

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
Data File : BG045146.D
Acq On : 23 Apr 2020 17:50
Operator : CG/JU
Sample : L2326-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

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-BG041520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.280	843	884	887	rVV2	24636261	216431587	100.00%	63.235%
2	9.208	1030	1042	1050	rBV2	1889435	4719945	2.18%	1.379%
3	9.872	1059	1155	1156	rBV	3329012	48418590	22.37%	14.147%
4	10.671	1248	1291	1296	rBV4	2529457	21614214	9.99%	6.315%
5	13.103	1674	1705	1709	rBV	2460798	13206975	6.10%	3.859%
6	13.273	1726	1734	1751	rVB	2717363	5177011	2.39%	1.513%
7	15.176	2035	2058	2062	rBV	3922683	16108634	7.44%	4.706%
8	16.616	2299	2303	2308	rVV	2609435	3823999	1.77%	1.117%
9	16.669	2308	2312	2322	rVB	1551415	2251065	1.04%	0.658%
10	19.899	2856	2862	2871	rBV	1623031	2231555	1.03%	0.652%
11	20.005	2874	2880	2886	rVB	4095993	5488339	2.54%	1.604%
12	22.478	3294	3301	3309	rVB	1666196	2792078	1.29%	0.816%

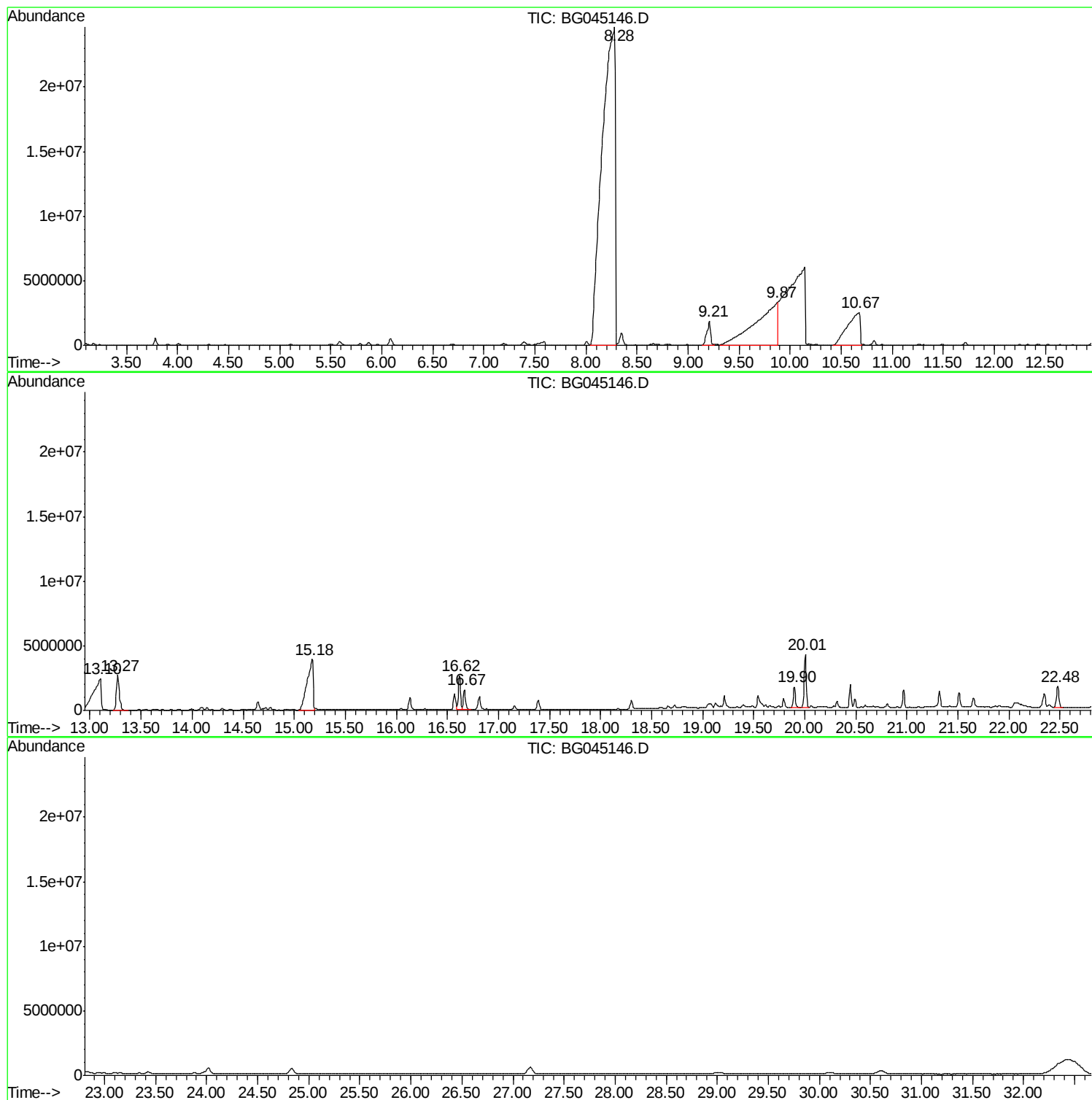
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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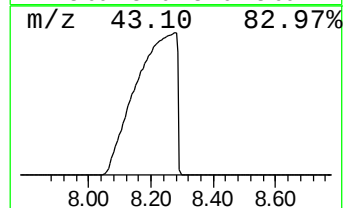
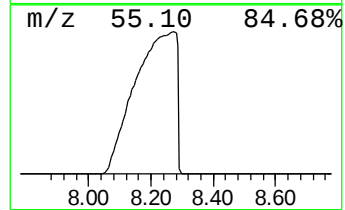
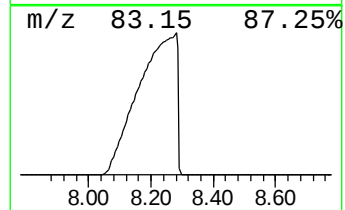
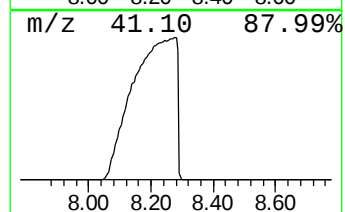
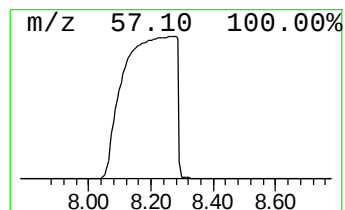
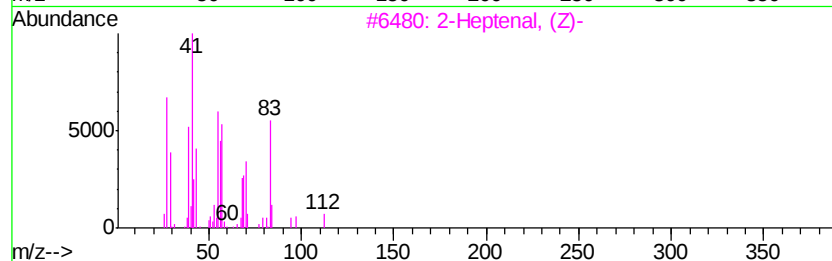
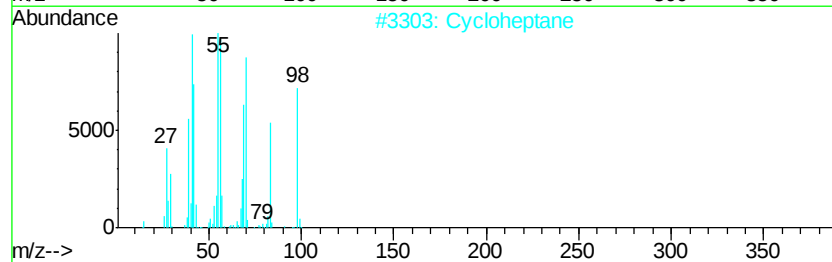
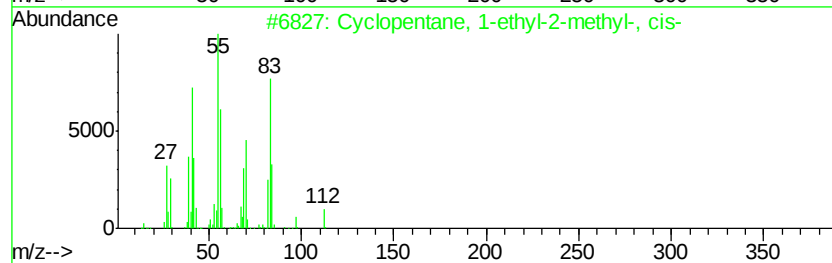
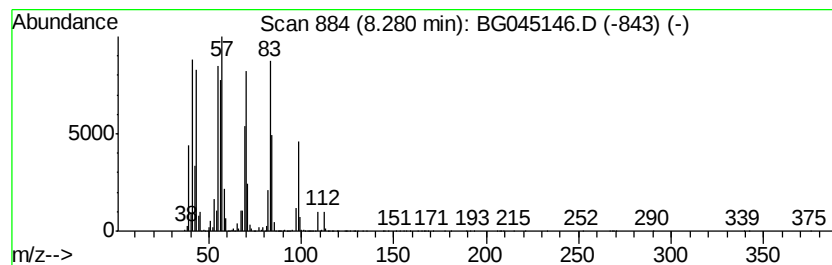
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentane, 1-ethyl-2-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	20.00 ng	216432000	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1-ethyl-2-methyl-, ...	112	C8H16	000930-89-2	58
2		Cycloheptane	98	C7H14	000291-64-5	46
3		2-Heptenal, (Z)-	112	C7H12O	057266-86-1	46
4		Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	43
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	38



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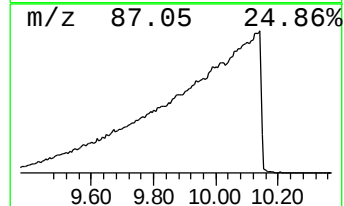
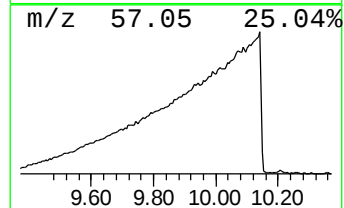
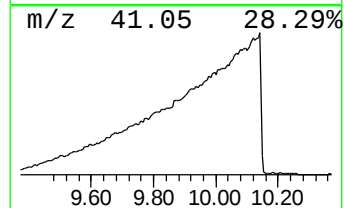
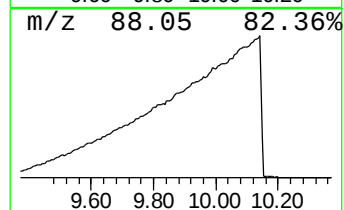
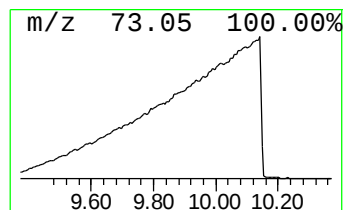
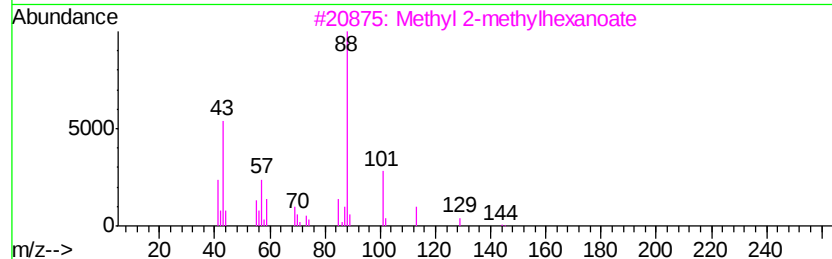
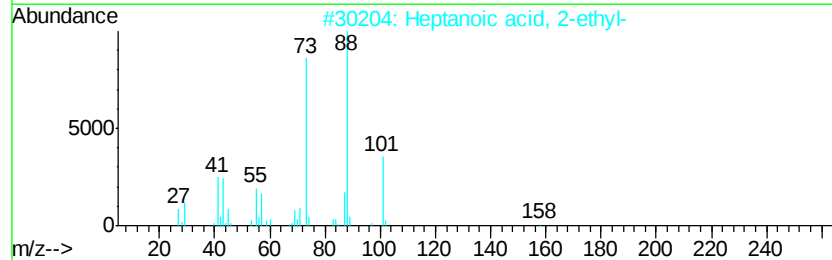
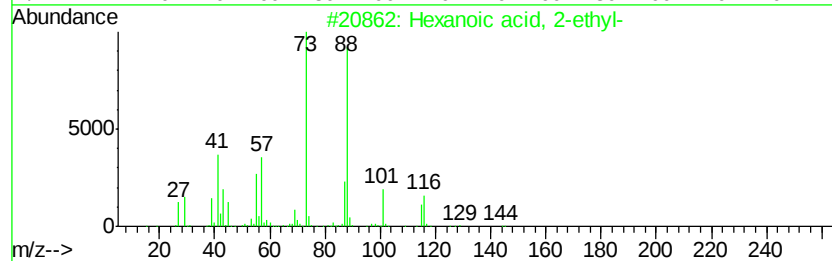
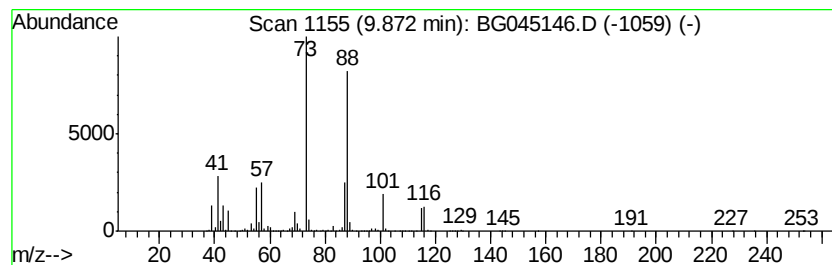
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	44.80 ng	48418600	Naphthalene-d8	10.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
3		Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	40
4		1,4-Dioxane	88	C4H8O2	000123-91-1	38
5		Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	33



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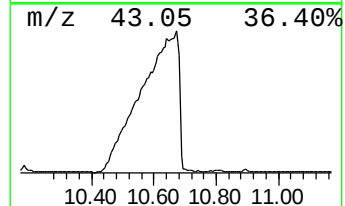
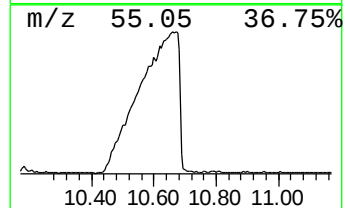
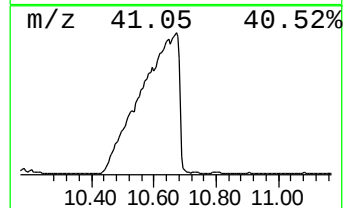
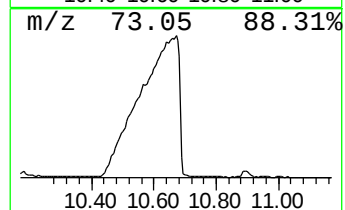
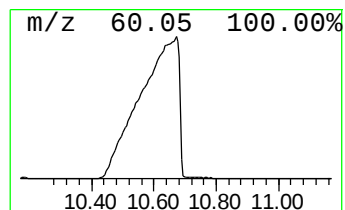
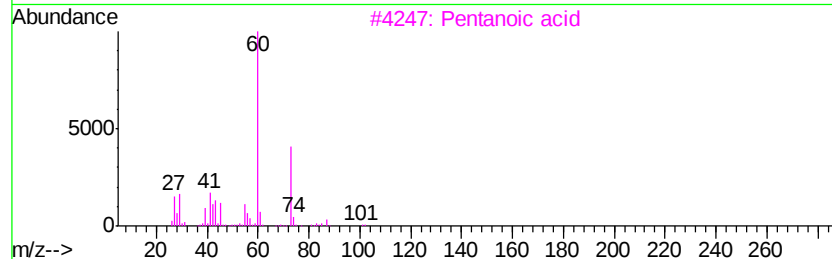
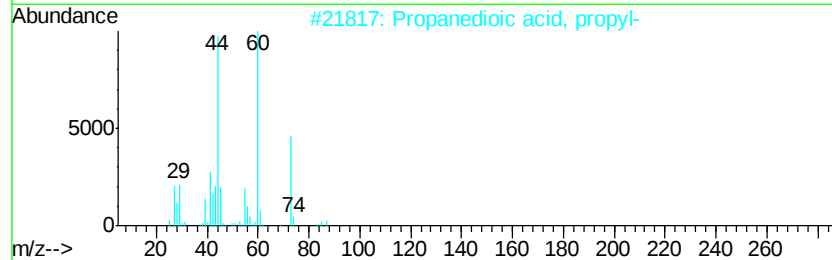
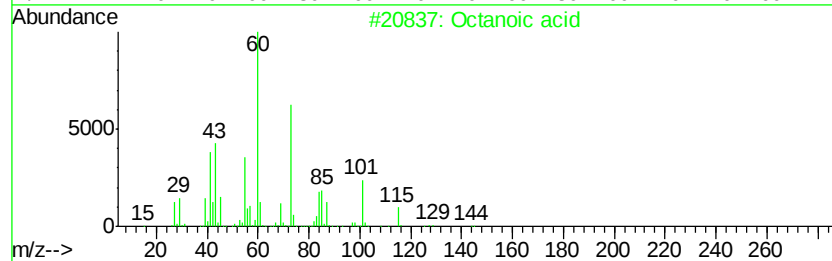
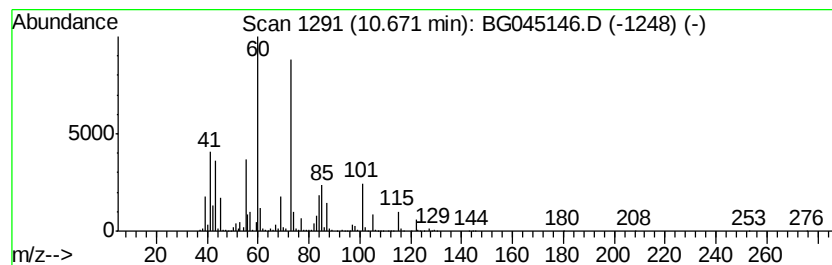
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Peak Number 3 Octanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	20.00 ng	21614200	Naphthalene-d8	10.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octanoic acid	144 C8H16O2	000124-07-2 95
2		Propanedioic acid, propyl-	146 C6H10O4	000616-62-6 53
3		Pentanoic acid	102 C5H10O2	000109-52-4 53
4		Hexanoic acid	116 C6H12O2	000142-62-1 50
5		Butanoic acid, 3-methyl-	102 C5H10O2	000503-74-2 38



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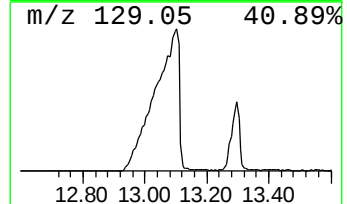
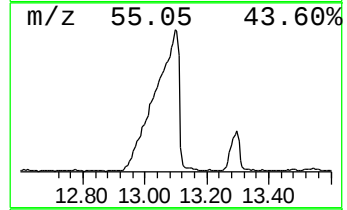
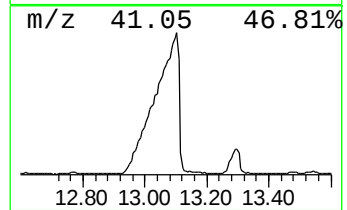
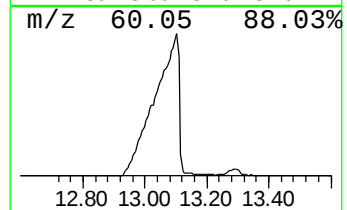
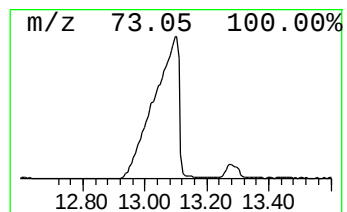
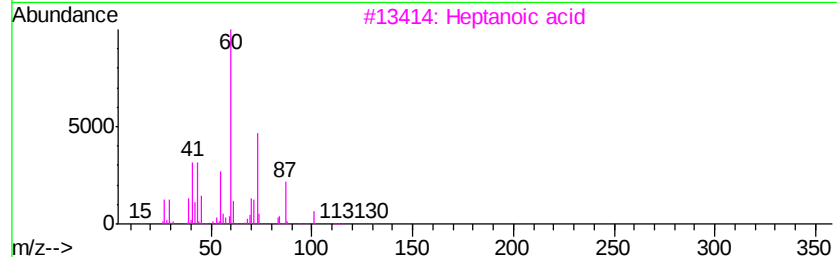
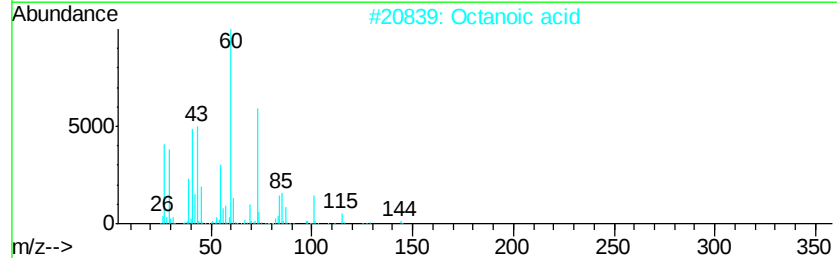
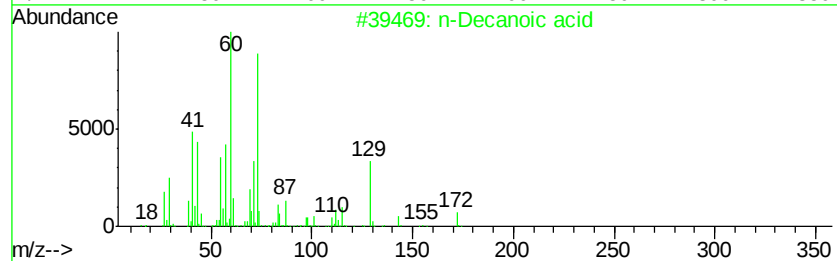
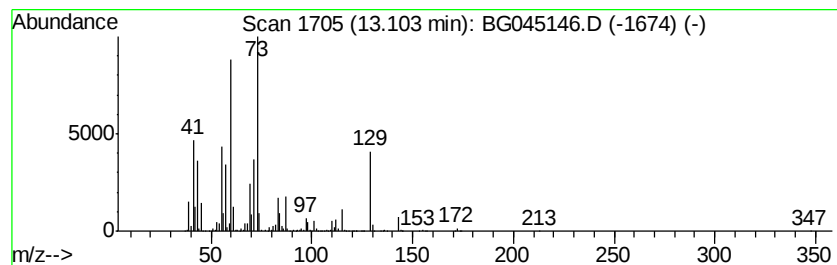
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Peak Number 4 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	16.40 ng	13207000	Acenaphthene-d10	14.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	94	
2	Octanoic acid	144	C8H16O2	000124-07-2	49	
3	Heptanoic acid	130	C7H14O2	000111-14-8	47	
4	Hexanoic acid	116	C6H12O2	000142-62-1	43	
5	D-Fucose	164	C6H12O5	003615-37-0	43	



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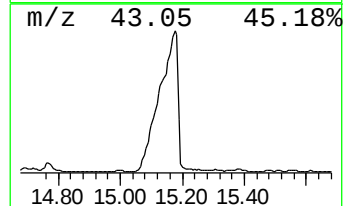
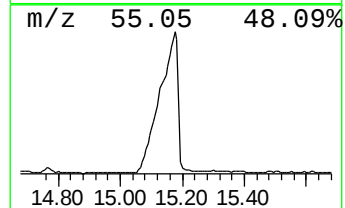
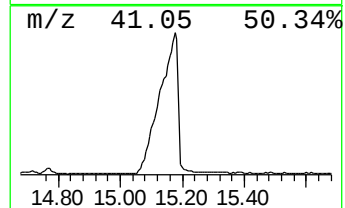
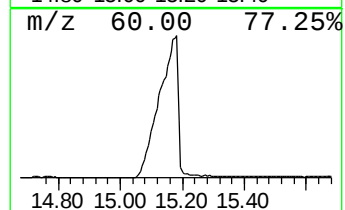
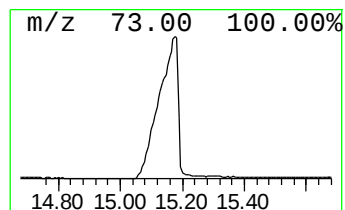
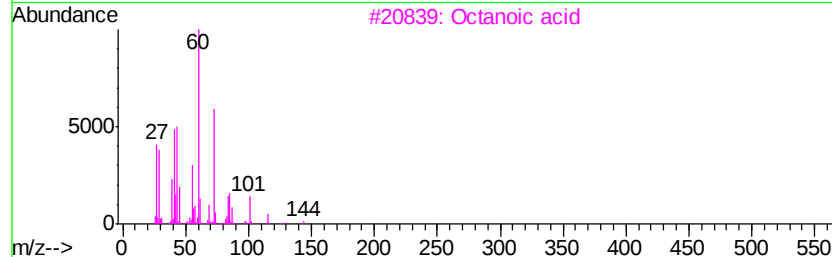
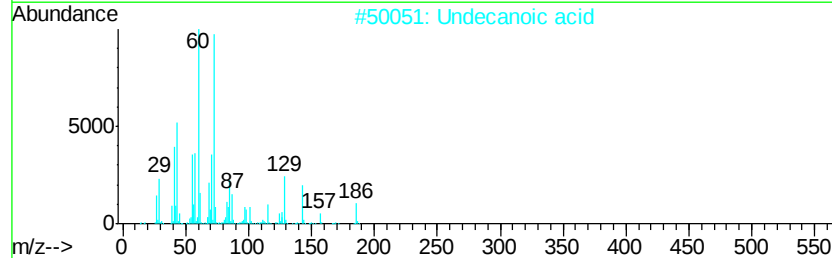
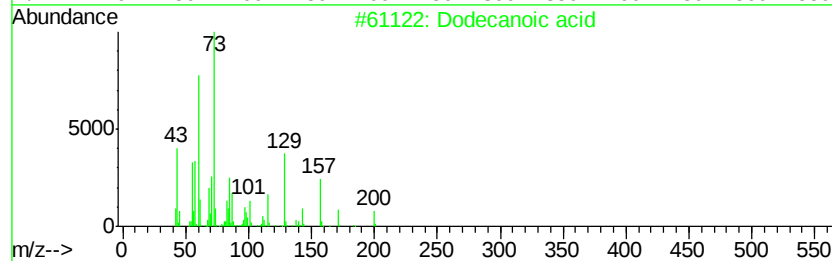
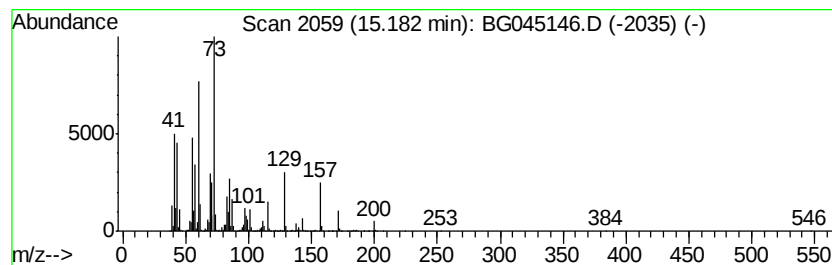
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Peak Number 5 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	20.00 ng	16108600	Acenaphthene-d10	14.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98	
2	Undecanoic acid	186	C11H22O2	000112-37-8	72	
3	Octanoic acid	144	C8H16O2	000124-07-2	49	
4	Nonanoic acid	158	C9H18O2	000112-05-0	46	
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	37	



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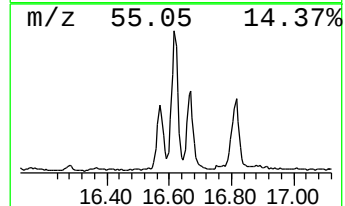
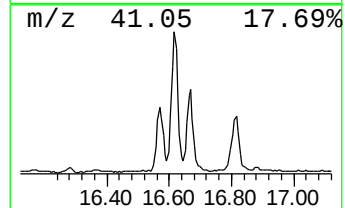
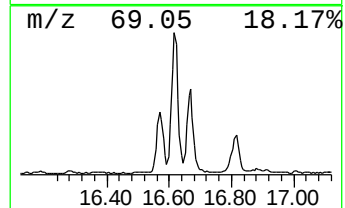
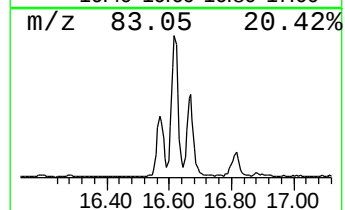
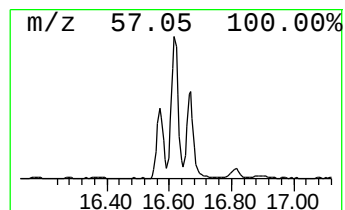
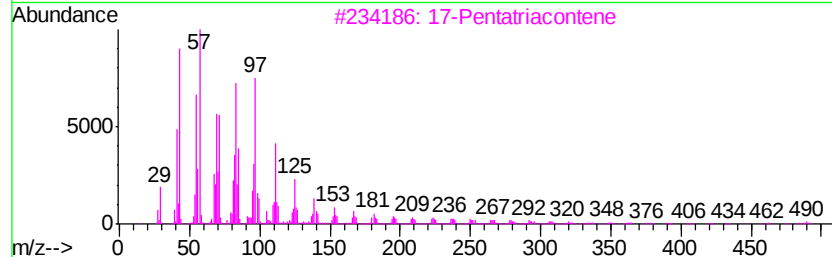
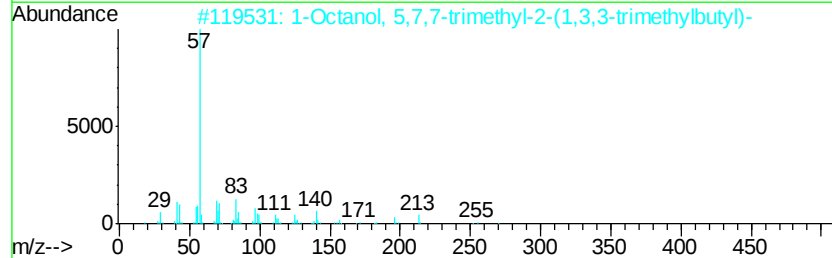
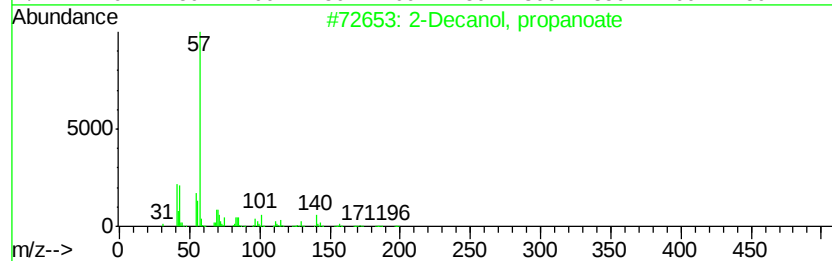
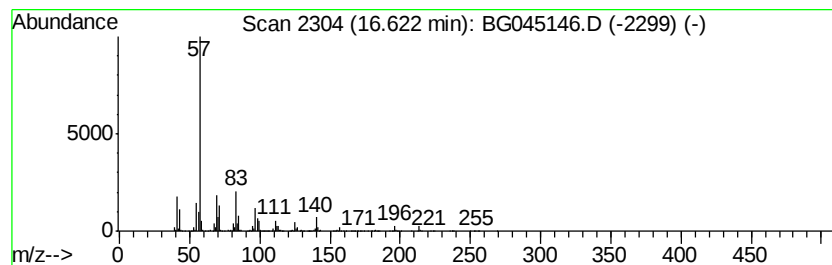
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Peak Number 6 2-Decanol, propanoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	33.98 ng	3824000	Phenanthrene-d10	17.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Decanol, propanoate	214	C13H26O2	055683-11-9	53
2		1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	47
3		17-Pentatriacontene	491	C35H70	006971-40-0	47
4		3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	47
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
Data File : BG045146.D
Acq On : 23 Apr 2020 17:50
Operator : CG/JU
Sample : L2326-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

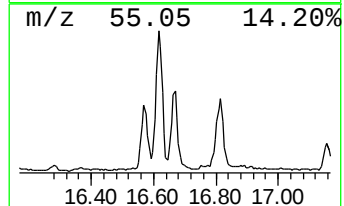
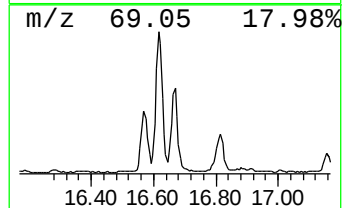
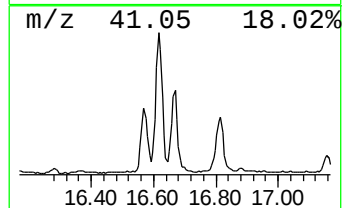
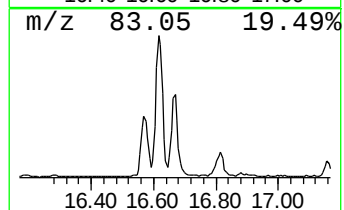
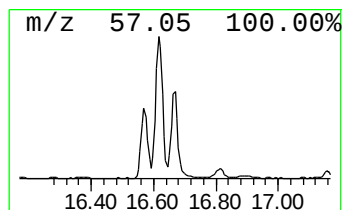
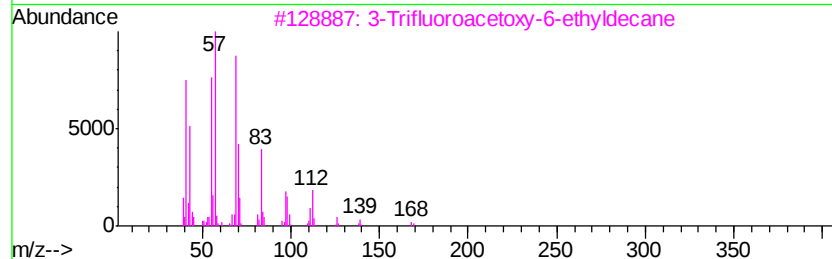
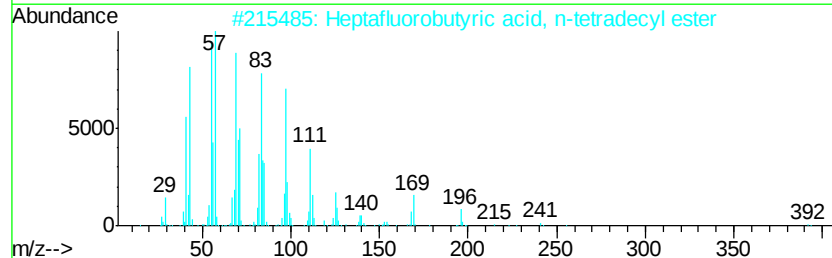
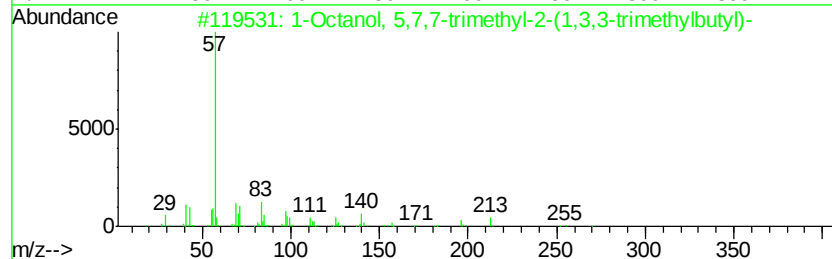
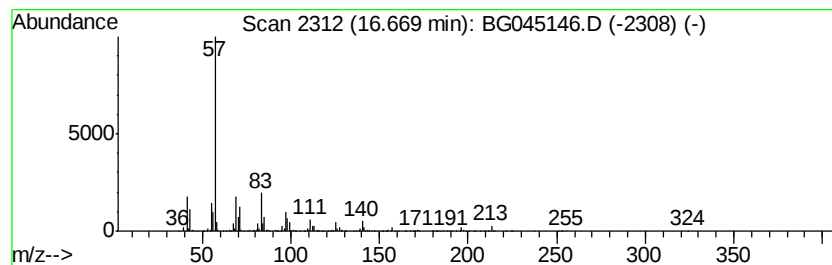
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	20.00 ng	2251070	Phenanthrene-d10	17.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	58
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	47
3		3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	47
4		3-Propionyloxytridecane	256	C16H32O2	1000245-62-5	47
5		Octacosanol	410	C28H58O	000557-61-9	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
Data File : BG045146.D
Acq On : 23 Apr 2020 17:50
Operator : CG/JU
Sample : L2326-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

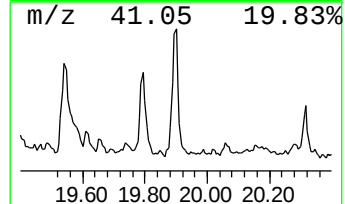
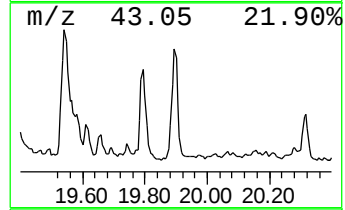
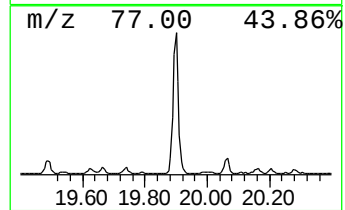
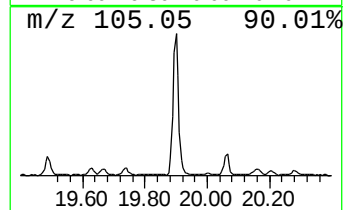
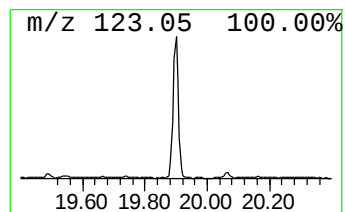
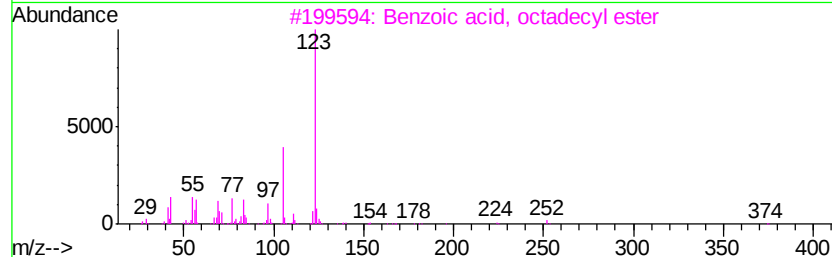
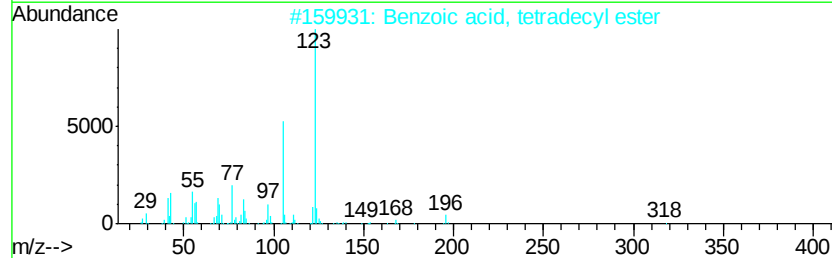
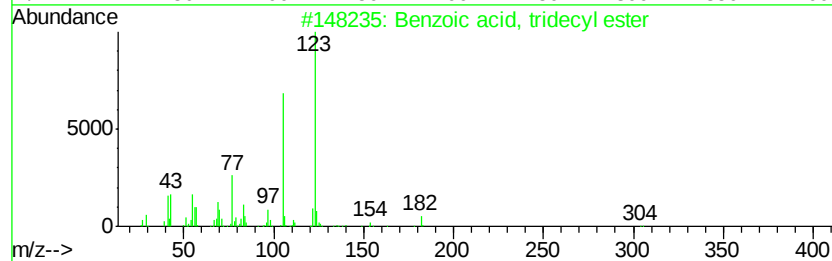
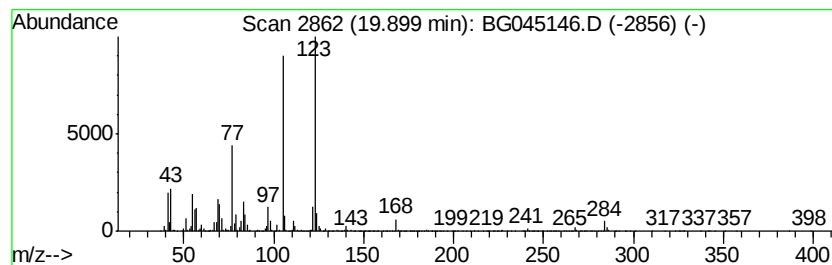
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzoic acid, tridecyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	15.98 ng	2231560	Chrysene-d12	21.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	83
2		Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	74
3		Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	68
4		Benzoic acid, eicosyl ester	402	C27H46O2	1000340-23-3	64
5		Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
Data File : BG045146.D
Acq On : 23 Apr 2020 17:50
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Sample : L2326-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

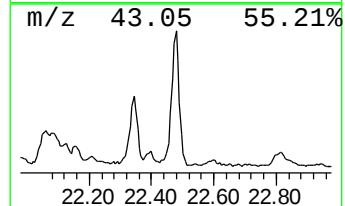
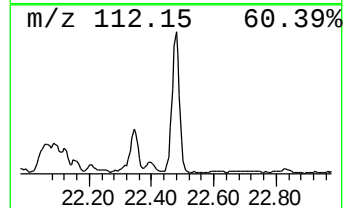
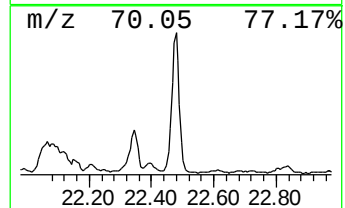
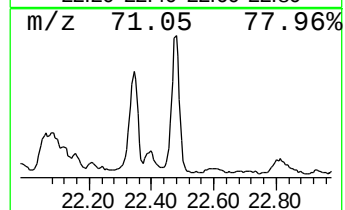
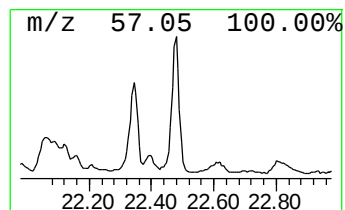
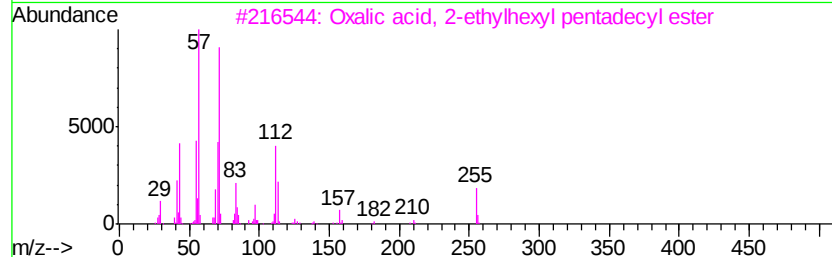
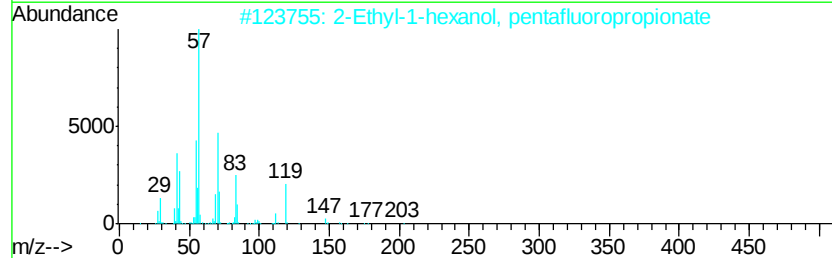
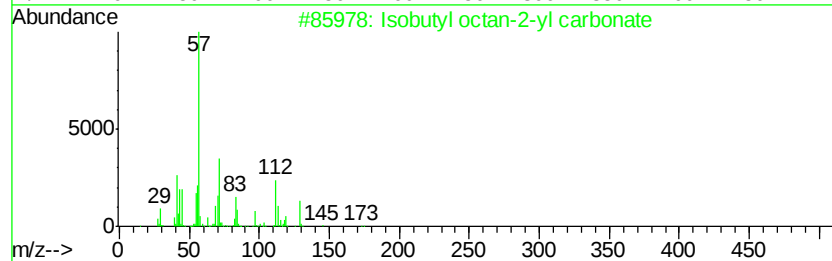
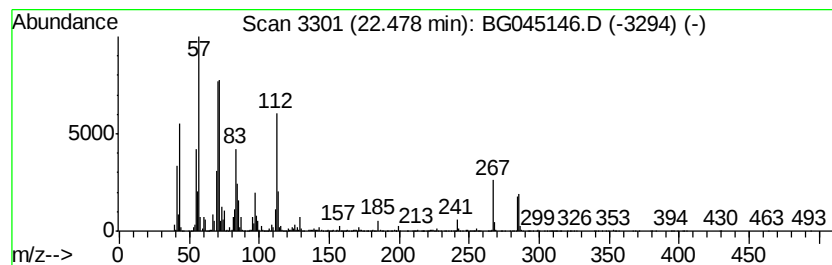
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Isobutyl octan-2-yl carbonate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	20.00 ng	2792080	Chrysene-d12	21.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	53
2		2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	43
3		Oxalic acid, 2-ethylhexyl pentad...	412	C25H48O4	1000309-39-8	43
4		Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	38
5		Formic acid, 2-ethylhexyl ester	158	C9H18O2	1000368-94-7	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
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 Sample : L2326-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, 1-e...	8.28	20.0	ng	216432000	1	8.00	216432000	20.0
Hexanoic acid, 2-...	9.87	44.8	ng	48418600	2	10.82	21614200	20.0
Octanoic acid	10.67	20.0	ng	21614200	2	10.82	21614200	20.0
n-Decanoic acid	13.10	16.4	ng	13207000	3	14.65	16108600	20.0
Dodecanoic acid	15.18	20.0	ng	16108600	3	14.65	16108600	20.0
2-Decanol, propan...	16.62	34.0	ng	3824000	4	17.39	2251070	20.0
1-Octanol, 5,7,7-...	16.67	20.0	ng	2251070	4	17.39	2251070	20.0
Benzoic acid, tri...	19.90	16.0	ng	2231560	5	21.65	2792080	20.0
Isobutyl octan-2-...	22.48	20.0	ng	2792080	5	21.65	2792080	20.0