LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102622\
Data File : BM037250.D
Acq On : 26 Oct 2022 22:49
Operator : CG/JU
Sample : N5218-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-2

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-BM102622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	318	323	330	rBV	58411	87766	1.19%	0.259%
2	5.457	395	403	415	rBV	378681	623239	8.48%	1.838%
3	7.063	668	676	685	rBV	446198	752279	10.24%	2.219%
4	7.887	811	816	823	rVB	95925	147766	2.01%	0.436%
5	9.051	1007	1014	1021	rBV	220687	380999	5.18%	1.124%
6	10.687	1285	1292	1302	rBV	163229	276486	3.76%	0.815%
7	13.145	1703	1710	1717	rBV	798682	1147304	15.61%	3.384%
8	14.522	1937	1944	1951	rBV	348533	521420	7.10%	1.538%
9	14.939	2009	2015	2025	rBV2	133912	351777	4.79%	1.037%
10	16.010	2190	2197	2205	rBV	2580260	3752894	51.07%	11.068%
11	16.474	2272	2276	2280	rVV	81379	148339	2.02%	0.437%
12	16.516	2281	2283	2293	rVB3	57549	129549	1.76%	0.382%
13	16.668	2304	2309	2329	rBV2	84620	325220	4.43%	0.959%
14	17.263	2404	2410	2415	rBV	665146	926764	12.61%	2.733%
15	18.157	2557	2562	2577	rBV	414709	985572	13.41%	2.907%
16	19.321	2752	2760	2761	rBV2	612249	998076	13.58%	2.943%
17	19.362	2761	2767	2776	rVV	3564656	7348532	100.00%	21.672%
18	19.433	2776	2779	2794	rVB	933631	1946218	26.48%	5.740%
19	19.668	2817	2819	2828	rVB3	168329	275919	3.75%	0.814%
20	19.880	2850	2855	2861	rVB	3897012	4692381	63.85%	13.838%
21	20.427	2945	2948	2957	rBV3	146127	268530	3.65%	0.792%
22	21.145	3067	3070	3079	rVB	315421	440986	6.00%	1.301%
23	21.433	3115	3119	3124	rBV	1794475	2334557	31.77%	6.885%
24	21.986	3209	3213	3219	rBV	934336	1511999	20.58%	4.459%
25	23.803	3516	3522	3537	rVB2	1747434	3533811	48.09%	10.422%

Sum of corrected areas: 33908383

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Instrument :
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ClientSampleId :
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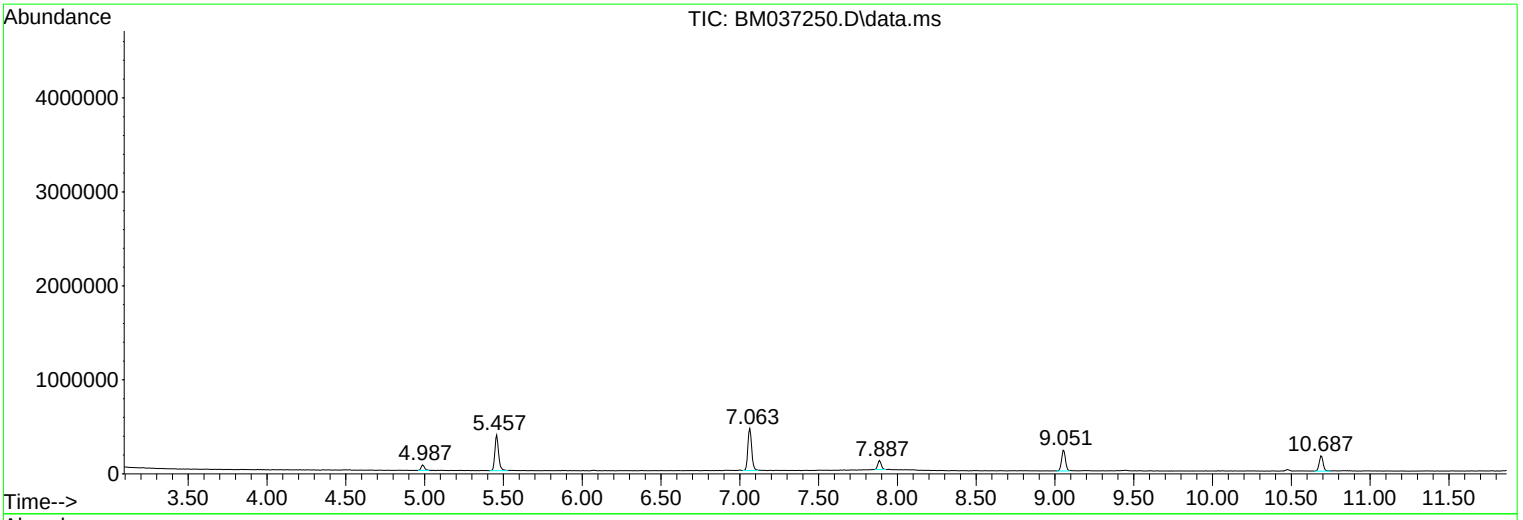
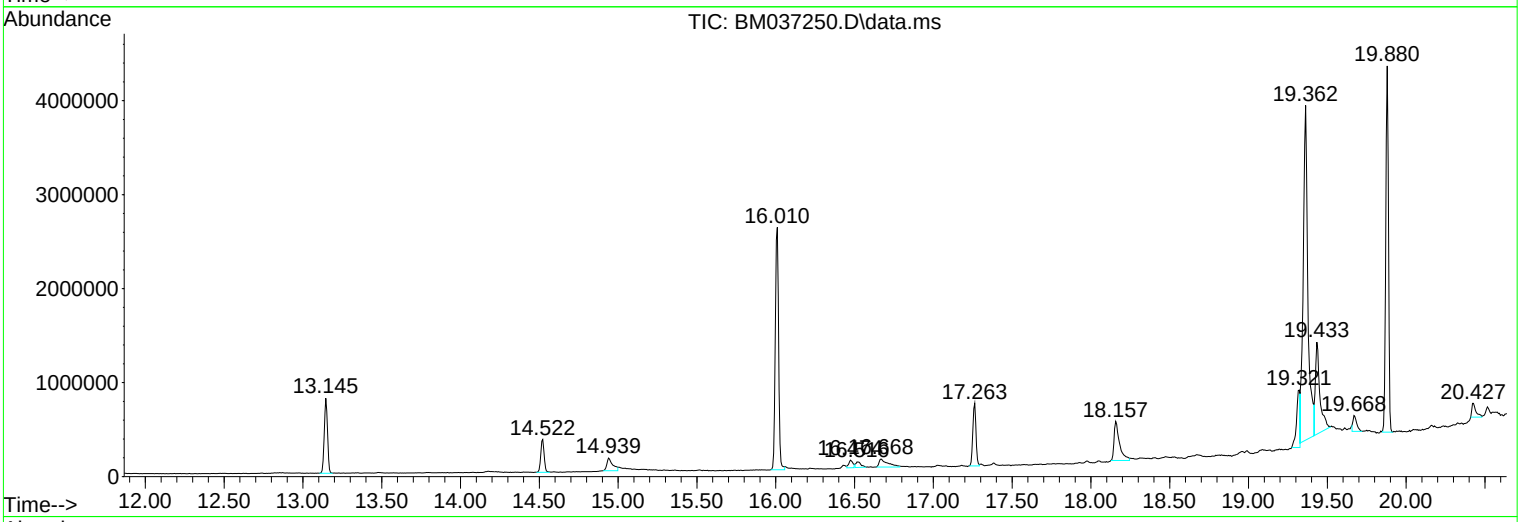
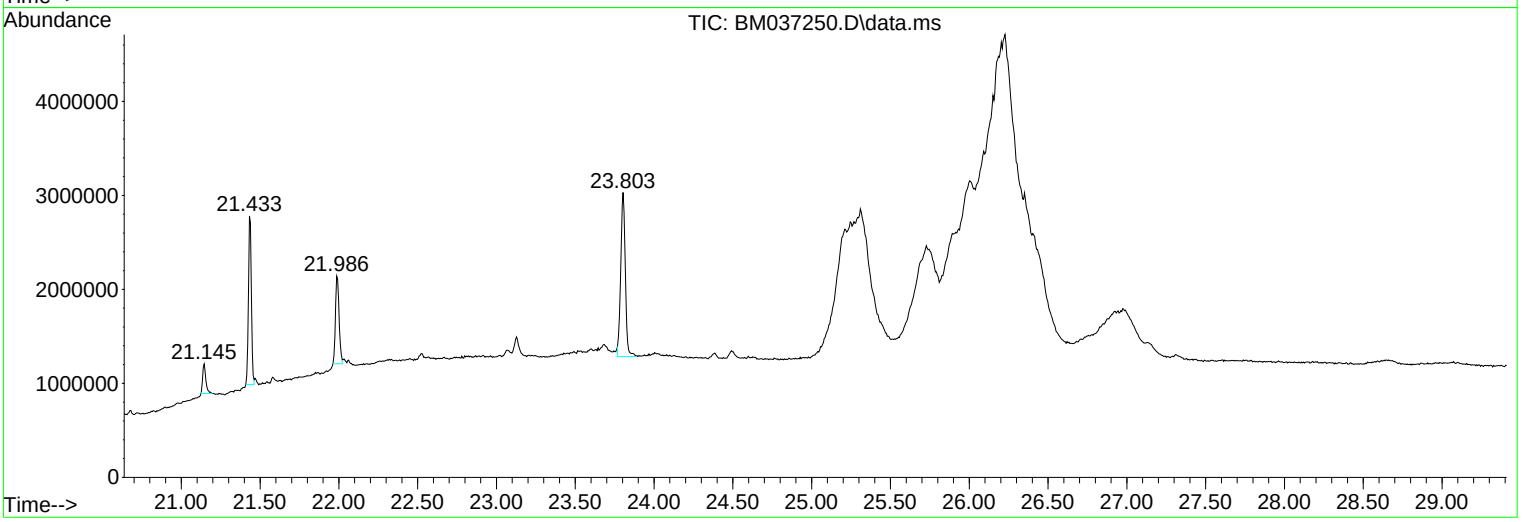
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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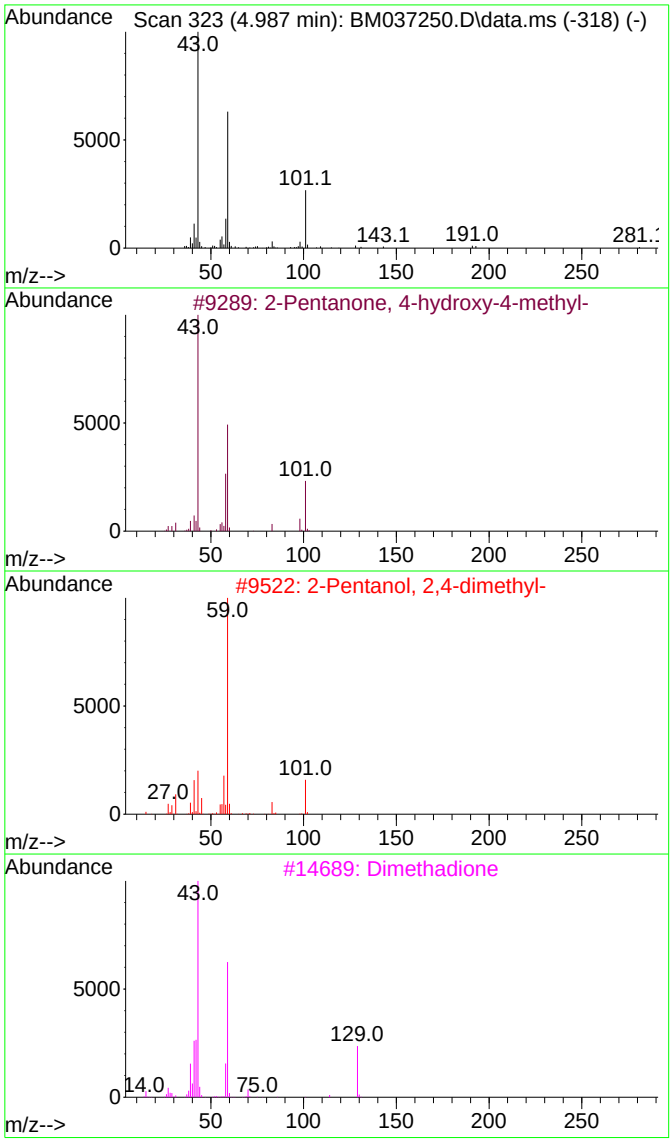
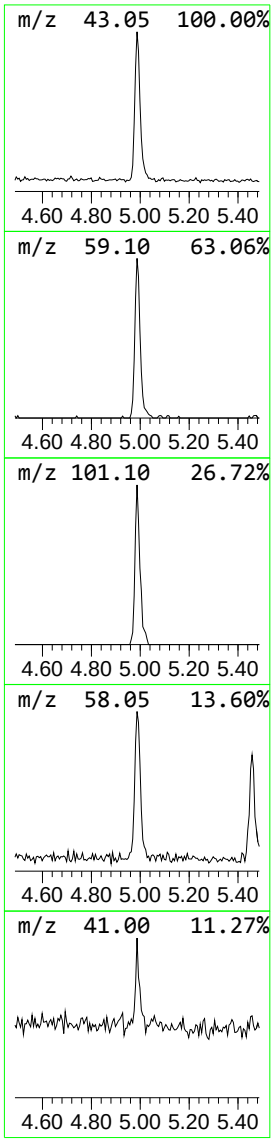
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	11.88 ng	87766	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	50
3	Dimethadione	129	C5H7NO3	000695-53-4	33
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27





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Operator : CG/JU
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Instrument :
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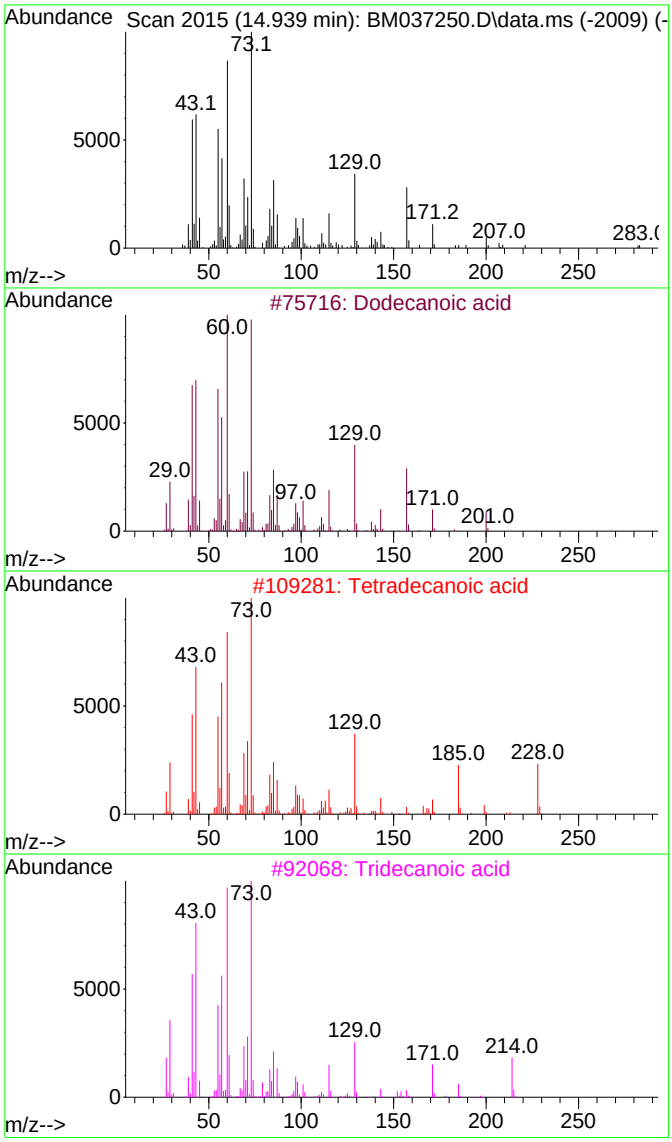
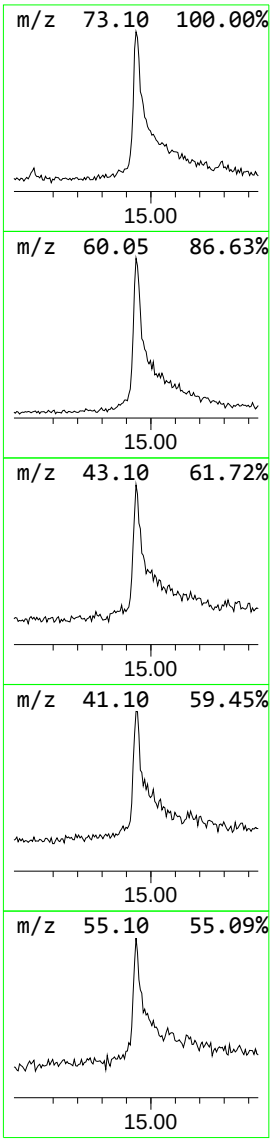
****

Peak Number 2 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	13.49 ng	351777	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	Nonanoic acid	158	C9H18O2	000112-05-0	46





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Instrument :
BNA_M
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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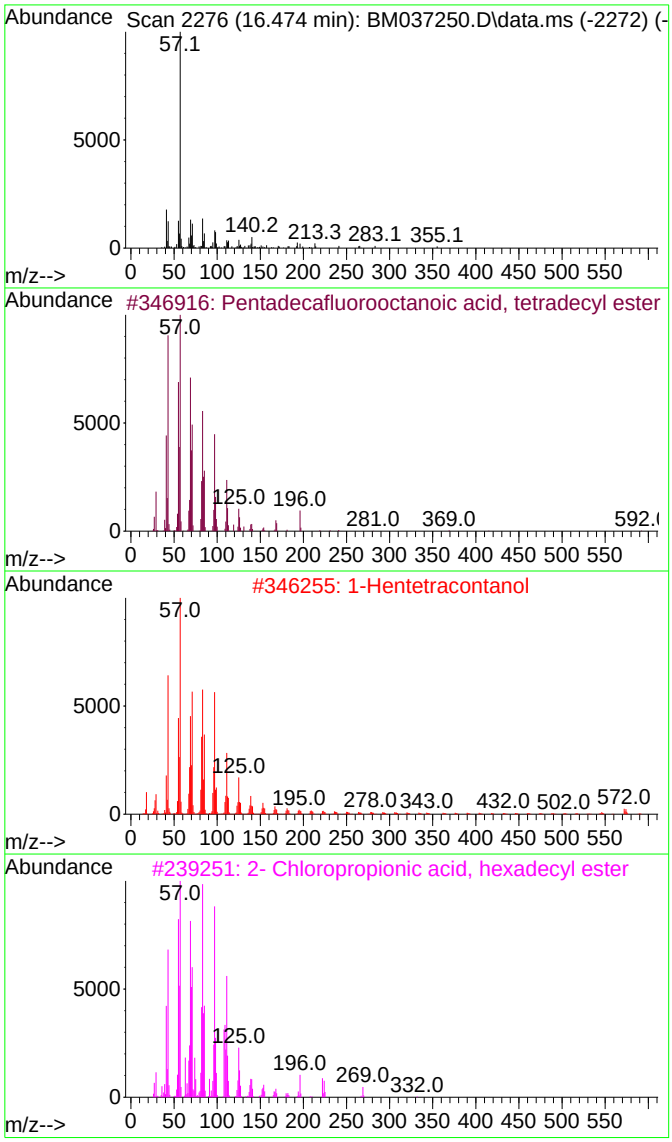
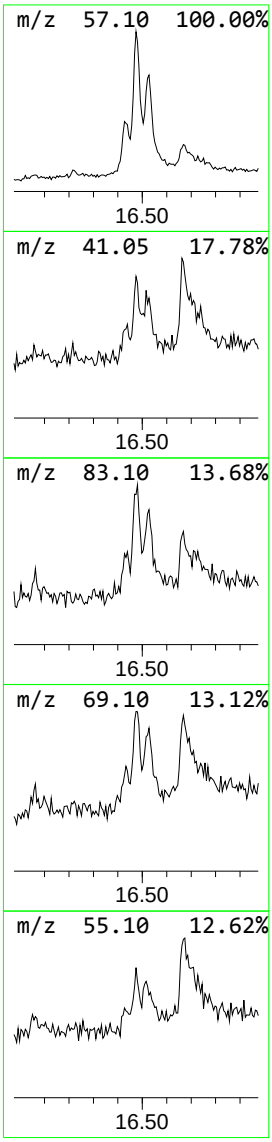
Peak Number 3 unknown16.474 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.474	3.20 ng	148339	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	49
2	1-Hentetracontanol	593	C41H84O	040710-42-7	47
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	47
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	43
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	43





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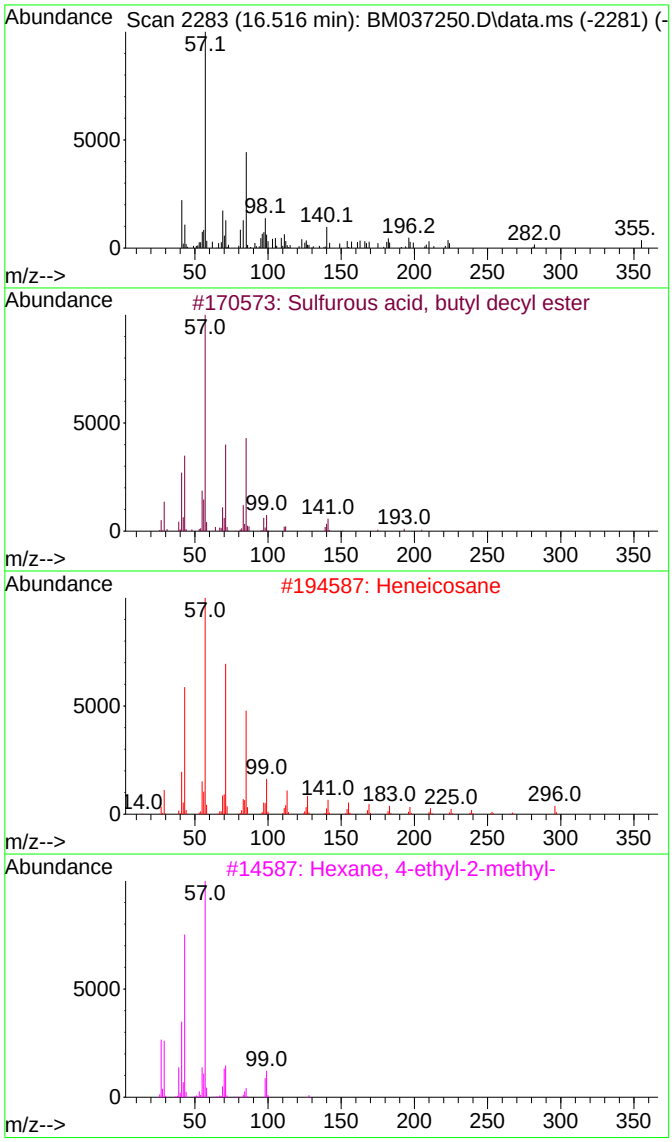
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

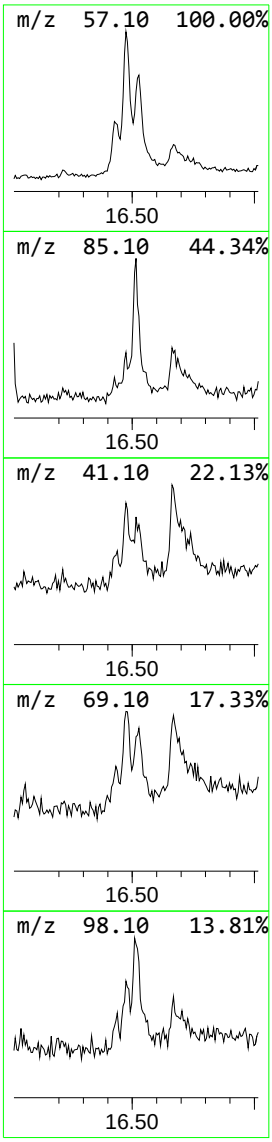
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Sulfurous acid, butyl decyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	2.80 ng	129549	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	50
2	Heneicosane	296	C21H44	000629-94-7	32
3	Hexane, 4-ethyl-2-methyl-	128	C9H20	003074-75-7	14
4	Diethylmalonic acid, butyl hept-...	314	C18H34O4	1000370-50-8	14
5	Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	12





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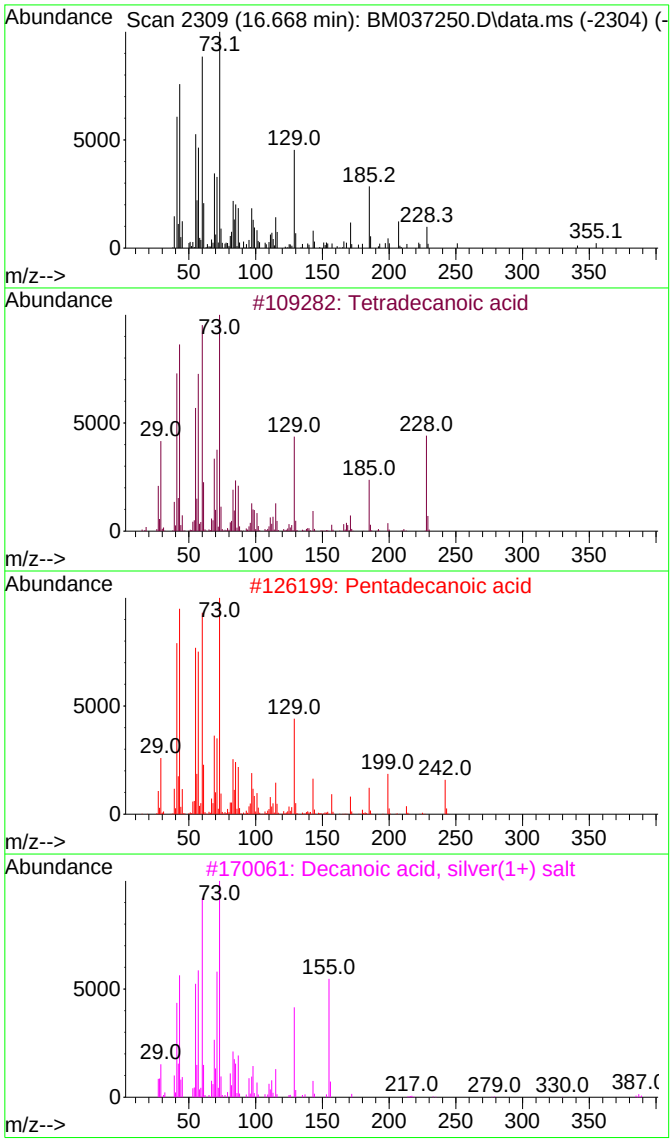
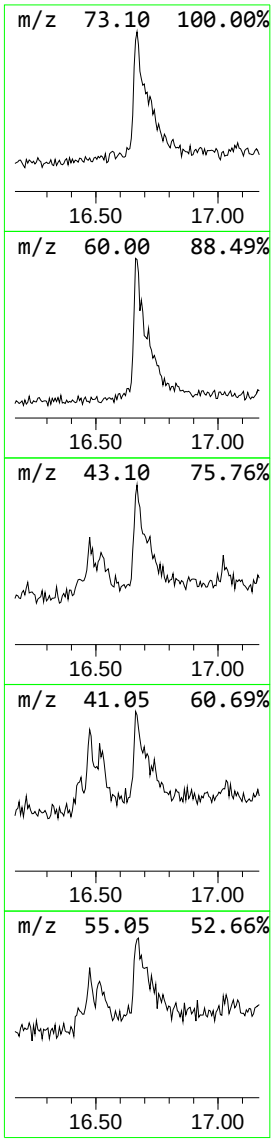
****

Peak Number 5 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.669	7.02 ng	325220	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	62
4	Dodecanoic acid	200	C12H24O2	000143-07-7	60
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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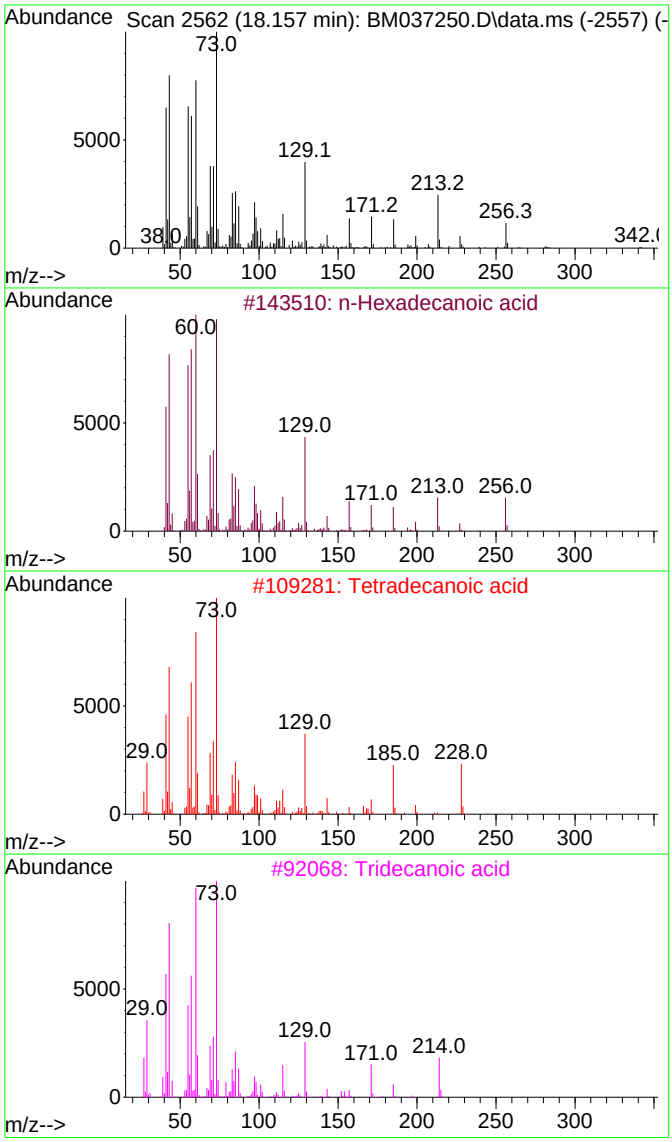
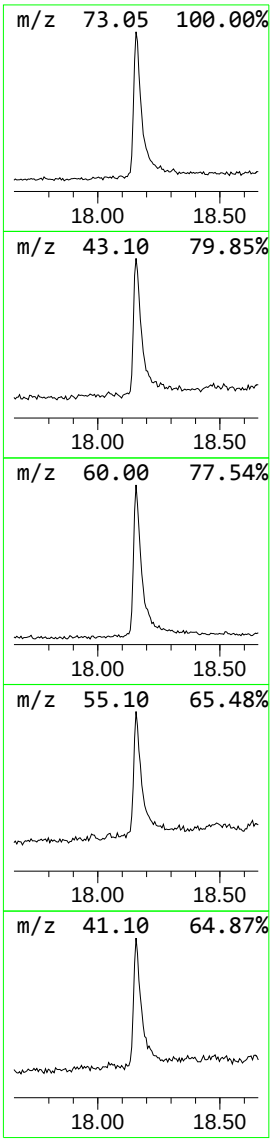
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	21.27 ng	985572	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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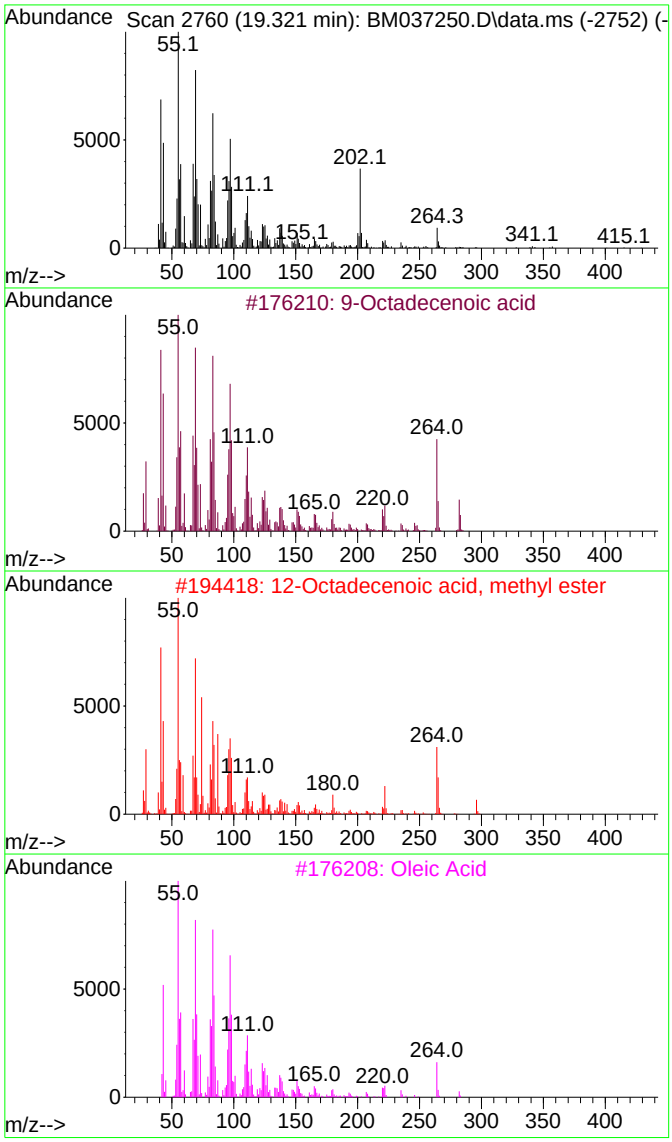
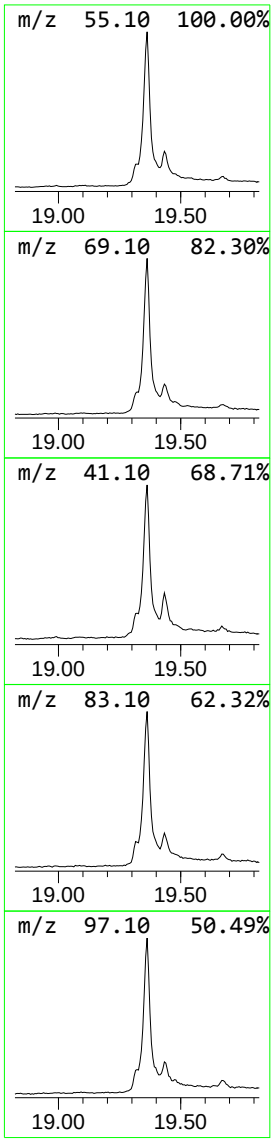
Peak Number 7 9-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	21.54 ng	998076	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid	282	C18H34O2	002027-47-6	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
3	Oleic Acid	282	C18H34O2	000112-80-1	90
4	cis-9-Octadecenoic acid, propyl ...	324	C21H40O2	1000405-15-0	87
5	9-Nonadecene	266	C19H38	031035-07-1	86





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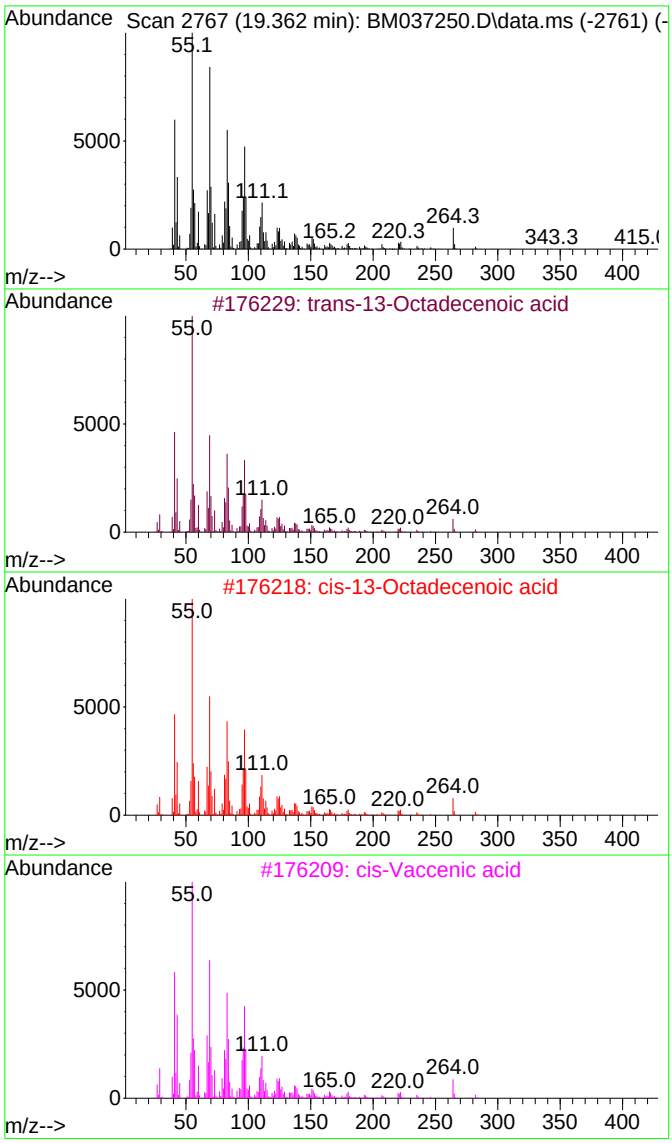
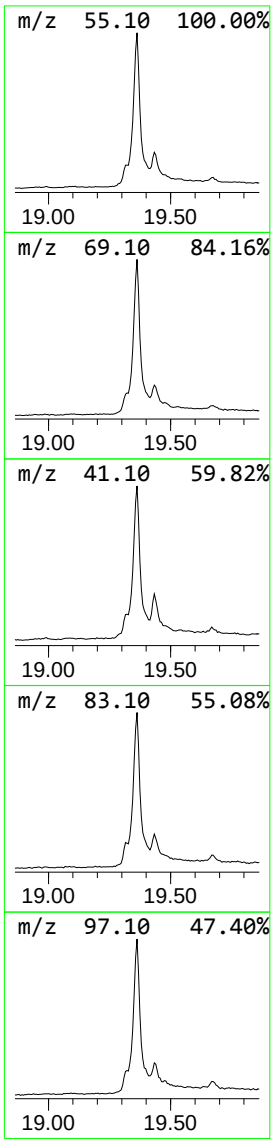
Peak Number 8 trans-13-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.362	62.95 ng	7348530	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	95
4	Palmitoleic acid	254	C16H30O2	000373-49-9	90
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	90





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TIC Library : C:\Database\NIST20.L
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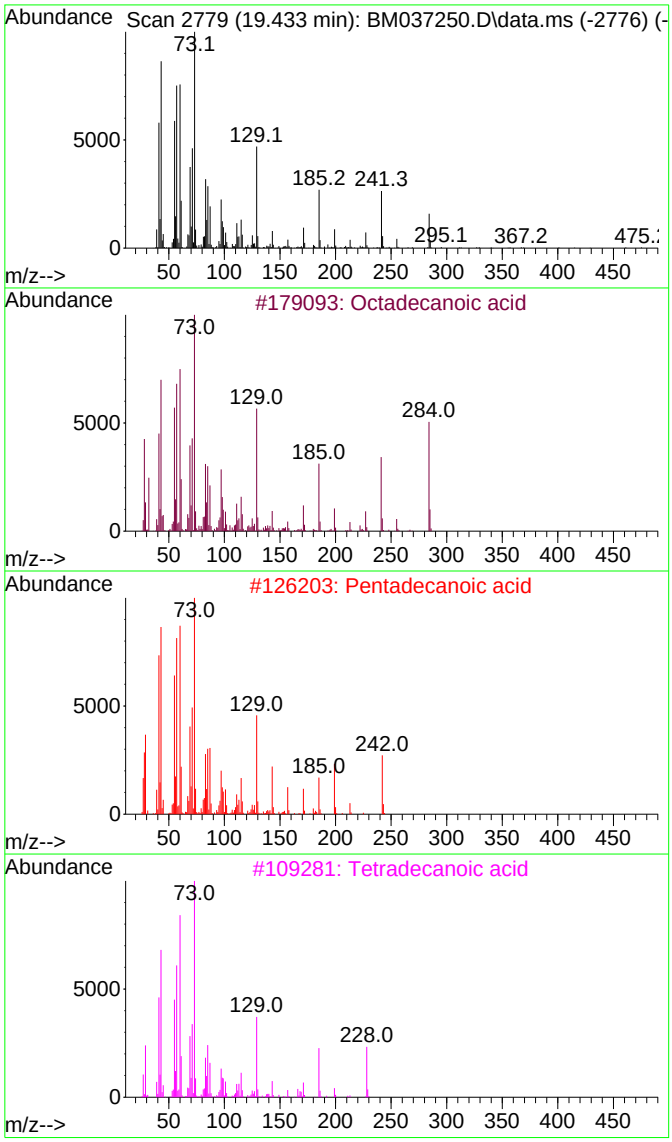
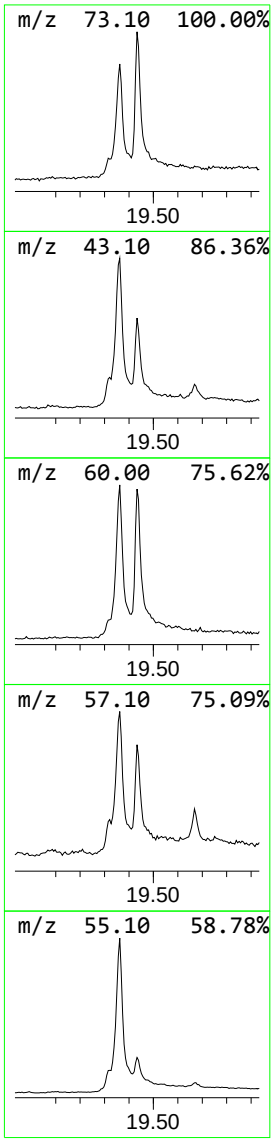
Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	16.67 ng	1946220	Chrysene-d12	21.433

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	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.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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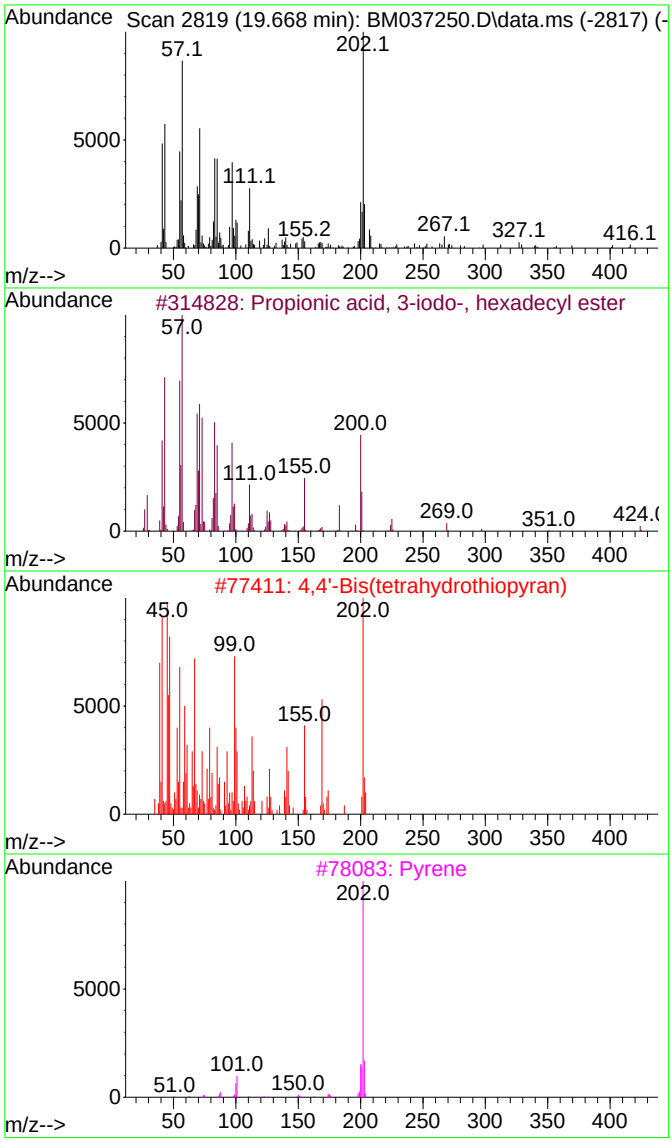
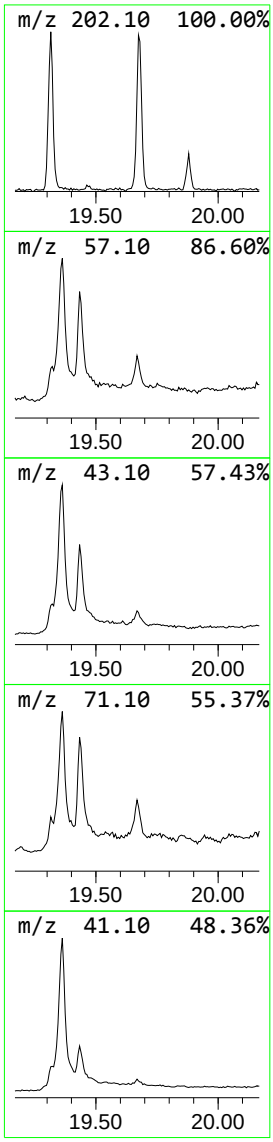
Peak Number 10 unknown19.668 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.668	2.36 ng	275919	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propionic acid, 3-iodo-, hexadec...	424	C19H37IO2	1000406-24-7	43
2	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	42
3	Pyrene	202	C16H10	000129-00-0	35
4	1-Octadecene	252	C18H36	000112-88-9	30
5	Tetradecane	198	C14H30	000629-59-4	25





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Data File : BM037250.D
Acq On : 26 Oct 2022 22:49
Operator : CG/JU
Sample : N5218-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.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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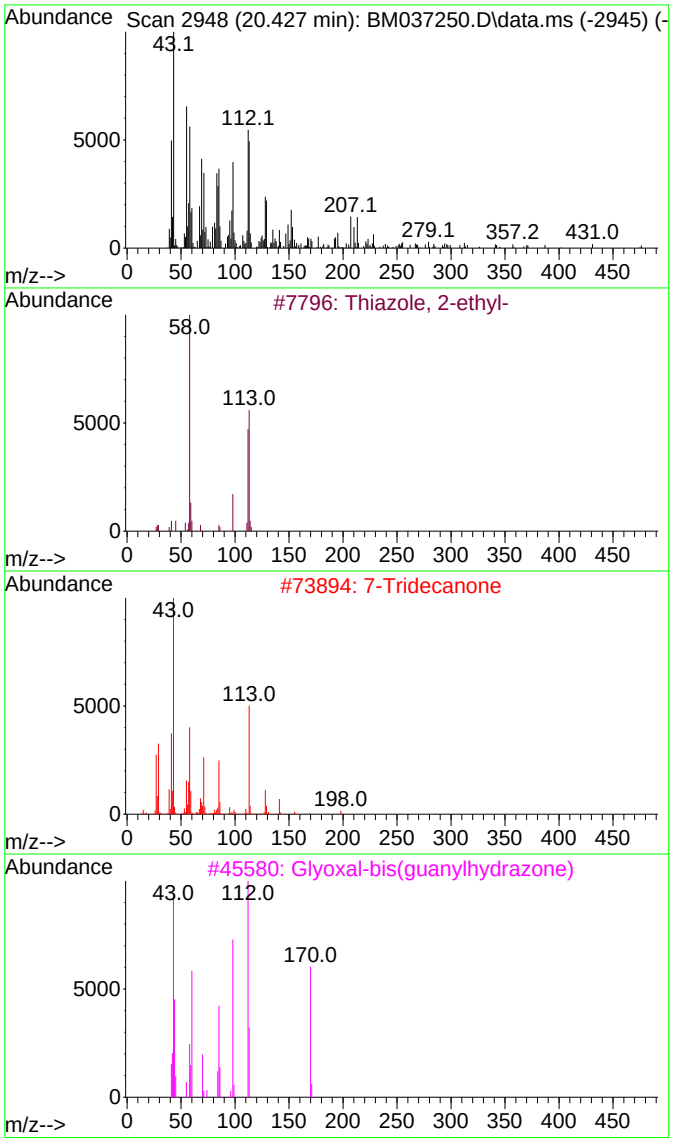
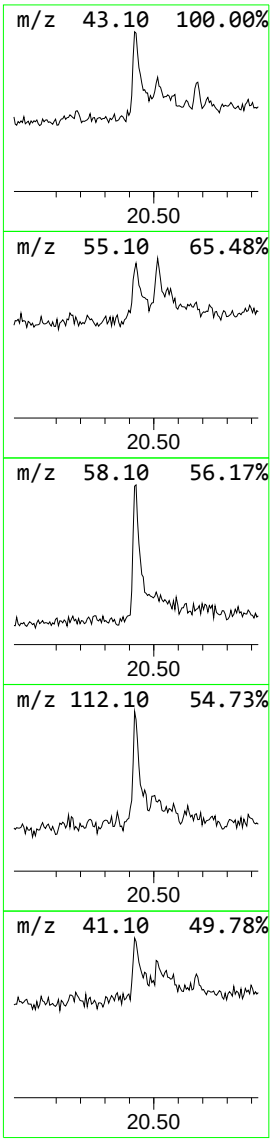
Peak Number 11 Thiazole, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.427	2.30 ng	268530	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, 2-ethyl-	113	C5H7NS	015679-09-1	58
2	7-Tridecanone	198	C13H26O	000462-18-0	38
3	Glyoxal-bis(guanylhydrazone)	170	C4H10N8	014358-42-0	27
4	7-Heptadecanone	254	C17H34O	006064-42-2	25
5	N-(2-(Dimethylamino)ethyl)-2-(pi...	242	C12H26N4O	1000498-57-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102622\
Data File : BM037250.D
Acq On : 26 Oct 2022 22:49
Operator : CG/JU
Sample : N5218-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.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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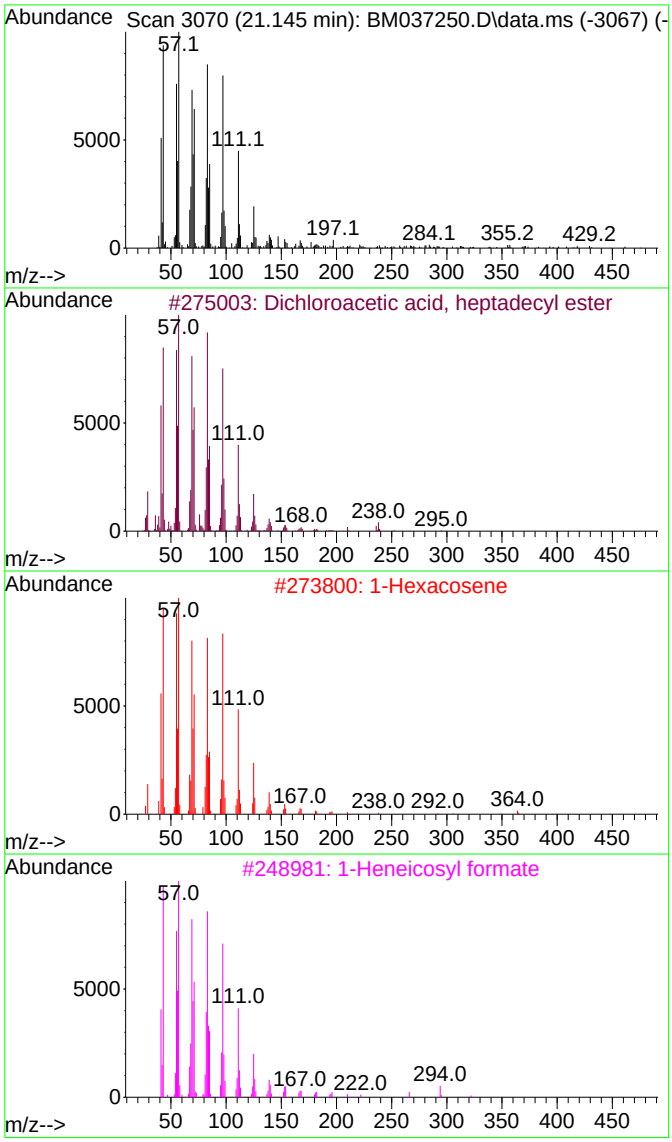
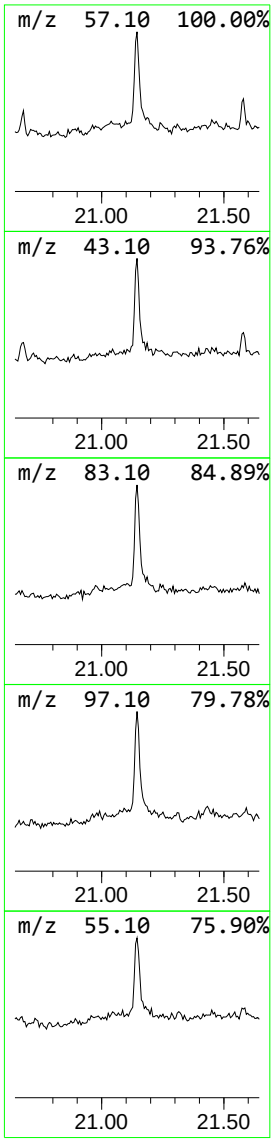
Peak Number 12 Dichloroacetic acid, heptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	3.78 ng	440986	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102622\
Data File : BM037250.D
Acq On : 26 Oct 2022 22:49
Operator : CG/JU
Sample : N5218-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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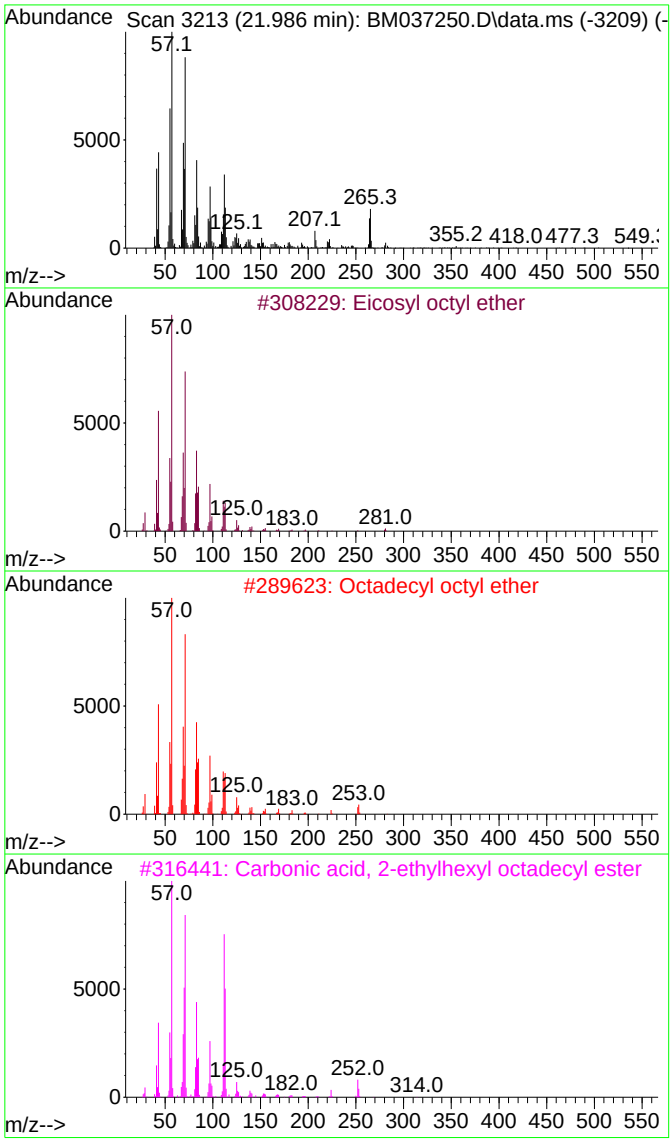
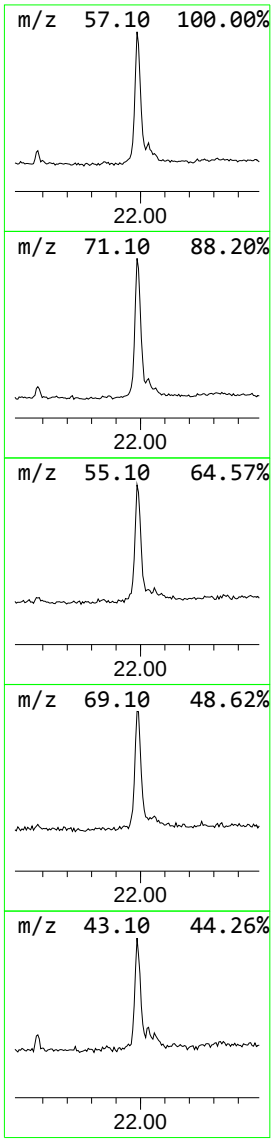
Peak Number 13 Eicosyl octyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.986	12.95 ng	1512000	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl octyl ether	410	C28H58O	1000406-38-8	64
2	Octadecyl octyl ether	382	C26H54O	1000406-38-7	64
3	Carbonic acid, 2-ethylhexyl octa...	426	C27H54O3	1000383-14-5	58
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	50
5	9-Octadecenoic acid (Z)-, pentyl...	352	C23H44O2	000142-57-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102622\
Data File : BM037250.D
Acq On : 26 Oct 2022 22:49
Operator : CG/JU
Sample : N5218-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102622.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
2-Pentanone, 4-...	4.987	11.9	ng	87766	1	7.887	147766	20.0
Dodecanoic acid	14.939	13.5	ng	351777	3	14.522	521420	20.0
unknown16.474	16.474	3.2	ng	148339	4	17.263	926764	20.0
Sulfurous acid,...	16.515	2.8	ng	129549	4	17.263	926764	20.0
Tetradecanoic acid	16.669	7.0	ng	325220	4	17.263	926764	20.0
n-Hexadecanoic ...	18.157	21.3	ng	985572	4	17.263	926764	20.0
9-Octadecenoic ...	19.321	21.5	ng	998076	4	17.263	926764	20.0
trans-13-Octade...	19.362	63.0	ng	7348530	5	21.433	2334560	20.0
Octadecanoic acid	19.433	16.7	ng	1946220	5	21.433	2334560	20.0
unknown19.668	19.668	2.4	ng	275919	5	21.433	2334560	20.0
Thiazole, 2-ethyl-	20.427	2.3	ng	268530	5	21.433	2334560	20.0
Dichloroacetic ...	21.145	3.8	ng	440986	5	21.433	2334560	20.0
Eicosyl octyl e...	21.986	12.9	ng	1512000	5	21.433	2334560	20.0