

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
 Data File : BM039157.D
 Acq On : 27 Mar 2023 12:16
 Operator : CG/JU
 Sample : PB151512BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB151512BL

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.422	189	193	201	rVB	329964	426742	2.81%	0.486%
2	5.040	292	298	309	rVB	3110689	4213080	27.73%	4.798%
3	5.504	371	377	392	rVB	7229527	10384548	68.36%	11.825%
4	7.116	643	651	668	rBV	6641205	10319169	67.93%	11.751%
5	7.945	785	792	802	rVB	1275591	1937735	12.76%	2.207%
6	9.116	983	991	1004	rBV	4010190	6501622	42.80%	7.404%
7	10.757	1262	1270	1283	rBV	1536907	2600363	17.12%	2.961%
8	13.216	1680	1688	1708	rBV	9329501	13214064	86.99%	15.047%
9	14.586	1914	1921	1933	rBV	2131717	3082477	20.29%	3.510%
10	16.074	2168	2174	2196	rBV	6265090	9005442	59.28%	10.255%
11	17.333	2381	2388	2401	rBV	2414083	3307806	21.78%	3.767%
12	18.227	2535	2540	2550	rBV	184474	367664	2.42%	0.419%
13	19.503	2753	2757	2766	rBV2	137355	280687	1.85%	0.320%
14	19.651	2778	2782	2786	rVB	158459	179557	1.18%	0.204%
15	19.956	2828	2834	2843	rBV	12616468	15190655	100.00%	17.298%
16	20.692	2956	2959	2964	rBV	230903	250960	1.65%	0.286%
17	21.515	3094	3099	3104	rBV	2441561	3201223	21.07%	3.645%
18	23.938	3505	3511	3521	rVB2	1689271	3354204	22.08%	3.819%

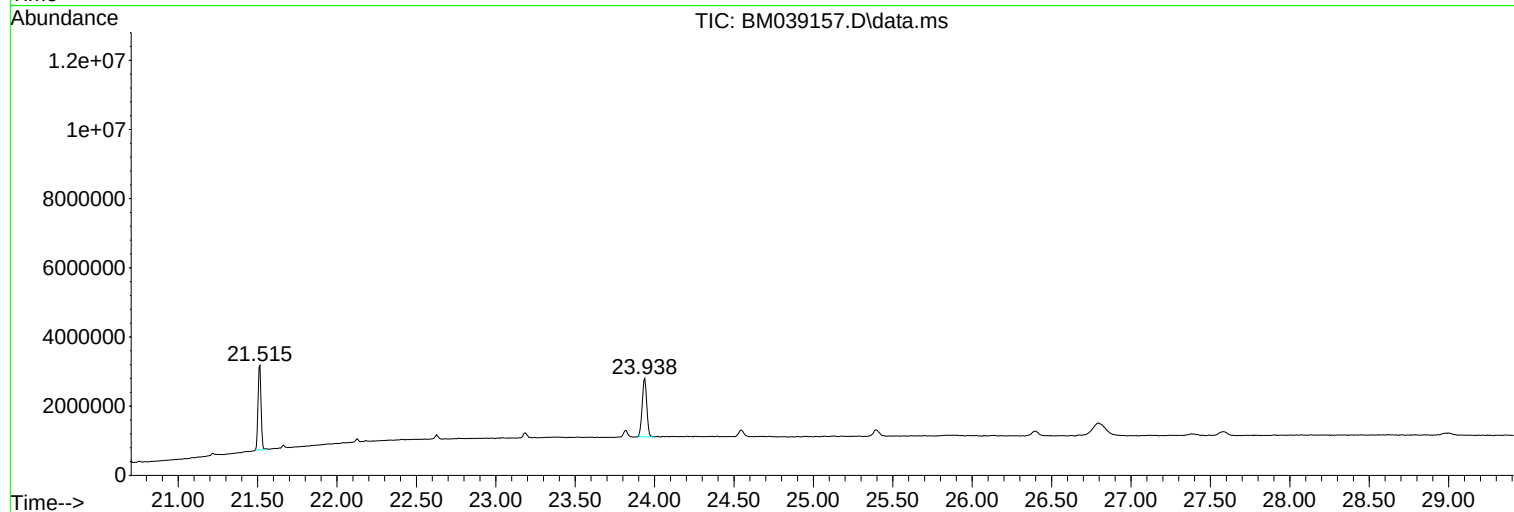
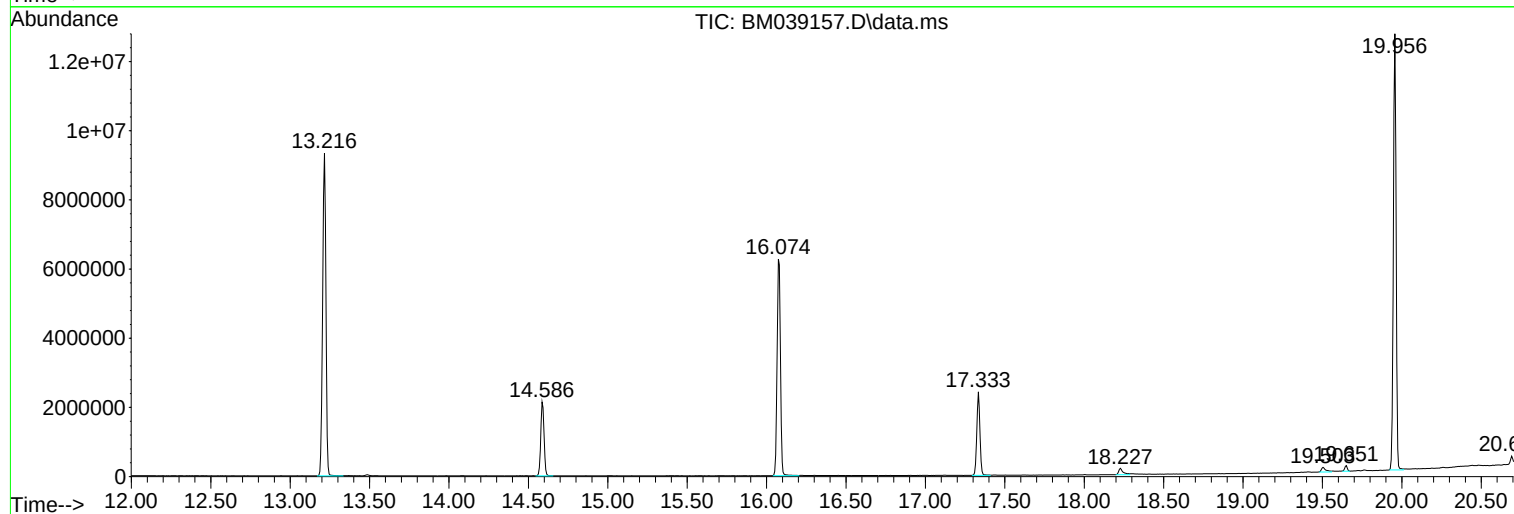
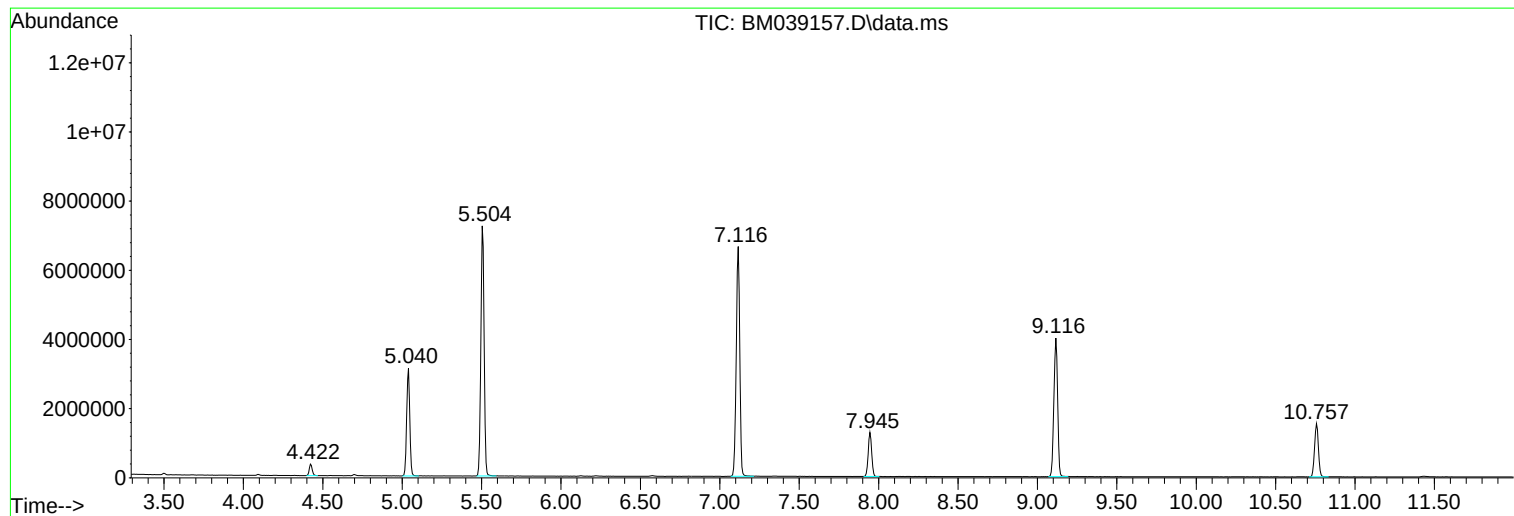
Sum of corrected areas: 87817998

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039157.D
Acq On : 27 Mar 2023 12:16
Operator : CG/JU
Sample : PB151512BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB151512BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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\BM032723\
Data File : BM039157.D
Acq On : 27 Mar 2023 12:16
Operator : CG/JU
Sample : PB151512BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB151512BL

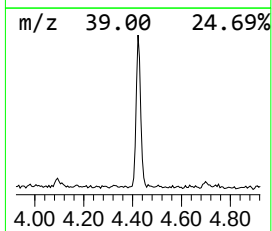
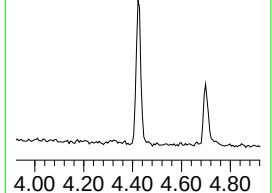
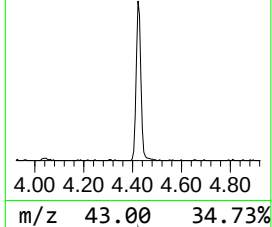
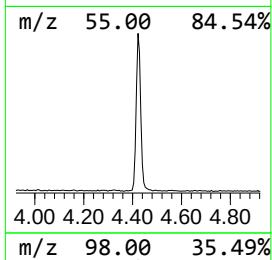
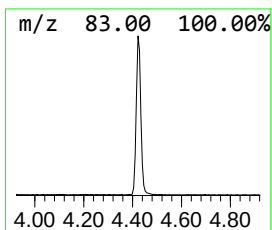
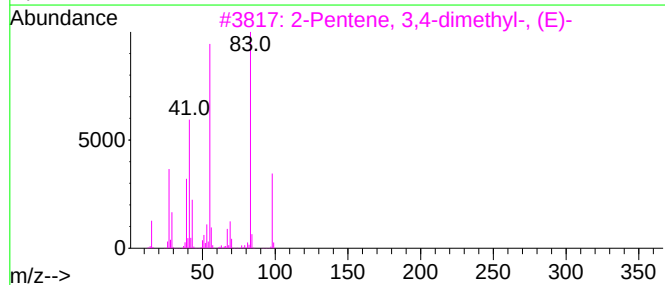
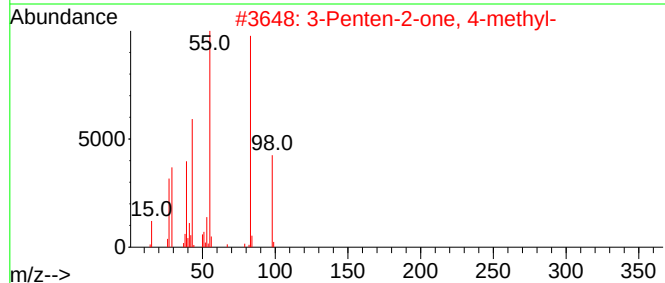
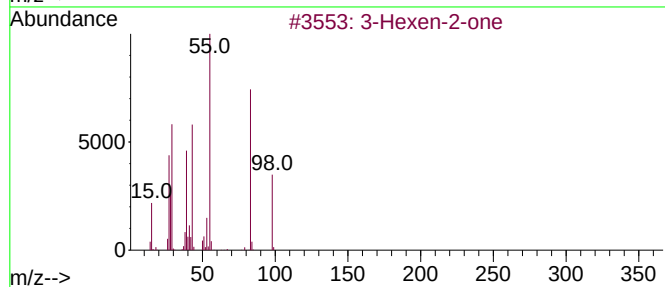
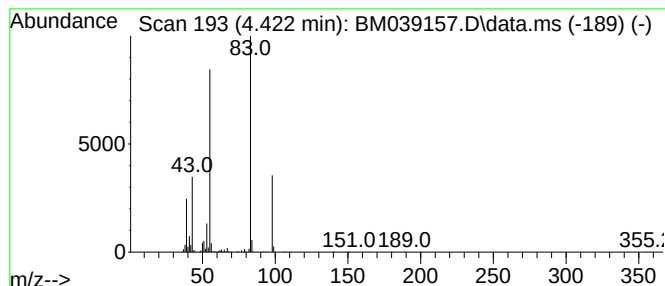
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.422	4.40 ng	426742	1,4-Dichlorobenzene-d4	7.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039157.D
Acq On : 27 Mar 2023 12:16
Operator : CG/JU
Sample : PB151512BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB151512BL

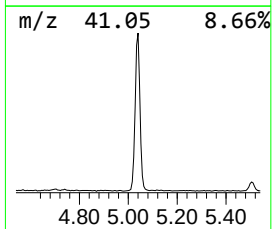
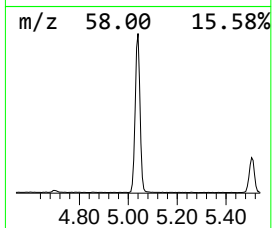
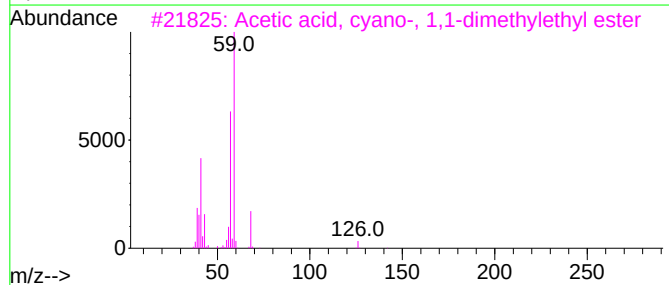
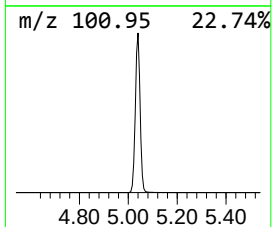
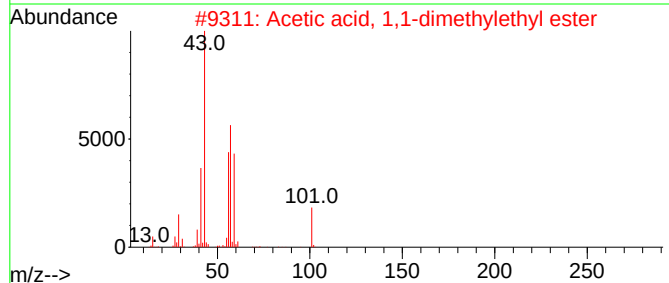
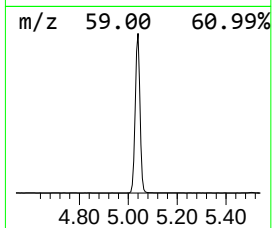
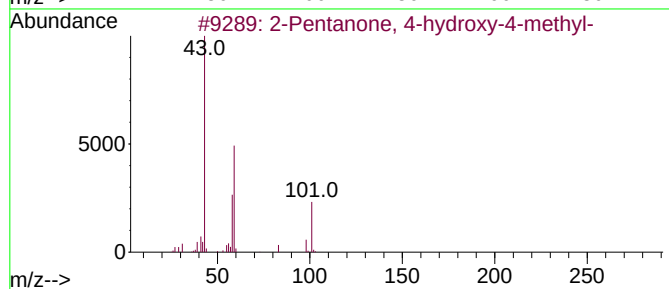
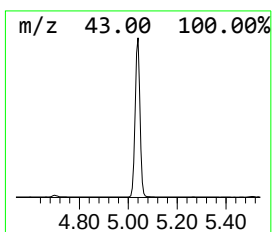
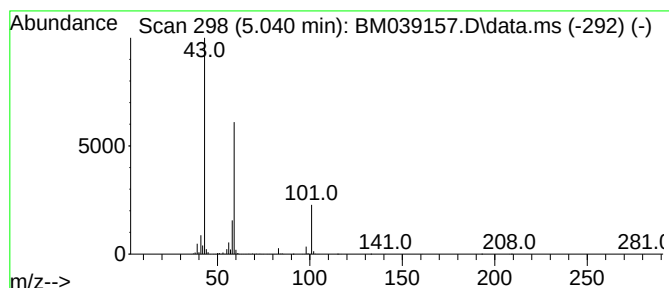
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	43.48 ng	4213080	1,4-Dichlorobenzene-d4	7.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039157.D
Acq On : 27 Mar 2023 12:16
Operator : CG/JU
Sample : PB151512BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

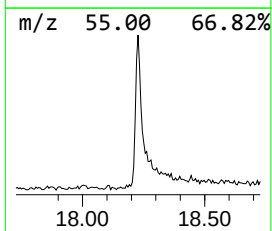
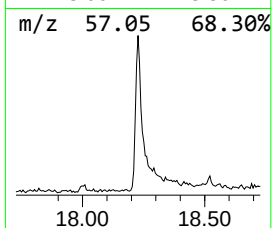
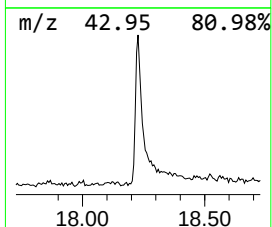
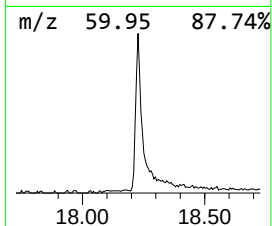
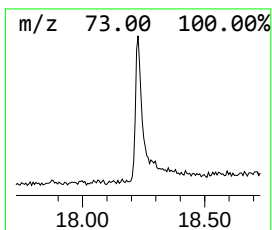
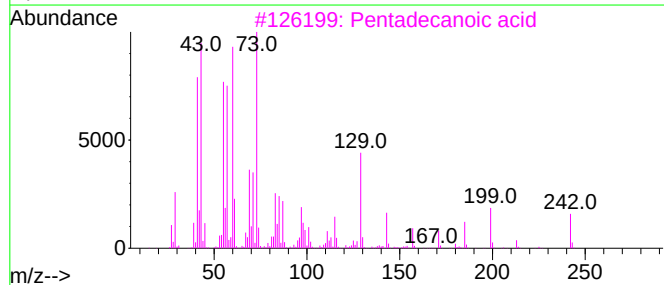
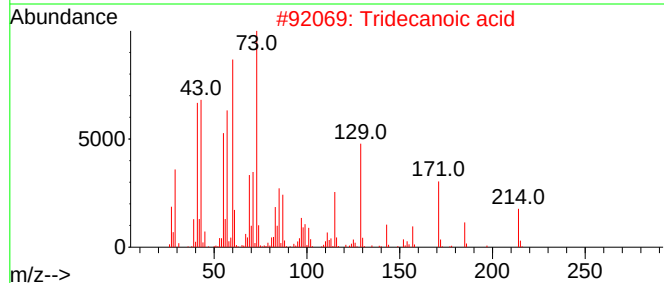
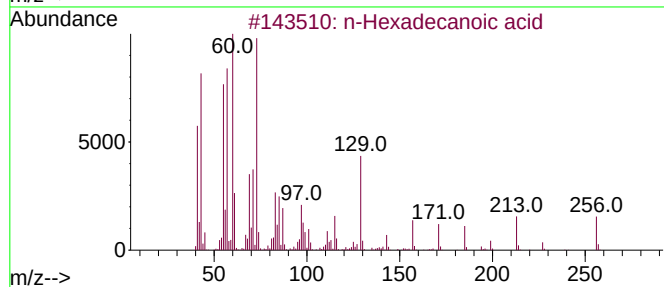
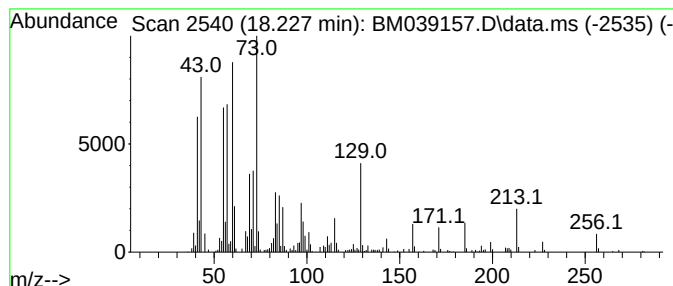
Instrument :
BNA_M
ClientSampleId :
PB151512BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.227	2.22 ng	367664	Phenanthrene-d10		17.333	
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	92
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039157.D
Acq On : 27 Mar 2023 12:16
Operator : CG/JU
Sample : PB151512BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB151512BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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
3-Hexen-2-one	4.422	4.4	ng	426742	1	7.945	1937740	20.0
2-Pentanone, 4-...	5.040	43.5	ng	4213080	1	7.945	1937740	20.0
n-Hexadecanoic ...	18.227	2.2	ng	367664	4	17.333	3307810	20.0