

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
 Data File : BG055985.D
 Acq On : 15 Dec 2022 20:33
 Operator : CG/JU
 Sample : N6055-01 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OK-2-121422

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_G\Methods\8270-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055985.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.413	16	21	27	rBV	7212	12152	4.07%	0.744%
2	5.422	358	363	370	rBB	6116	8787	2.95%	0.538%
3	5.892	438	443	451	rBB	49406	81486	27.32%	4.992%
4	7.502	711	717	724	rBB	54180	93136	31.23%	5.706%
5	8.377	860	866	873	rBB	34440	57770	19.37%	3.539%
6	9.547	1059	1065	1072	rBB2	33753	58543	19.63%	3.586%
7	11.215	1342	1349	1355	rBB	44938	79304	26.59%	4.858%
8	13.612	1751	1757	1764	rBB	115069	171178	57.40%	10.487%
9	14.987	1984	1991	1997	rBB	76190	122672	41.13%	7.515%
10	16.462	2236	2242	2248	rBV	120878	183997	61.70%	11.272%
11	17.719	2450	2456	2461	rBV	102643	159809	53.59%	9.790%
12	17.766	2461	2464	2468	rVB	7453	9674	3.24%	0.593%
13	18.565	2594	2600	2608	rBV5	14195	28749	9.64%	1.761%
14	18.636	2610	2612	2615	rVB3	2999	3655	1.23%	0.224%
15	19.077	2684	2687	2691	rBV5	4276	4129	1.38%	0.253%
16	19.253	2715	2717	2720	rVV4	2509	3140	1.05%	0.192%
17	19.488	2754	2757	2761	rBV5	5446	8952	3.00%	0.548%
18	19.611	2776	2778	2780	rBV3	3737	4029	1.35%	0.247%
19	19.670	2786	2788	2791	rBV4	4560	5290	1.77%	0.324%
20	19.752	2797	2802	2806	rBV	19279	30756	10.31%	1.884%
21	19.817	2809	2813	2816	rBV5	8160	14142	4.74%	0.866%
22	20.105	2860	2862	2868	rVB	17296	26157	8.77%	1.602%
23	20.293	2888	2894	2900	rBV	217748	298219	100.00%	18.269%
24	22.032	3185	3190	3197	rVB2	96581	166617	55.87%	10.207%

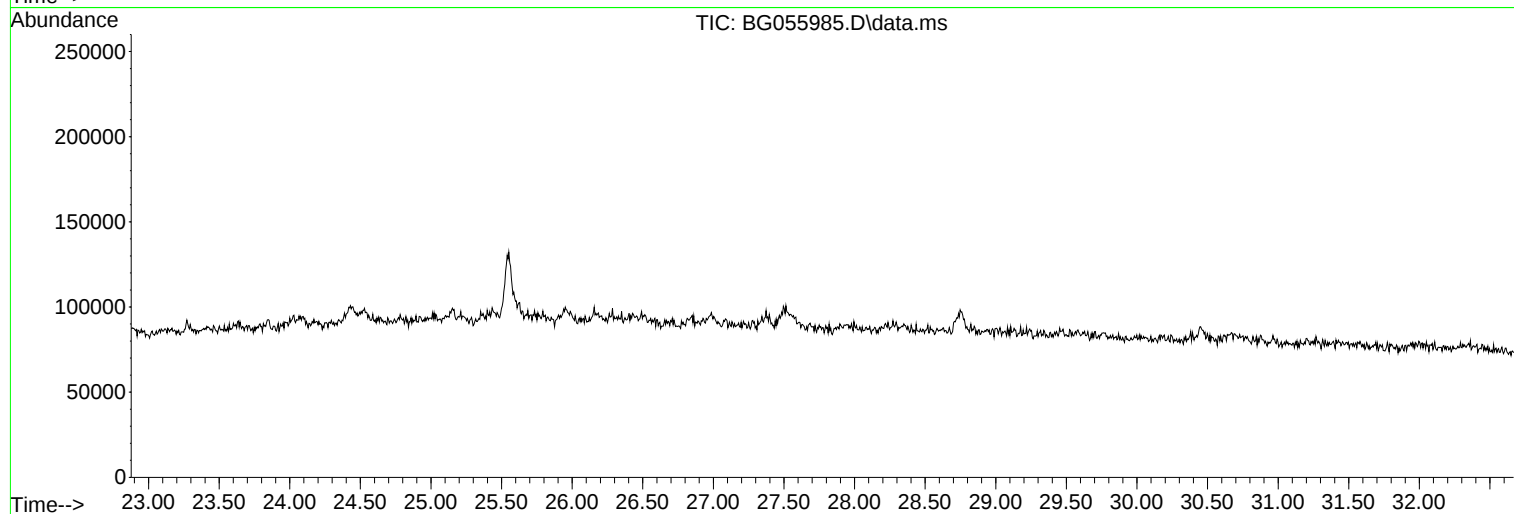
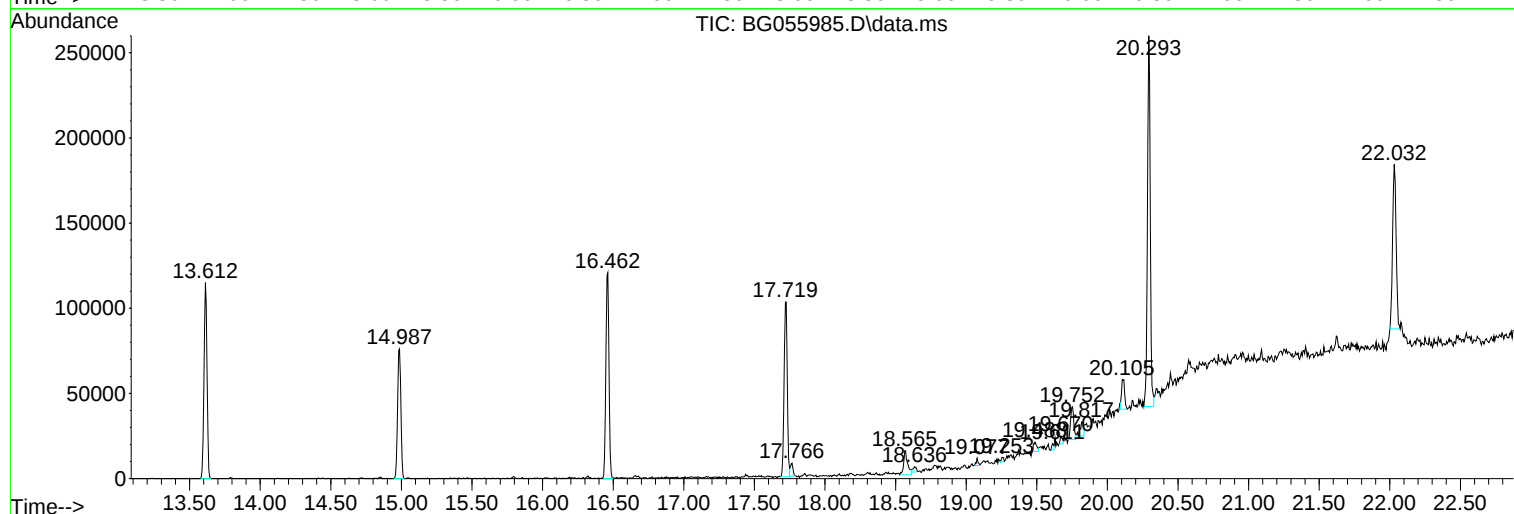
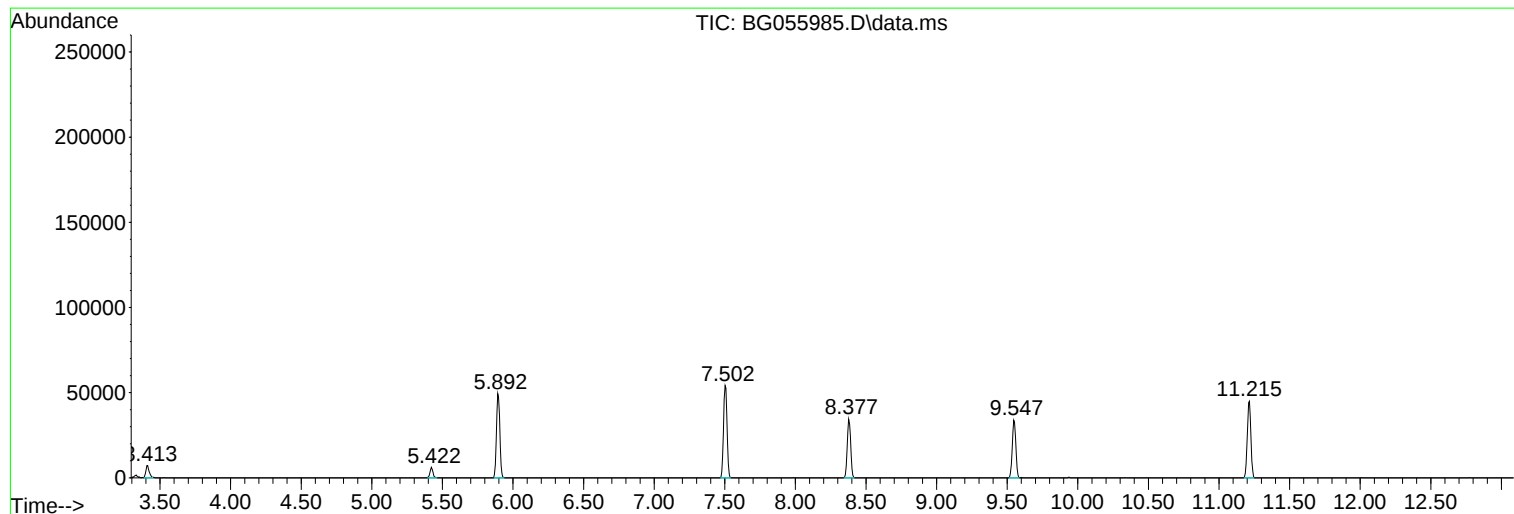
Sum of corrected areas: 1632343

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055985.D
Acq On : 15 Dec 2022 20:33
Operator : CG/JU
Sample : N6055-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-2-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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_G\Data\BG121522\
Data File : BG055985.D
Acq On : 15 Dec 2022 20:33
Operator : CG/JU
Sample : N6055-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-2-121422

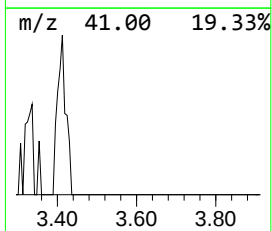
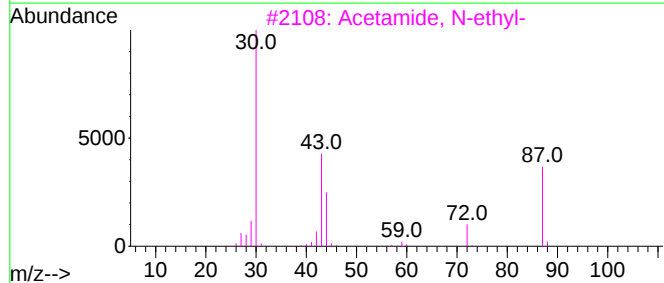
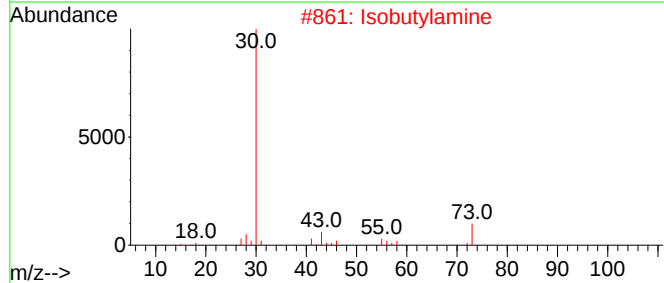
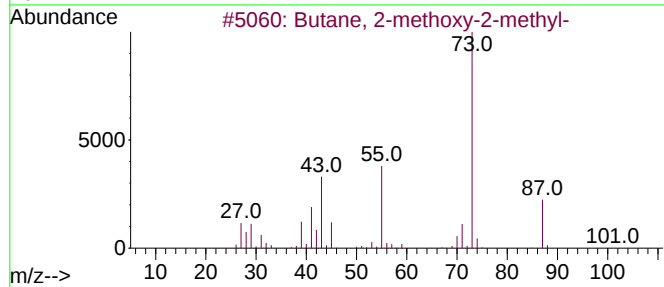
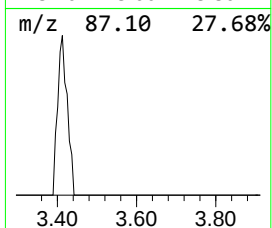
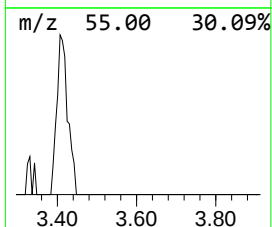
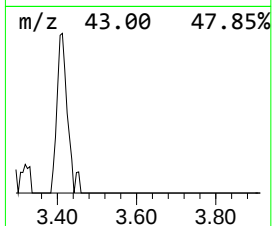
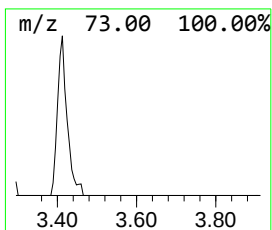
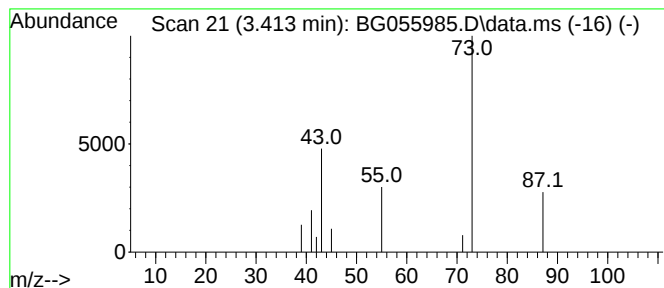
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.413 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.413	4.21 ng	12152	1,4-Dichlorobenzene-d4	8.377

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
4			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055985.D
Acq On : 15 Dec 2022 20:33
Operator : CG/JU
Sample : N6055-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-2-121422

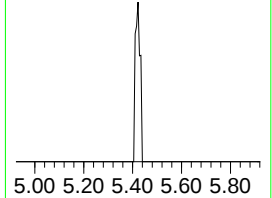
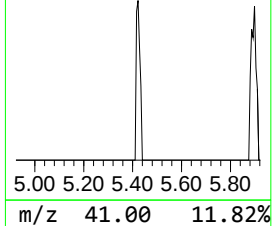
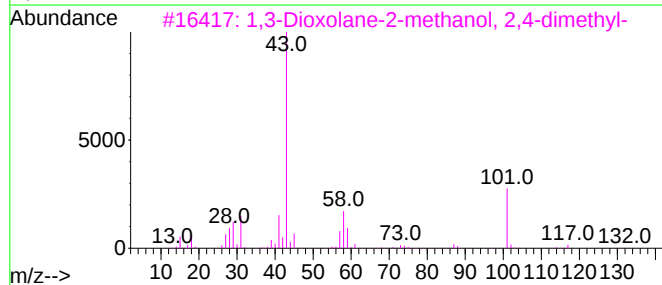
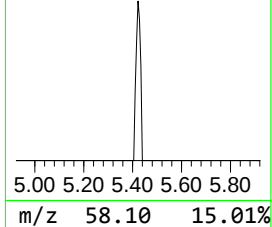
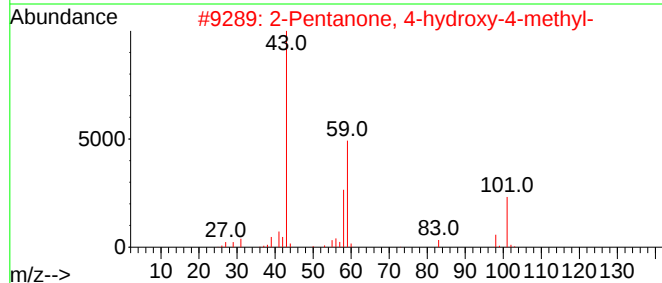
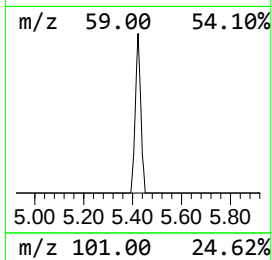
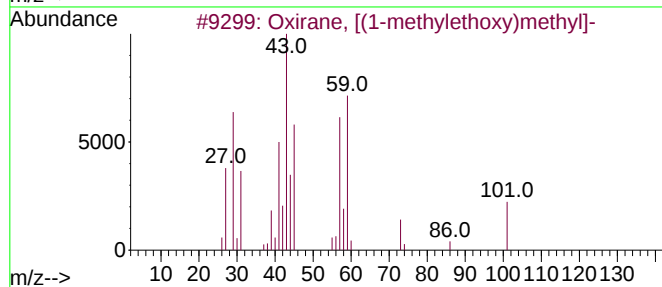
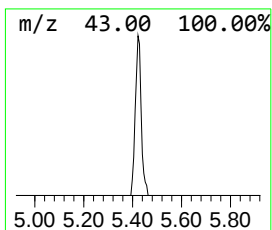
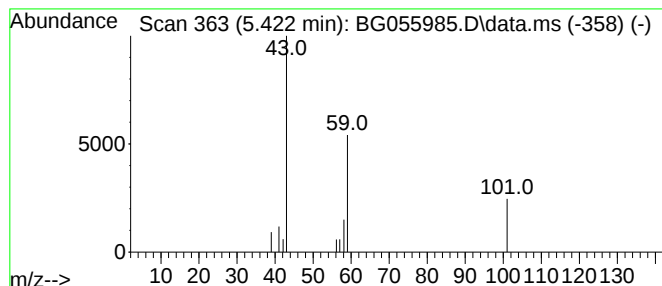
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.422	3.04 ng	8787	1,4-Dichlorobenzene-d4	8.377

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	64
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9
4			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	5
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055985.D
Acq On : 15 Dec 2022 20:33
Operator : CG/JU
Sample : N6055-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-2-121422

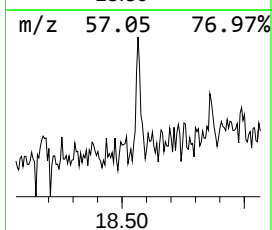
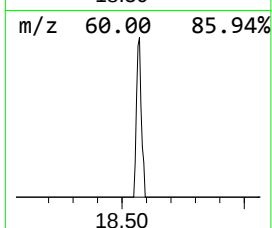
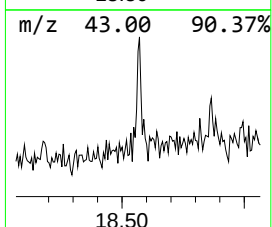
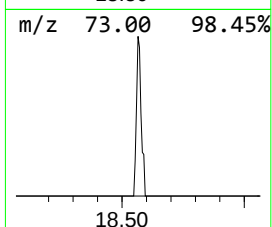
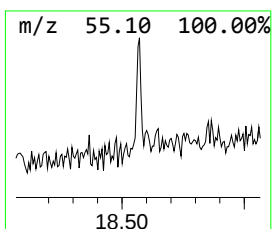
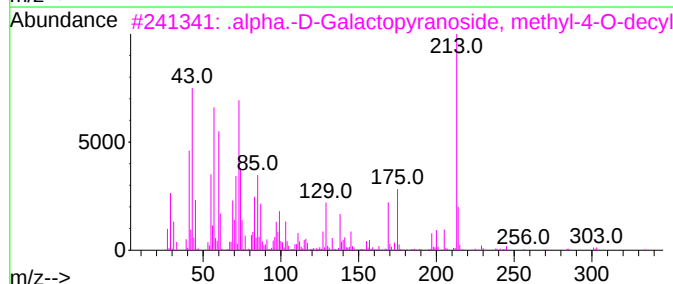
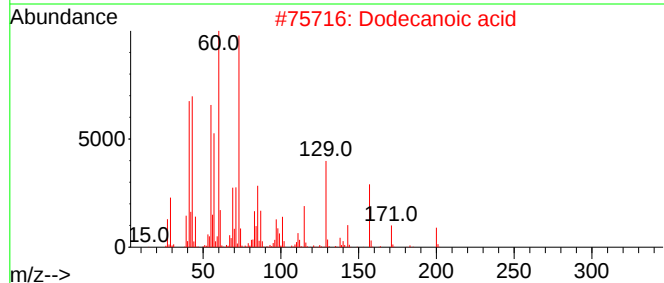
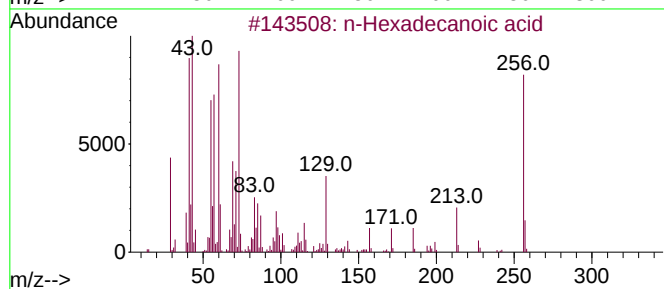
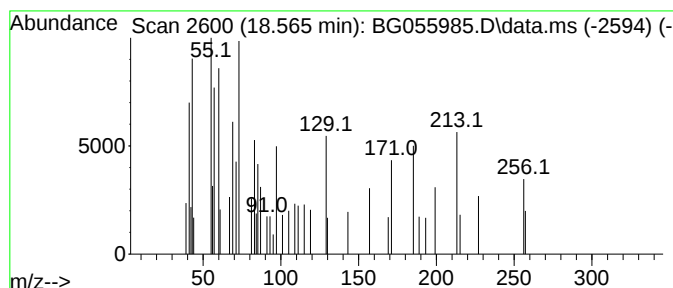
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.566	3.60 ng	28749	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
2			Dodecanoic acid	200	C12H24O2	000143-07-7	35
3			.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	35
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5			Tridecanoic acid	214	C13H26O2	000638-53-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055985.D
Acq On : 15 Dec 2022 20:33
Operator : CG/JU
Sample : N6055-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-2-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
unknown3.413	3.413	4.2	ng	12152	1	8.377	57770	20.0
Oxirane, [(1-me...	5.422	3.0	ng	8787	1	8.377	57770	20.0
n-Hexadecanoic ...	18.566	3.6	ng	28749	4	17.725	159809	20.0