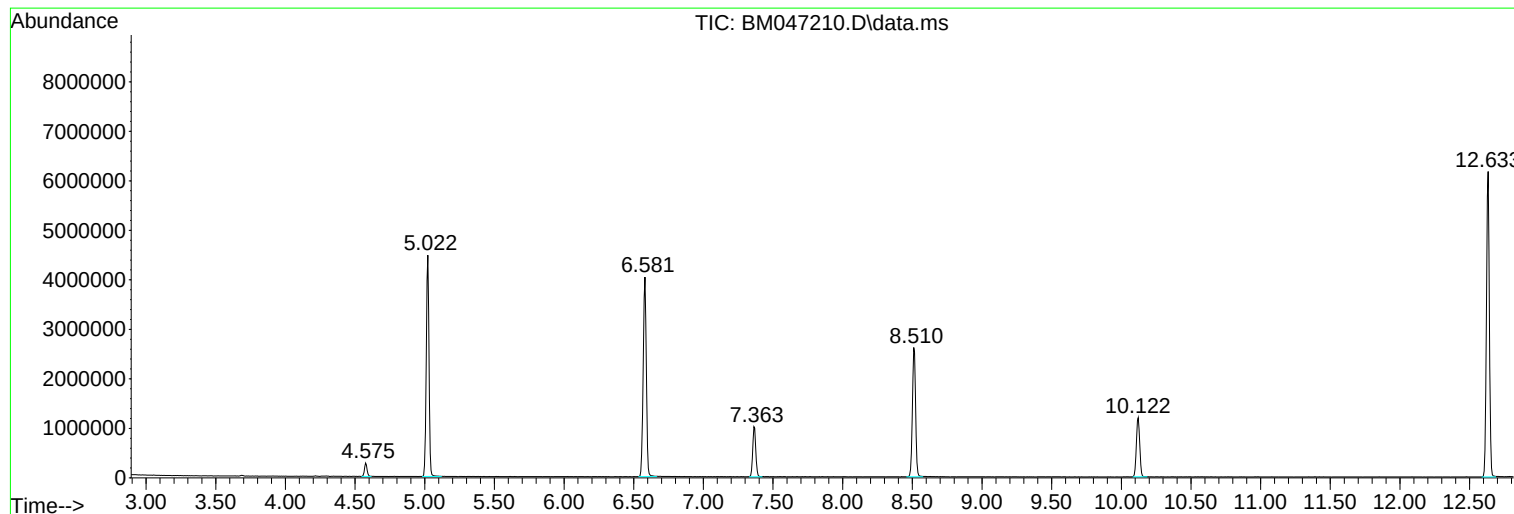
Sum of corrected areas: 60294587

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081524\
Data File : BM047210.D
Acq On : 15 Aug 2024 11:31
Operator : RC/JU
Sample : PB162717BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB162717BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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\BM081524\
Data File : BM047210.D
Acq On : 15 Aug 2024 11:31
Operator : RC/JU
Sample : PB162717BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB162717BL

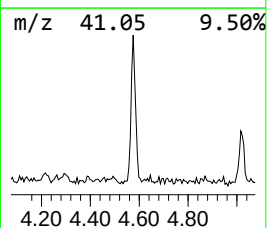
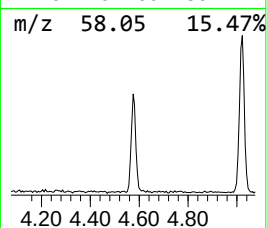
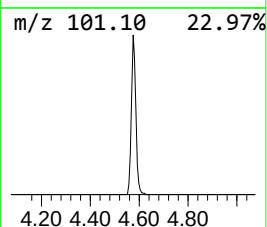
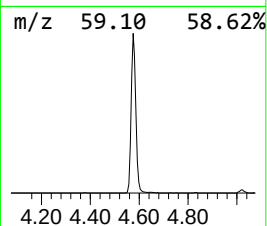
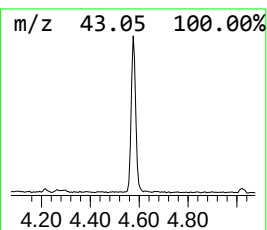
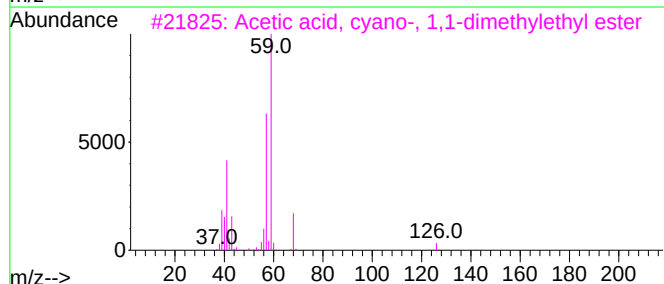
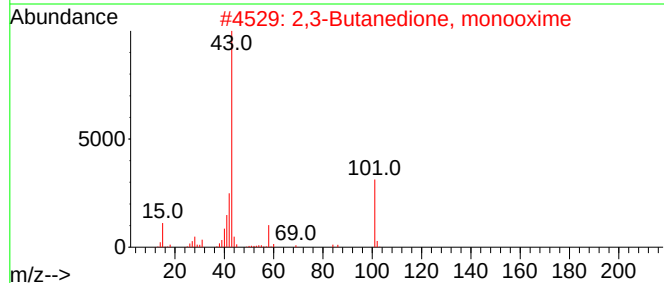
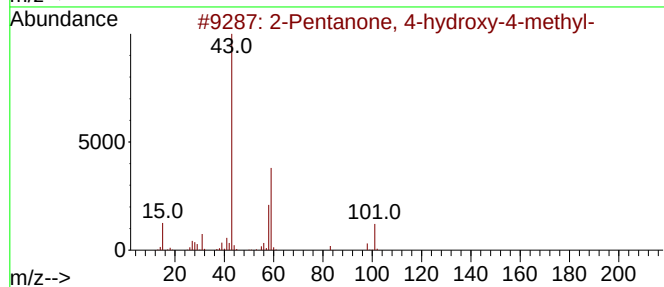
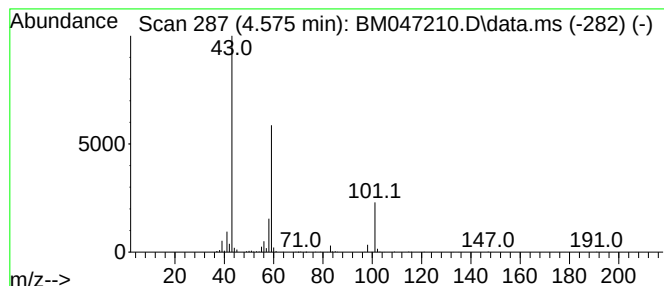
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	4.57 ng	355233	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Hexanamide	115	C6H13NO	000628-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081524\
Data File : BM047210.D
Acq On : 15 Aug 2024 11:31
Operator : RC/JU
Sample : PB162717BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB162717BL

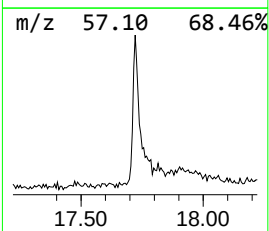
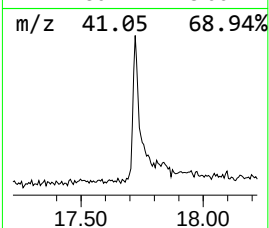
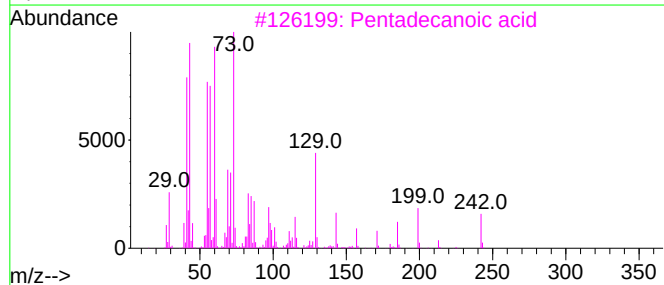
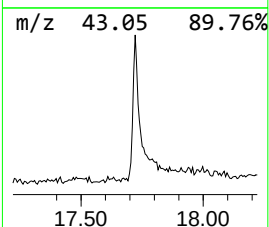
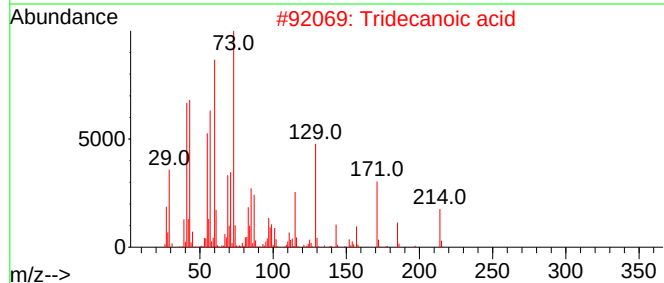
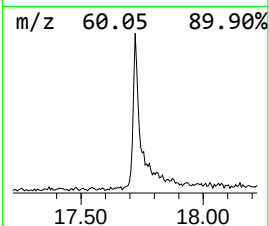
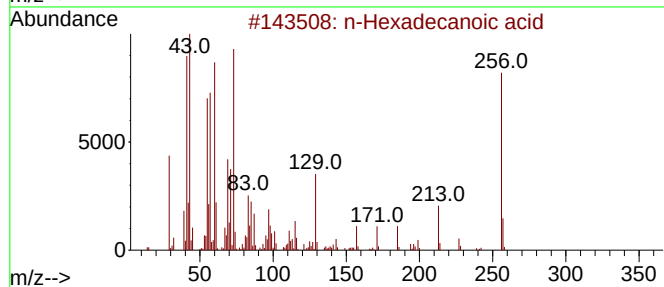
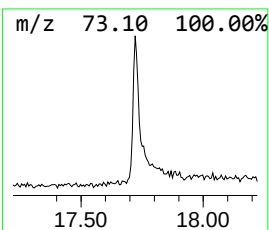
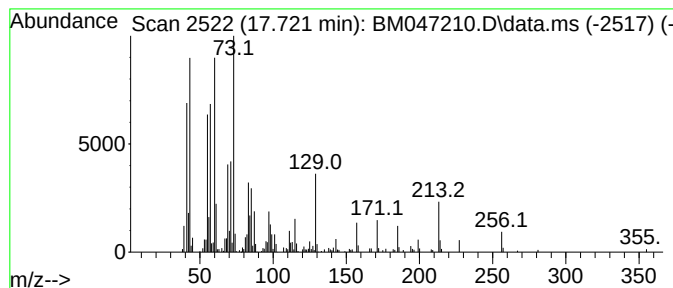
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	2.61 ng	365825	Phenanthrene-d10	16.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081524\
Data File : BM047210.D
Acq On : 15 Aug 2024 11:31
Operator : RC/JU
Sample : PB162717BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB162717BL

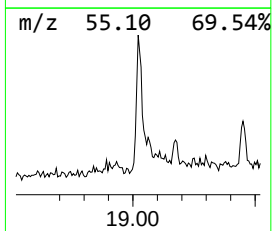
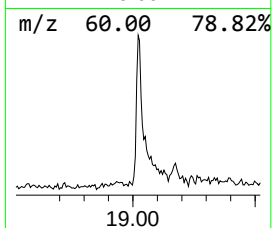
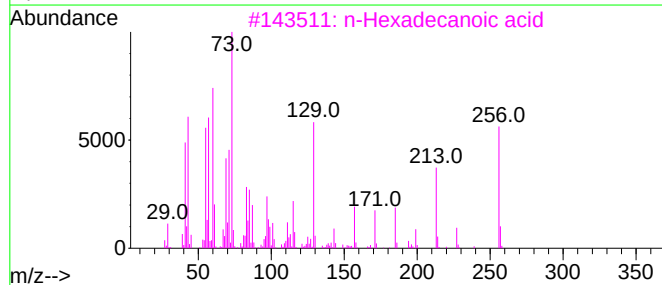
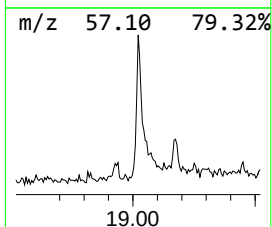
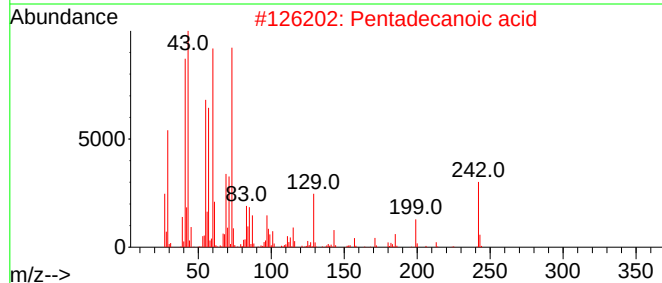
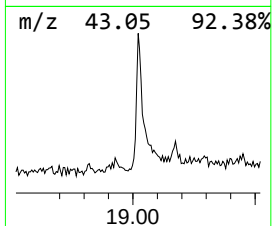
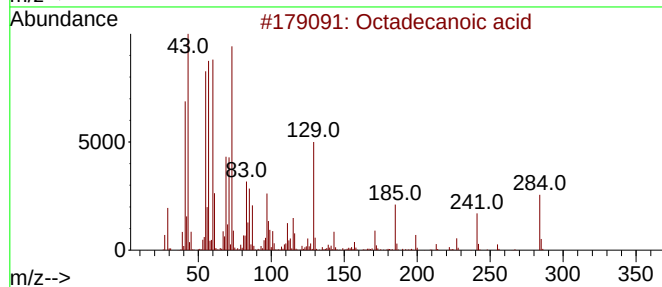
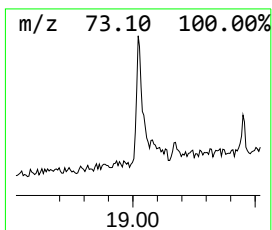
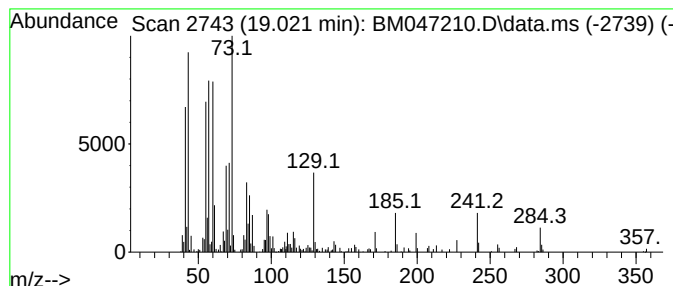
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	2.37 ng	347832	Chrysene-d12	21.021

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	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081524\
Data File : BM047210.D
Acq On : 15 Aug 2024 11:31
Operator : RC/JU
Sample : PB162717BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB162717BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.575	4.6	ng	355233	1	7.363	1553590	20.0
n-Hexadecanoic ...	17.721	2.6	ng	365825	4	16.786	2806140	20.0
Octadecanoic acid	19.021	2.4	ng	347832	5	21.021	2938850	20.0