LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061022\
Data File : BG053875.D
Acq On : 10 Jun 2022 15:00
Operator : CG/JU
Sample : N3287-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-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_G\Methods\8270-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.182	297	305	314	rBV2	11542	22034	1.20%	0.253%
2	5.652	378	385	395	rVB	304157	516793	28.19%	5.923%
3	7.244	647	656	665	rBV	300761	542968	29.61%	6.223%
4	8.091	793	800	806	rVB	58825	101775	5.55%	1.166%
5	9.248	989	997	1006	rBV	186369	344770	18.80%	3.952%
6	10.899	1270	1278	1286	rVB	79035	143816	7.84%	1.648%
7	13.337	1686	1693	1700	rBV	588556	905739	49.40%	10.381%
8	13.925	1790	1793	1798	rVB3	13657	19918	1.09%	0.228%
9	14.712	1919	1927	1934	rBV	126092	207422	11.31%	2.377%
10	16.193	2172	2179	2191	rBV	509981	852763	46.51%	9.774%
11	16.504	2212	2232	2247	rBV8	91643	694649	37.89%	7.962%
12	17.456	2387	2394	2402	rVB	181811	297707	16.24%	3.412%
13	18.314	2534	2540	2541	rBV6	15526	28815	1.57%	0.330%
14	18.343	2541	2545	2559	rVB6	40147	113473	6.19%	1.301%
15	19.606	2750	2760	2781	rVB3	131505	533629	29.10%	6.116%
16	20.065	2831	2838	2843	rBV	1263103	1833536	100.00%	21.015%
17	21.369	3055	3060	3067	rBV	89303	141337	7.71%	1.620%
18	21.727	3115	3121	3128	rBV	253432	464718	25.35%	5.326%
19	21.968	3153	3162	3171	rVB2	45160	119345	6.51%	1.368%
20	22.932	3319	3326	3333	rVB	139044	265412	14.48%	3.042%
21	23.455	3411	3415	3422	rVB2	22993	42402	2.31%	0.486%
22	23.596	3434	3439	3450	rVB3	25140	62391	3.40%	0.715%
23	25.000	3669	3678	3687	rBV2	136683	376559	20.54%	4.316%
24	29.013	4351	4361	4364	rBV8	32382	92998	5.07%	1.066%

Sum of corrected areas: 8724969

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061022\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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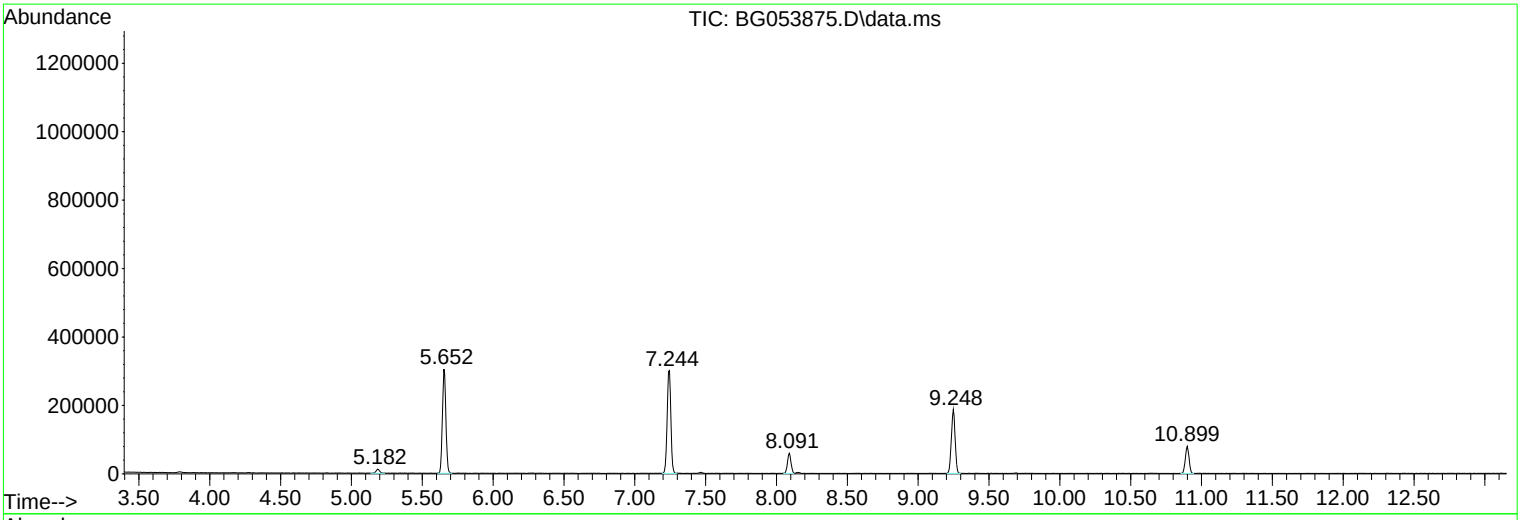
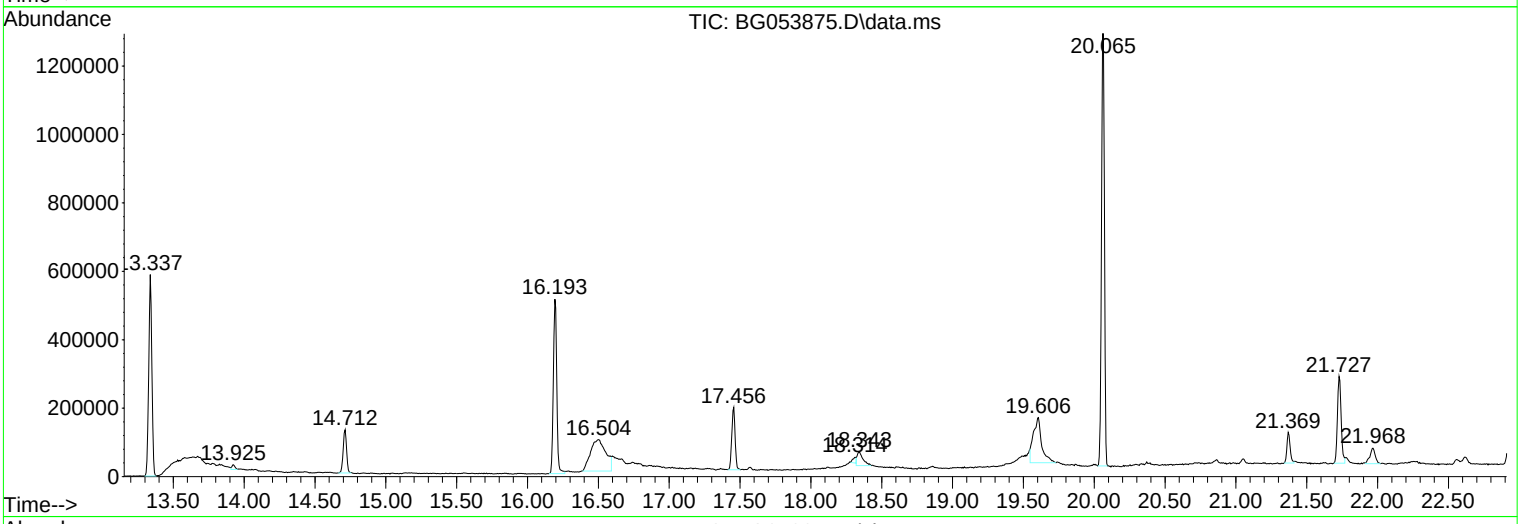
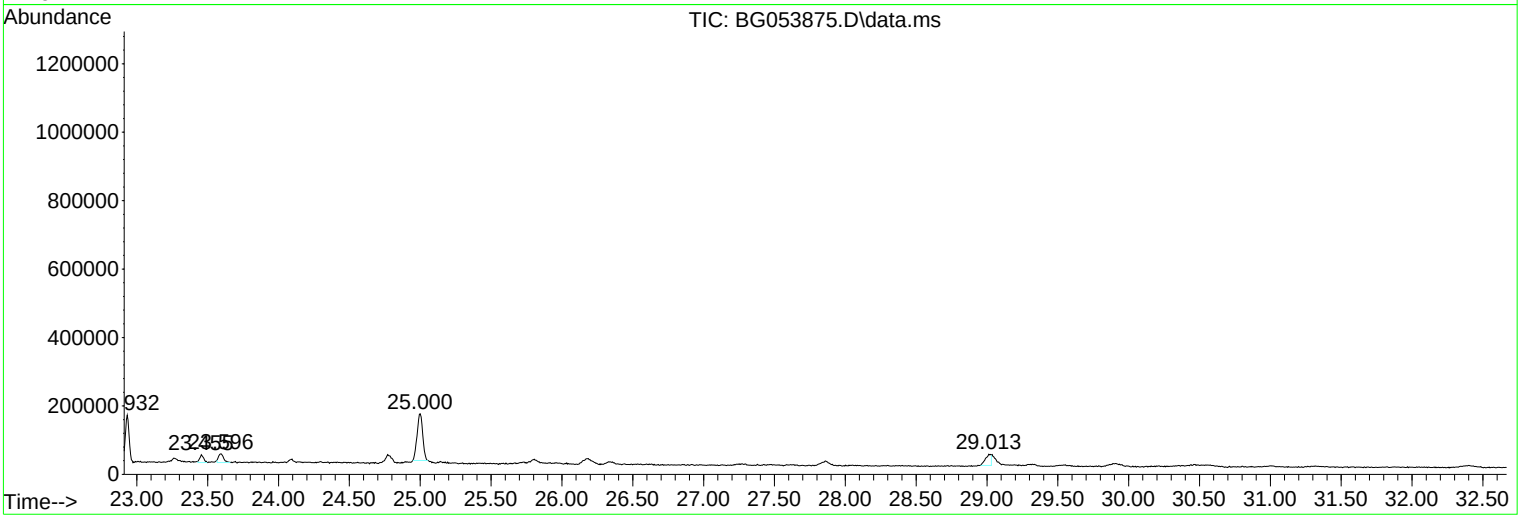
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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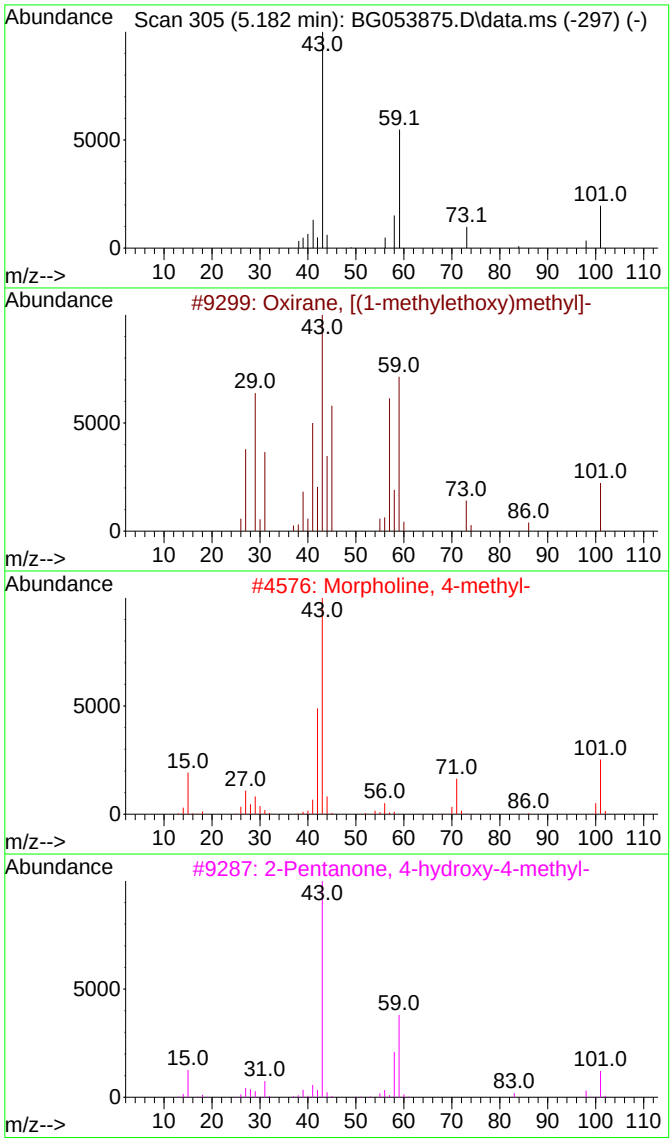
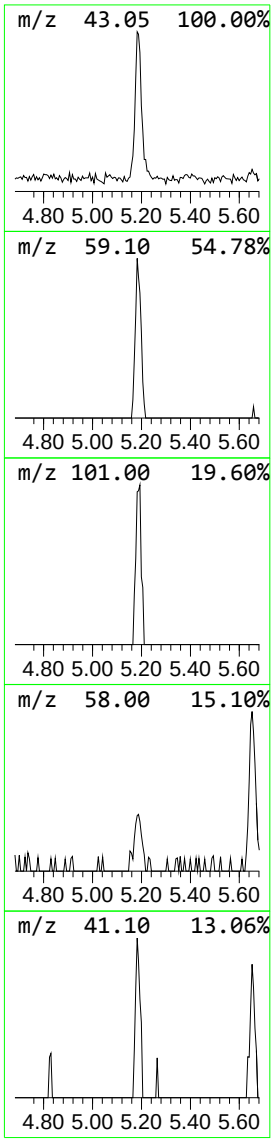
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Oxirane, [(1-methylethoxy)m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.182	4.33 ng	22034	1,4-Dichlorobenzene-d4	8.091

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	5
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	5





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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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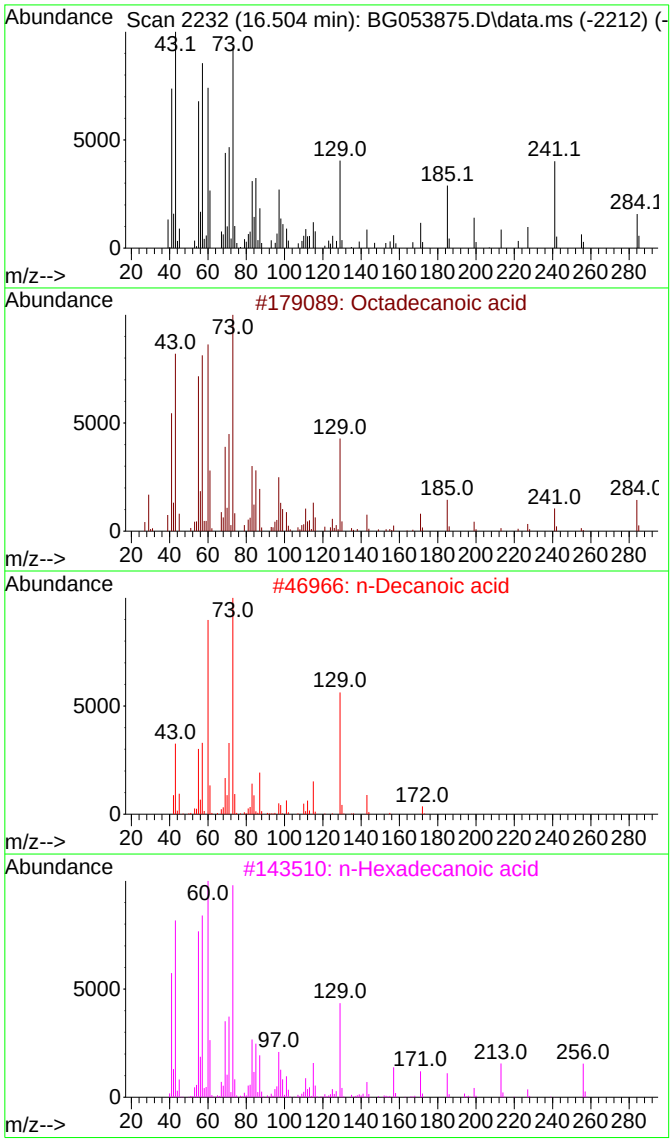
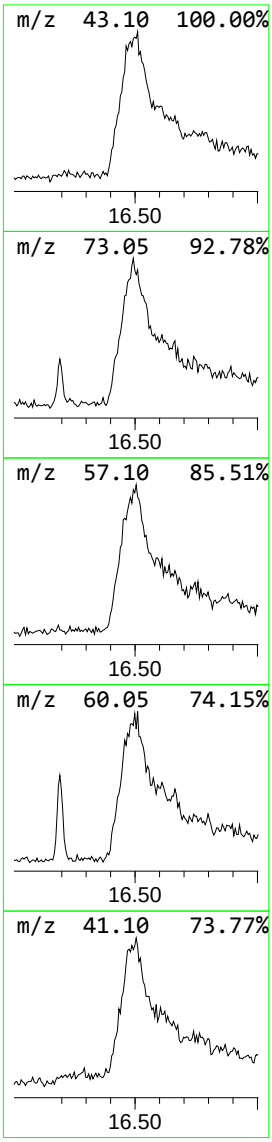
****

Peak Number 2 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.504	46.67 ng	694649	Phenanthrene-d10	17.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Acq On : 10 Jun 2022 15:00
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
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TIC Library : C:\Database\NIST20.L
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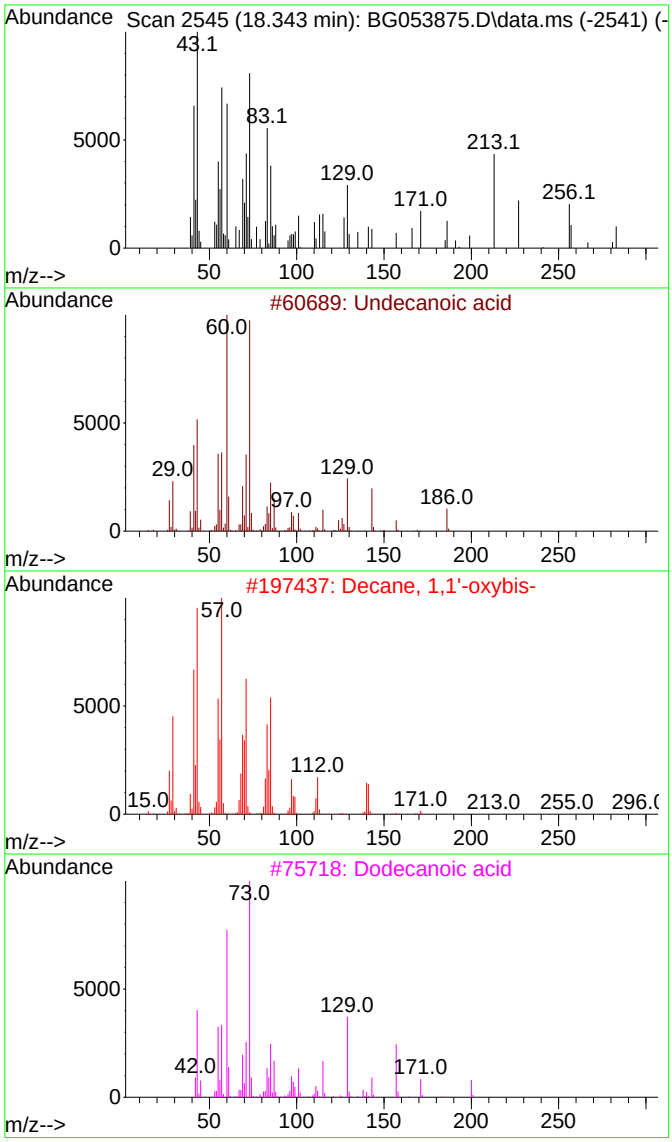
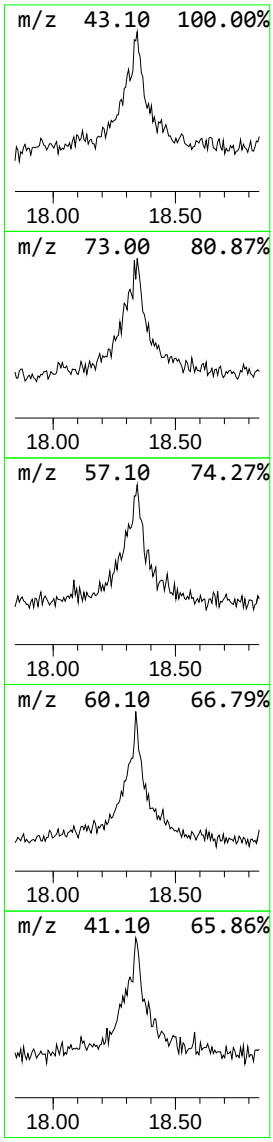
****

Peak Number 3 unknown18.343 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.343	7.62 ng	113473	Phenanthrene-d10	17.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	22
2	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	22
3	Dodecanoic acid	200	C12H24O2	000143-07-7	22
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	22
5	3-Pentadecanone	226	C15H30O	018787-66-1	22





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Operator : CG/JU
Sample : N3287-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

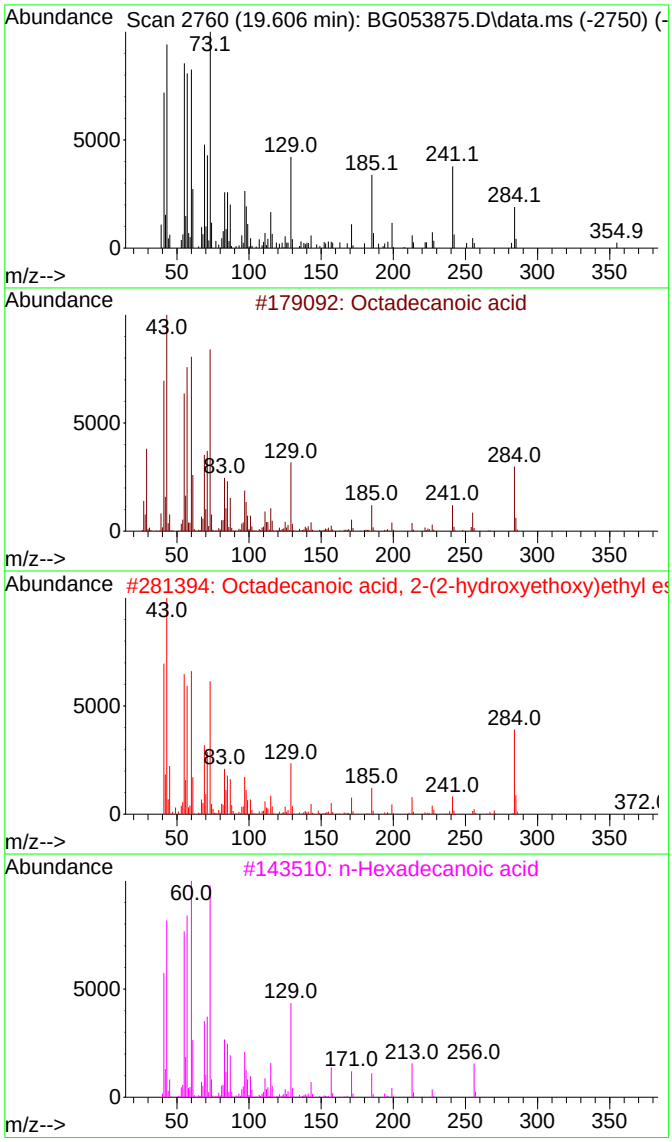
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

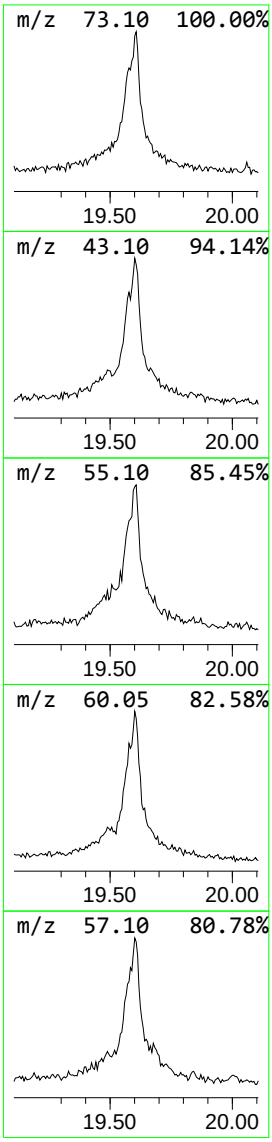
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid, 2-(2-hyd... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.606	22.97 ng	533629	Chrysene-d12	21.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Sample : N3287-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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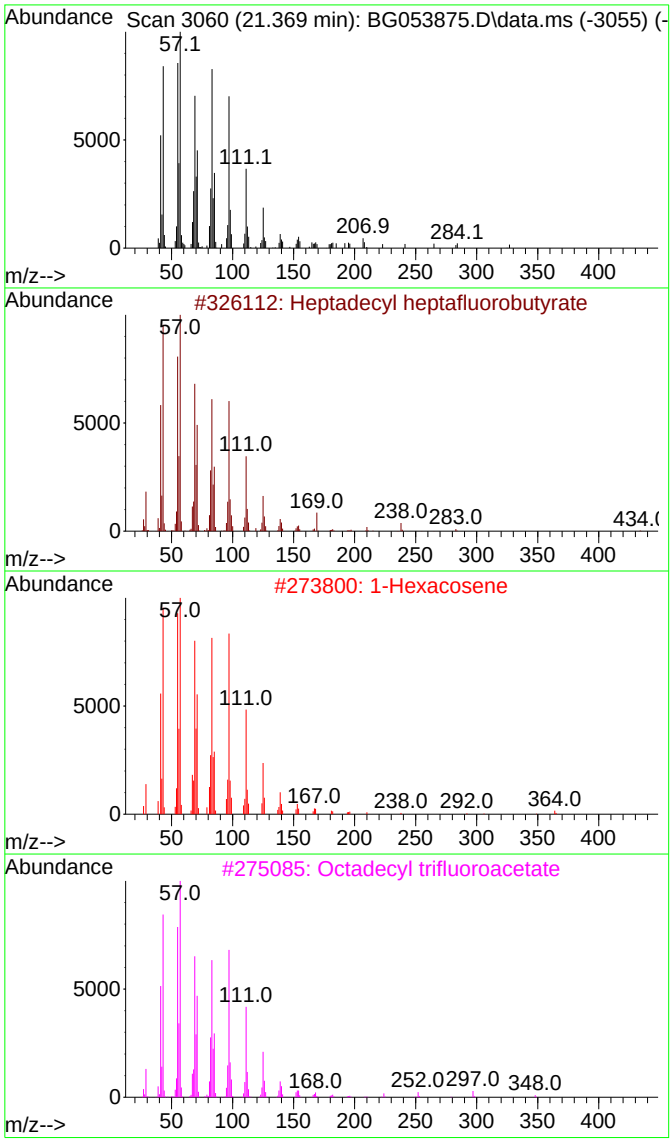
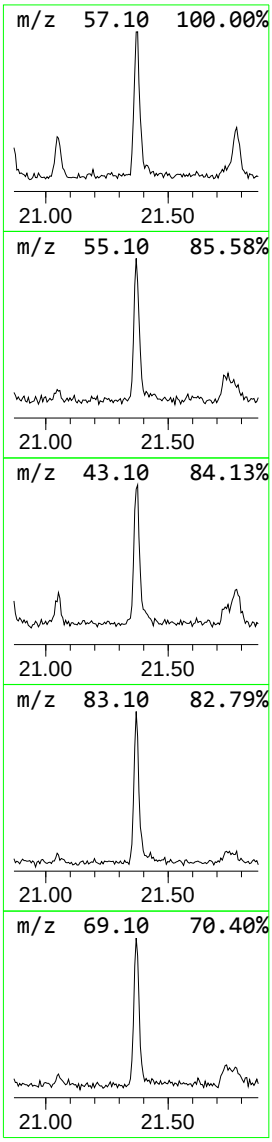
****
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	6.08 ng	141337	Chrysene-d12	21.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





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TIC Library : C:\Database\NIST20.L
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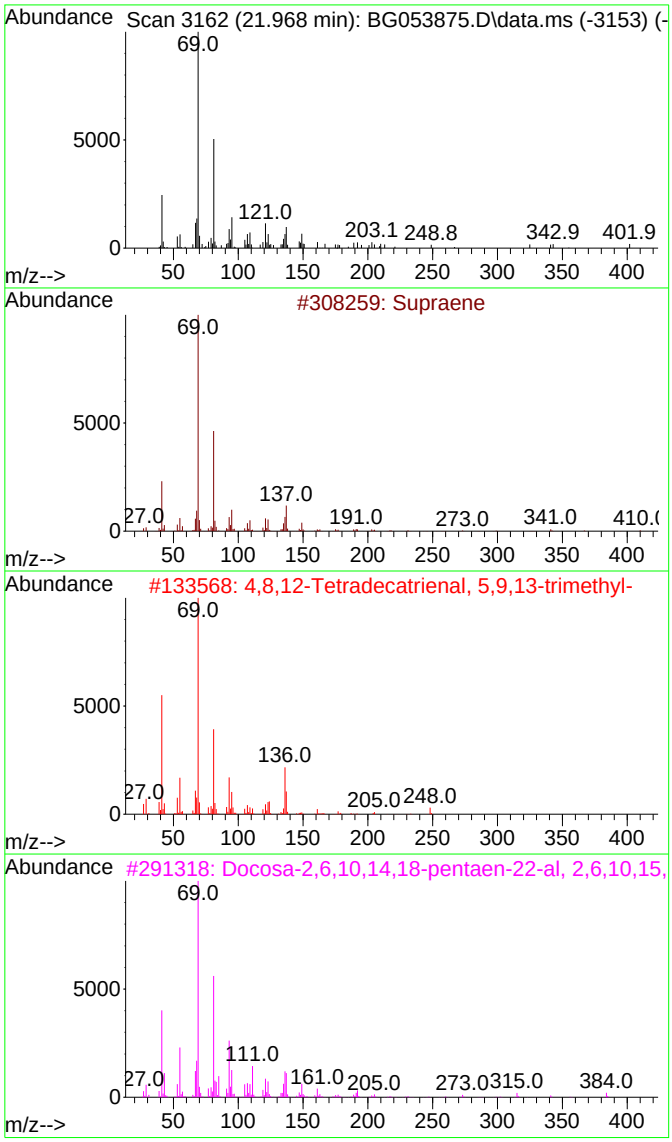
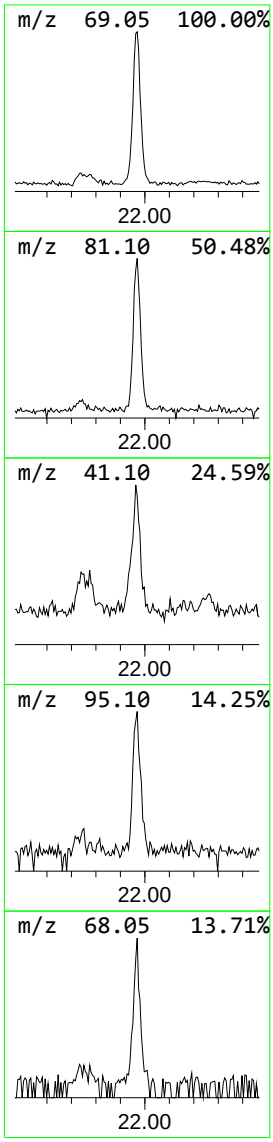
****

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.968	5.14 ng	119345	Chrysene-d12	21.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
5	trans-Farnesol	222	C15H26O	000106-28-5	64





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Instrument :
BNA_G
ClientSampleId :
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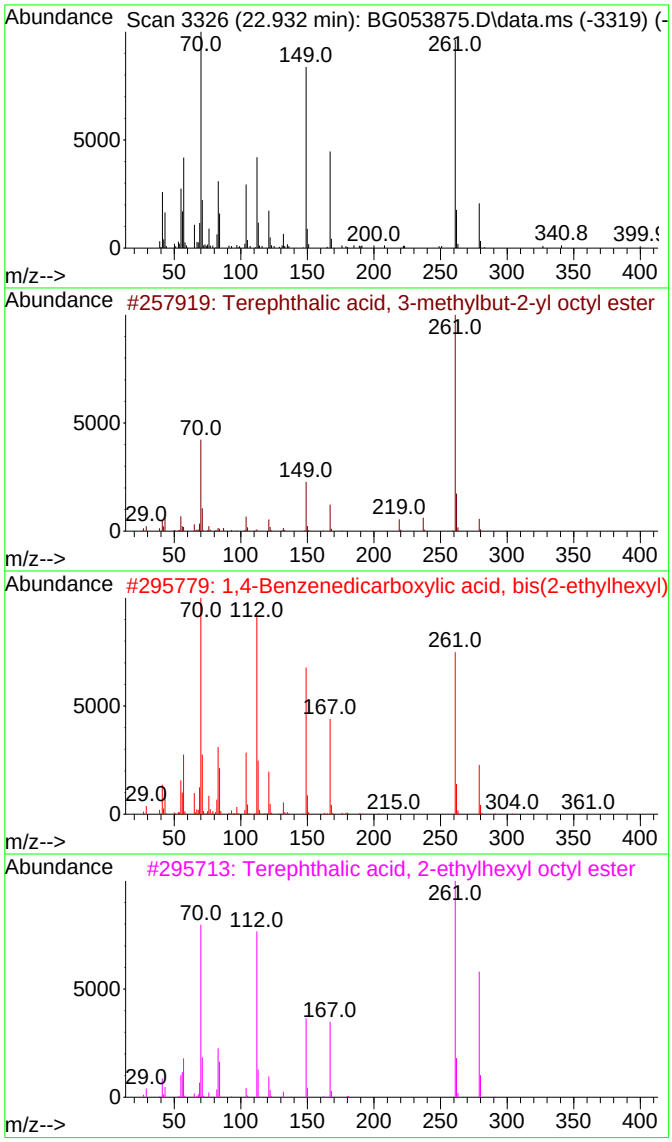
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

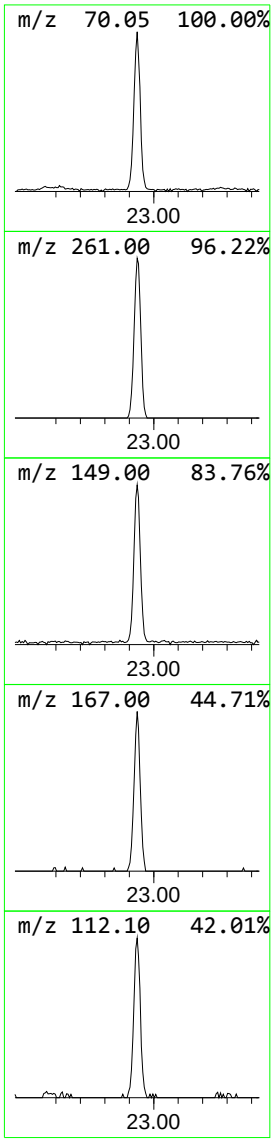
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Terephthalic acid, 3-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.932	11.42 ng	265412	Chrysene-d12	21.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	52
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
5	Terephthalic acid, 4-chloro-3-me...	402	C23H27ClO4	1000323-70-4	43





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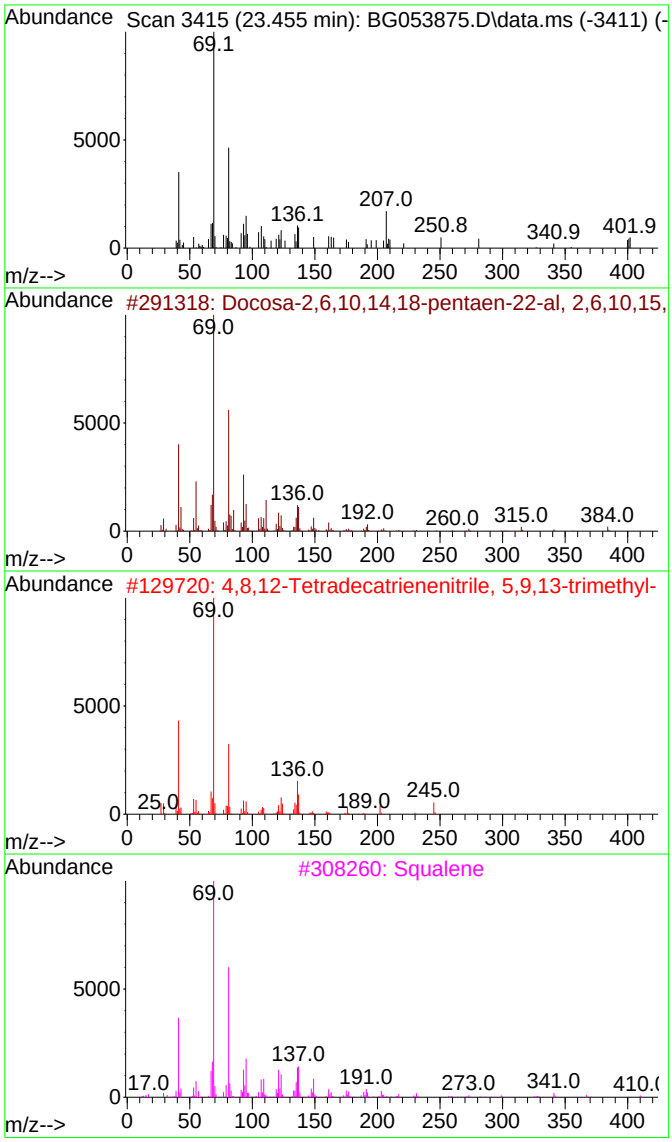
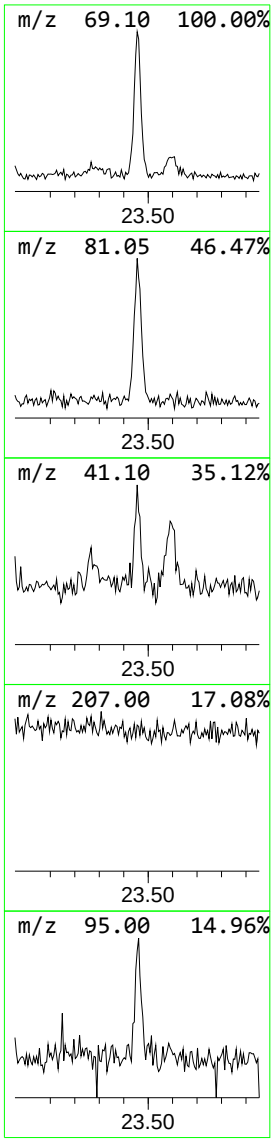
****
Peak Number 8 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.455	2.25 ng	42402	Perylene-d12	25.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	53
2	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	53
3	Squalene	410	C30H50	000111-02-4	53
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	53
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	49





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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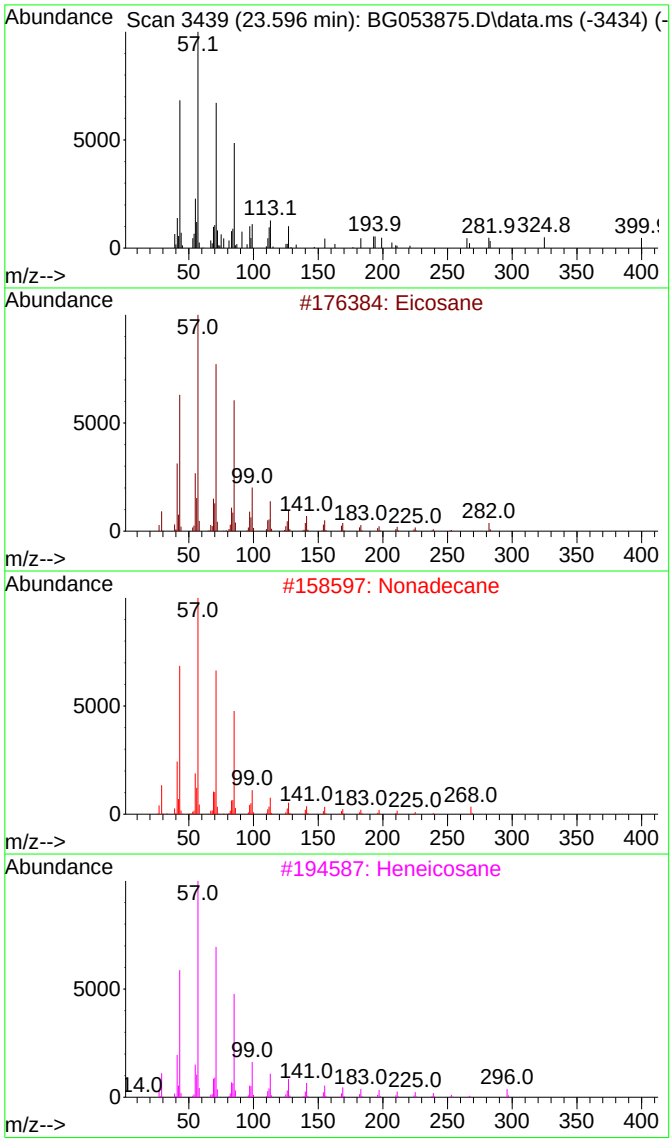
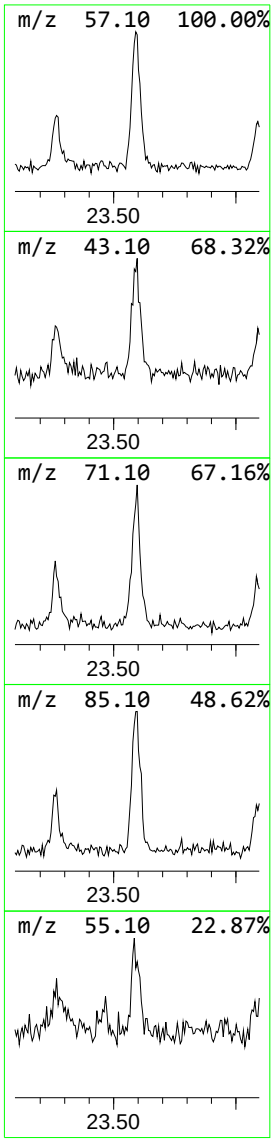
****

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.596	3.31 ng	62391	Perylene-d12	25.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	76
2	Nonadecane	268	C19H40	000629-92-5	64
3	Heneicosane	296	C21H44	000629-94-7	64
4	Octadecane	254	C18H38	000593-45-3	64
5	Heptadecane	240	C17H36	000629-78-7	64





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Data File : BG053875.D
Acq On : 10 Jun 2022 15:00
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

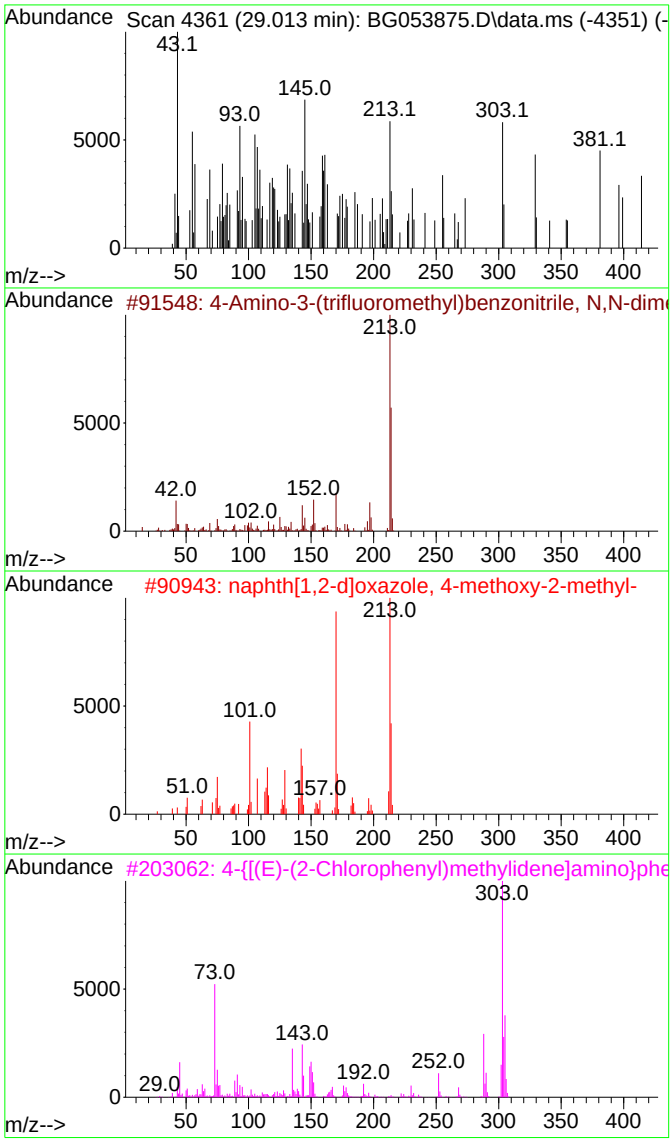
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

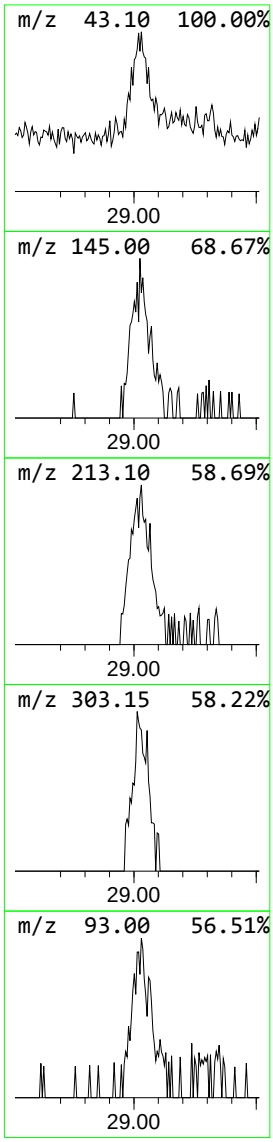
****

Peak Number 10 unknown29.013 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.013	4.94 ng	92998	Perylene-d12	25.000

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-3-(trifluoromethyl)benzo...	214	C10H9F3N2	071145-96-5	11
2	naphth[1,2-d]oxazole, 4-methoxy-...	213	C13H11NO2	1000396-17-8	11
3	4-{[(E)-(2-Chlorophenyl)methylid...	303	C16H18ClNOSi	1000511-13-9	10
4	N-(4-(Methylthio)-1-naphthyl)ace...	303	C16H21NOSSi	1000332-14-9	10
5	3,5-Dimethoxy-4-[4-nitrophenoxy]...	303	C15H13NO6	1010252-84-5	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061022\
Data File : BG053875.D
Acq On : 10 Jun 2022 15:00
Operator : CG/JU
Sample : N3287-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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
Oxirane, [(1-me...	5.182	4.3	ng	22034	1	8.091	101775	20.0
Octadecanoic acid	16.504	46.7	ng	694649	4	17.456	297707	20.0
unknown18.343	18.343	7.6	ng	113473	4	17.456	297707	20.0
Octadecanoic ac...	19.606	23.0	ng	533629	5	21.727	464718	20.0
Heptadecyl hept...	21.369	6.1	ng	141337	5	21.727	464718	20.0
Supraene	21.968	5.1	ng	119345	5	21.727	464718	20.0
Terephthalic ac...	22.932	11.4	ng	265412	5	21.727	464718	20.0
Docosa-2,6,10,1...	23.455	2.3	ng	42402	6	25.000	376559	20.0
Eicosane	23.596	3.3	ng	62391	6	25.000	376559	20.0
unknown29.013	29.013	4.9	ng	92998	6	25.000	376559	20.0