

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
 Data File : BM027182.D
 Acq On : 21 Aug 2020 22:41
 Operator : JU/CG
 Sample : L3729-17
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-4-(3-4)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BM082120.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	5.234	376	382	391	rBV	1390441	1991372	38.83%	5.887%
2	6.798	641	648	663	rBV	1430148	2138307	41.70%	6.321%
3	7.610	779	786	794	rVB	468712	741944	14.47%	2.193%
4	8.757	973	981	989	rBV	888287	1476587	28.79%	4.365%
5	10.381	1250	1257	1264	rBV	586432	978347	19.08%	2.892%
6	12.869	1673	1680	1687	rBV	2341615	3313064	64.61%	9.794%
7	13.710	1817	1823	1833	rVB	219916	315719	6.16%	0.933%
8	13.969	1862	1867	1870	rBV	34704	56337	1.10%	0.167%
9	14.251	1908	1915	1923	rBV	916855	1330764	25.95%	3.934%
10	14.698	1981	1991	1999	rBV2	194378	385594	7.52%	1.140%
11	15.739	2162	2168	2180	rBV	1891275	2688177	52.42%	7.946%
12	16.198	2241	2246	2249	rBV	153459	247486	4.83%	0.732%
13	16.245	2249	2254	2259	rVV2	400428	815562	15.90%	2.411%
14	16.292	2259	2262	2276	rVV	249779	453909	8.85%	1.342%
15	16.427	2280	2285	2295	rVB2	97727	166608	3.25%	0.492%
16	16.792	2343	2347	2355	rVB3	85657	148916	2.90%	0.440%
17	16.951	2369	2374	2377	rBV	134594	202729	3.95%	0.599%
18	16.992	2377	2381	2386	rVV	1089686	1565398	30.53%	4.627%
19	17.033	2386	2388	2396	rVB	115800	151124	2.95%	0.447%
20	17.504	2466	2468	2475	rVB	33273	53844	1.05%	0.159%
21	17.804	2515	2519	2524	rBV	50993	85307	1.66%	0.252%
22	17.915	2533	2538	2556	rBV	964434	1465540	28.58%	4.332%
23	19.056	2728	2732	2735	rBV	328093	444912	8.68%	1.315%
24	19.209	2753	2758	2769	rBV	726505	1039604	20.27%	3.073%
25	19.421	2790	2794	2805	rVB	357477	537137	10.47%	1.588%
26	19.639	2826	2831	2843	rVB	4355467	5128112	100.00%	15.159%
27	20.345	2945	2951	2956	rBV	1061507	1294741	25.25%	3.827%
28	20.927	3046	3050	3056	rBV2	553894	757275	14.77%	2.239%
29	21.192	3090	3095	3099	rBV	1498207	2066641	40.30%	6.109%
30	23.380	3461	3467	3473	rBV	1019930	1788126	34.87%	5.286%

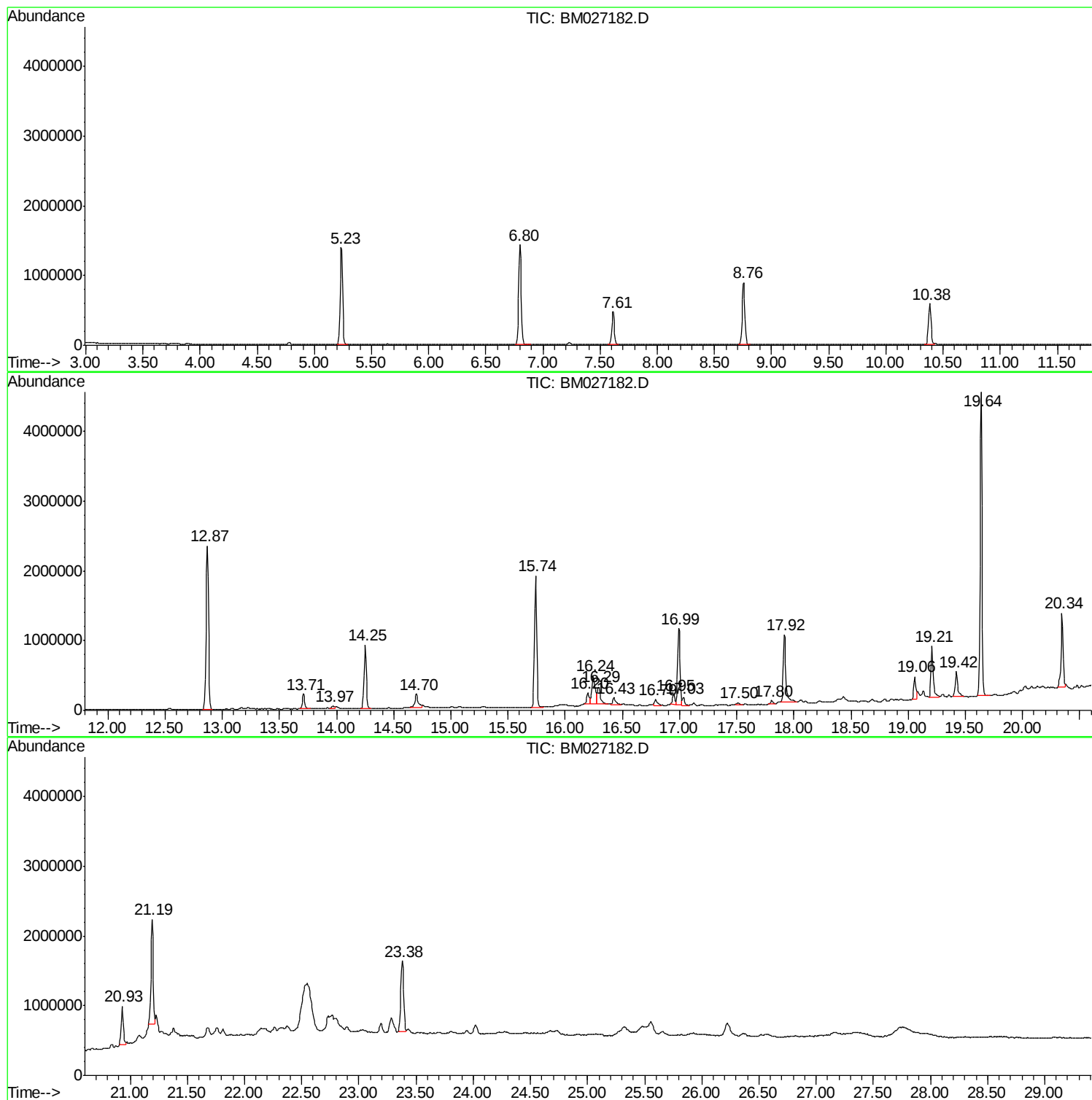
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COMP-4-(3-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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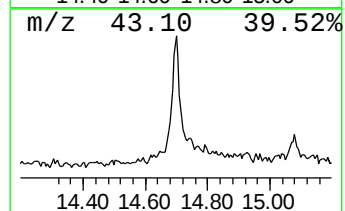
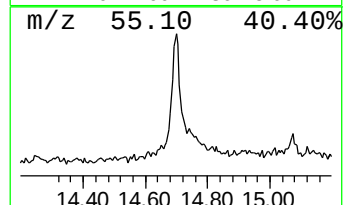
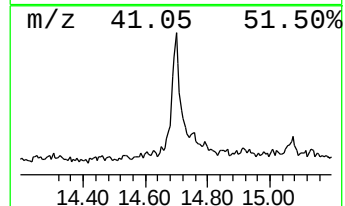
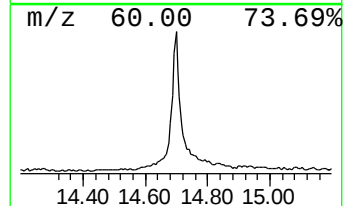
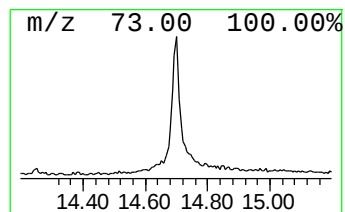
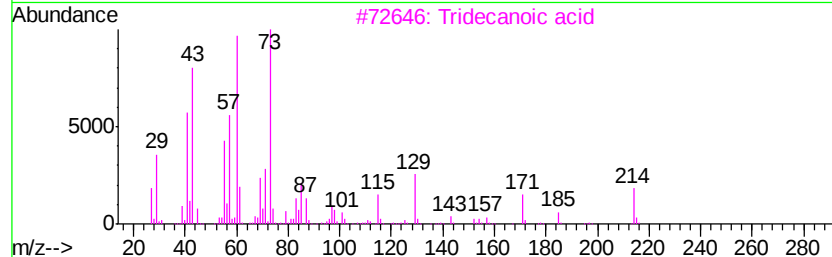
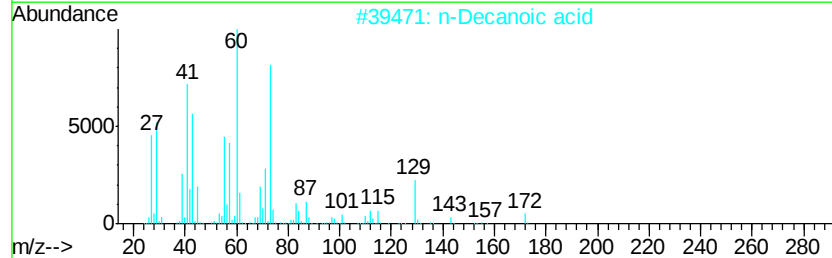
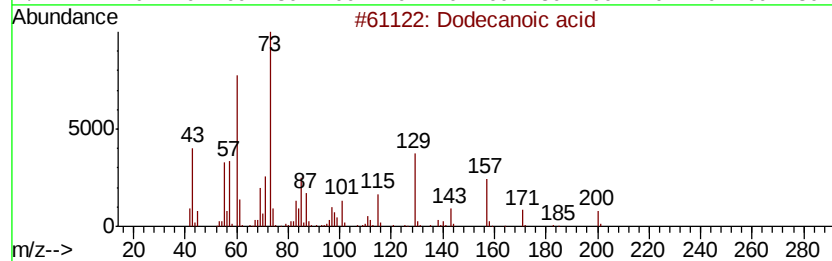
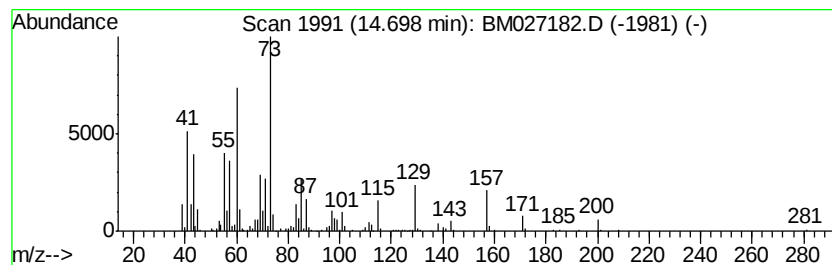
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.70	5.80 ng	385594	Acenaphthene-d10		14.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	96
2	n-Decanoic acid	172	C10H20O2	000334-48-5	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52



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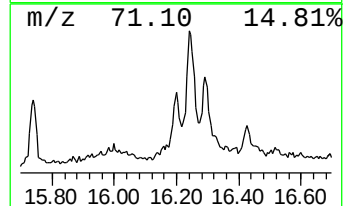
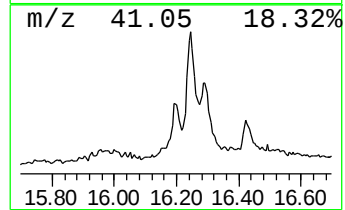
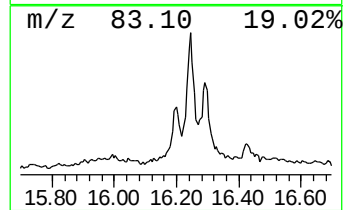
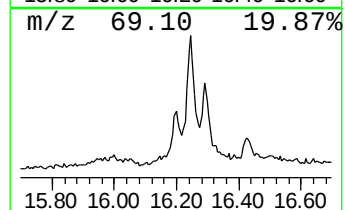
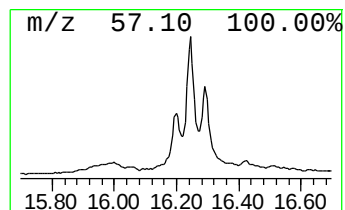
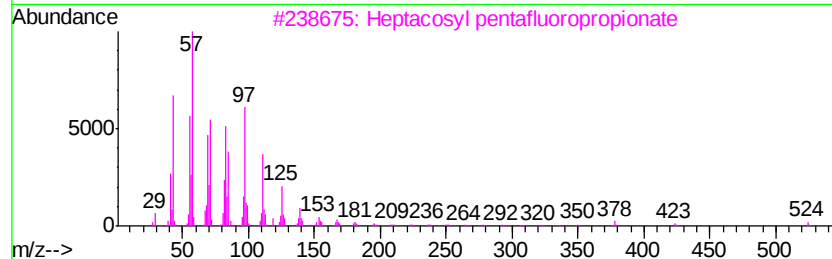
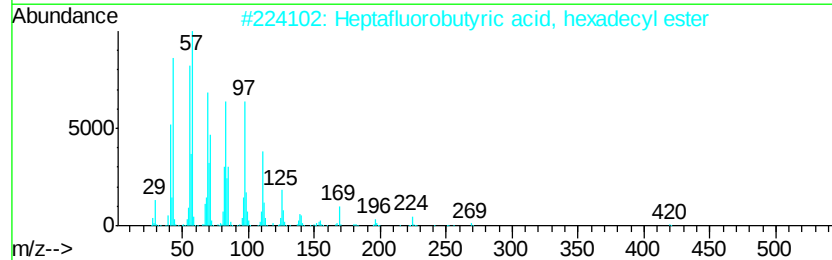
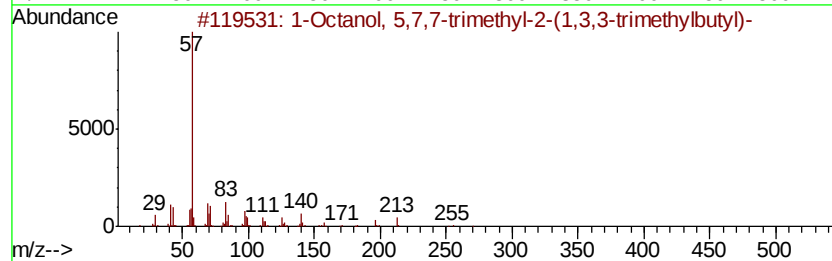
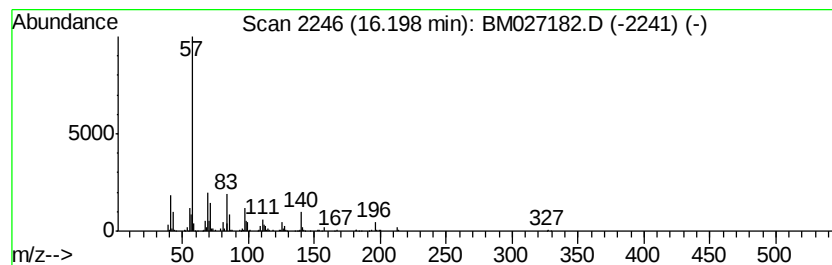
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Peak Number 2 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.20	3.16 ng	247486	Phenanthrene-d10	16.99		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	50	
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	49	
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	47	
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	47	
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	47	



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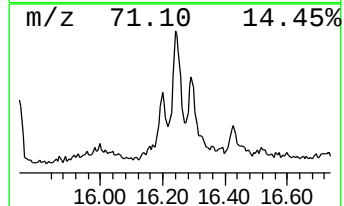
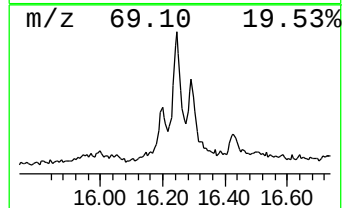
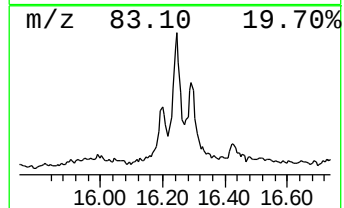
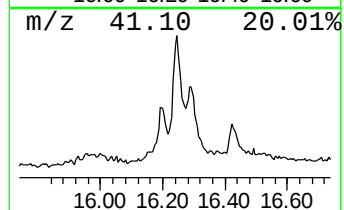
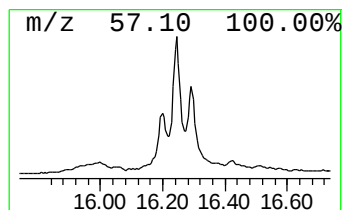
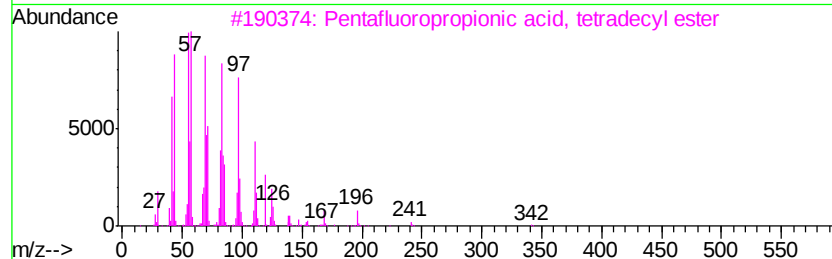
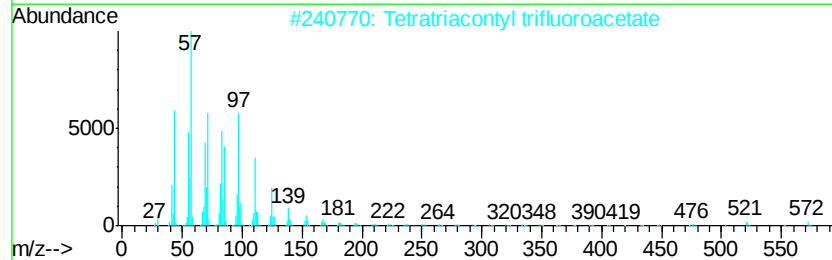
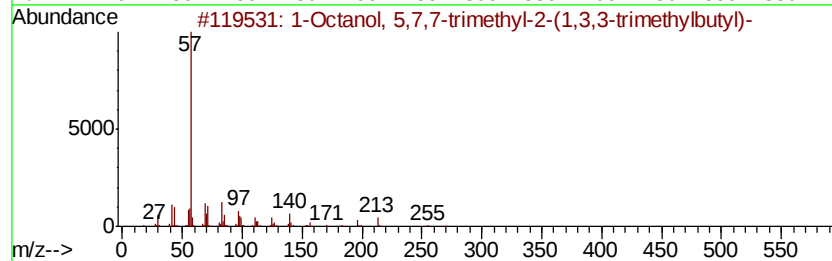
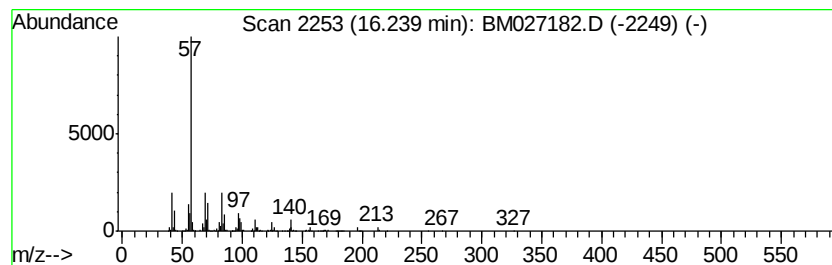
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Peak Number 3 unknown16.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	10.42 ng	815562	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	72
2		Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	47
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	47
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47
5		17-Pentatriacontene	491	C35H70	006971-40-0	47



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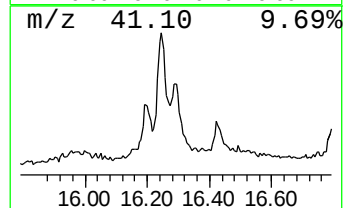
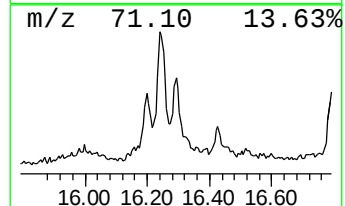
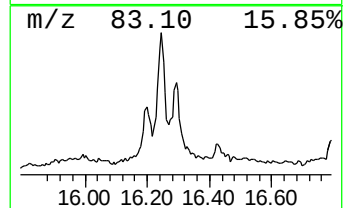
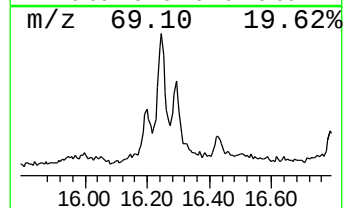
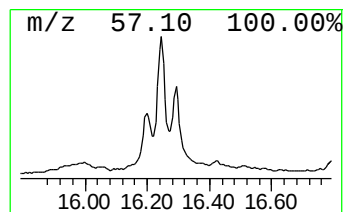
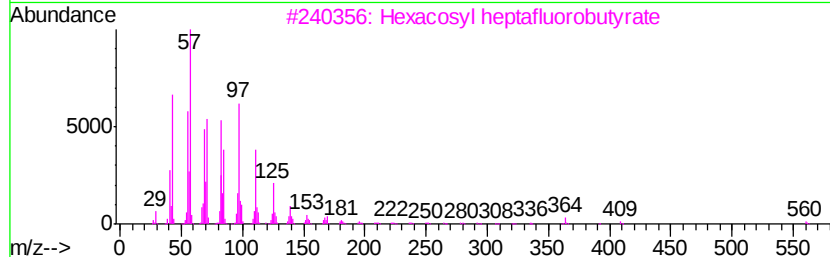
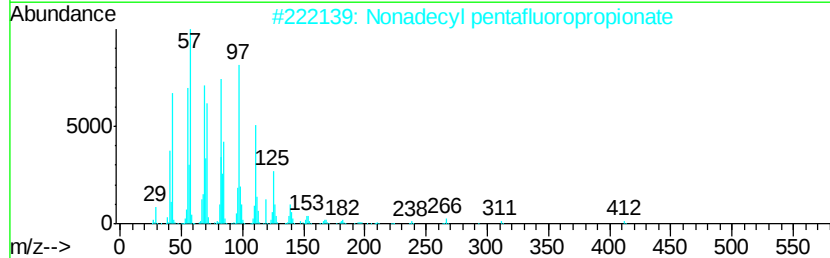
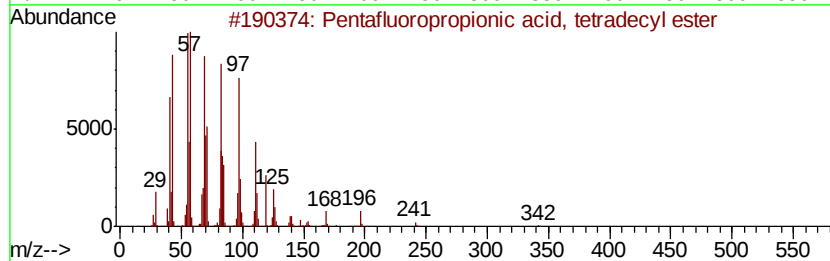
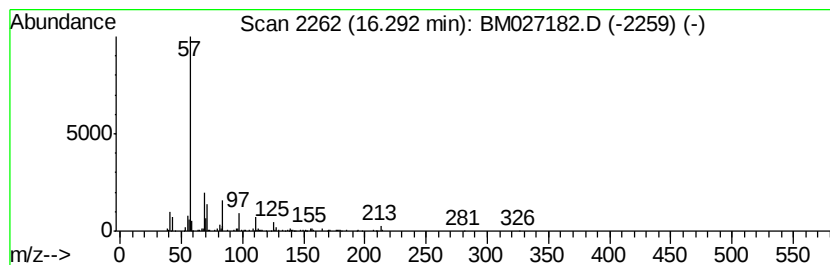
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.29	5.80 ng	453909	Phenanthrene-d10	16.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	58
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	53
3	Hexacosyl heptafluorobutyrte	578	C30H53F7O2	1000351-83-3	53
4	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	53
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	53



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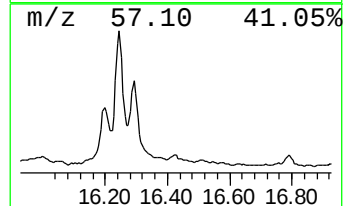
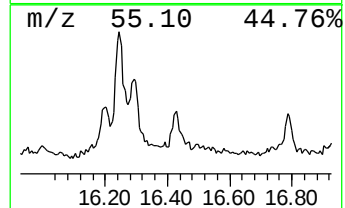
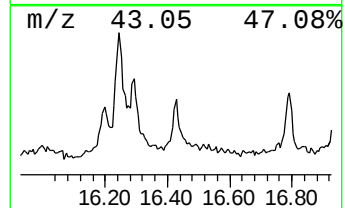
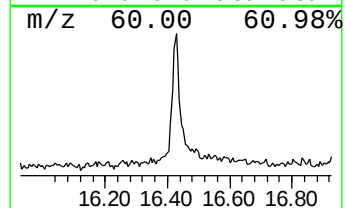
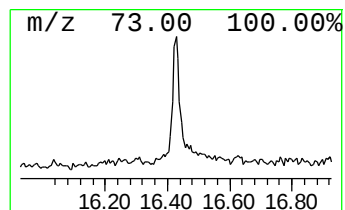
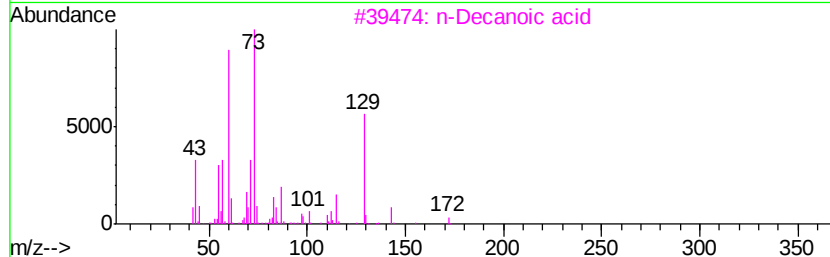
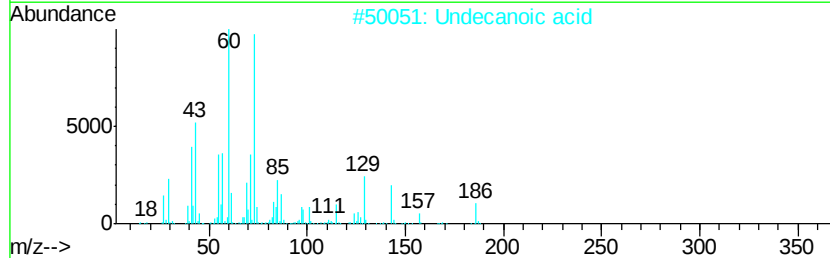
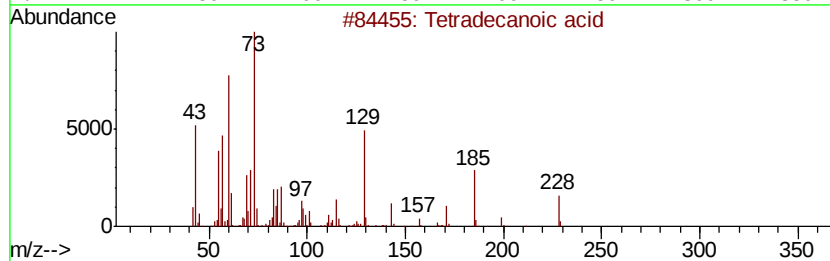
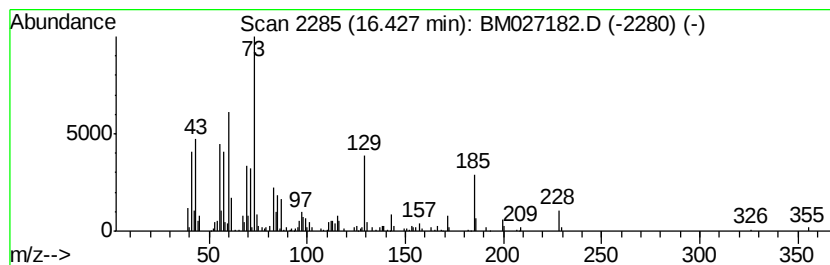
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Peak Number 5 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.13 ng	166608	Phenanthrene-d10	16.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2		Undecanoic acid	186	C11H22O2	000112-37-8	55
3		n-Decanoic acid	172	C10H20O2	000334-48-5	49
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
5		Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	47



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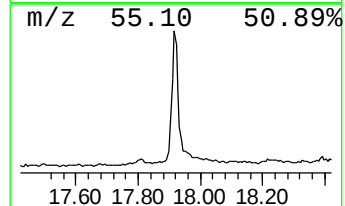
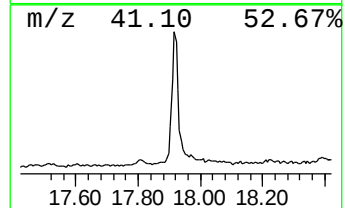
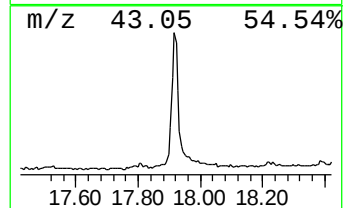
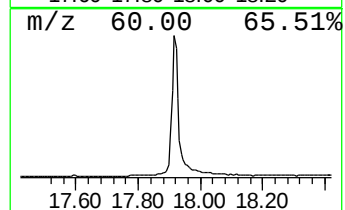
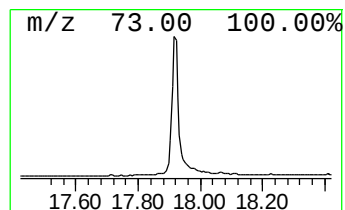
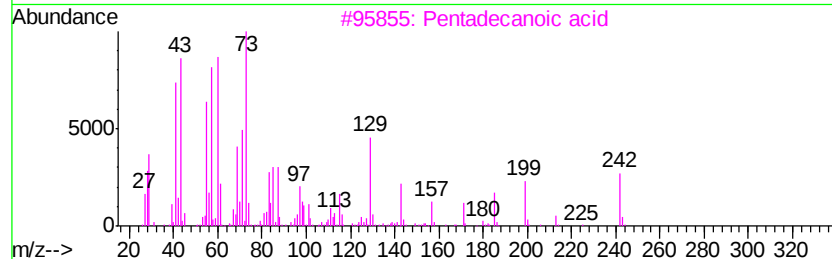
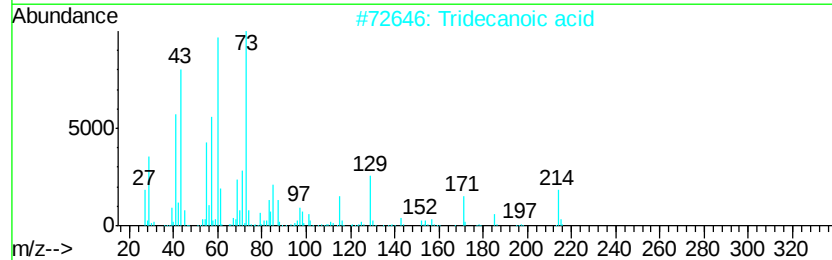
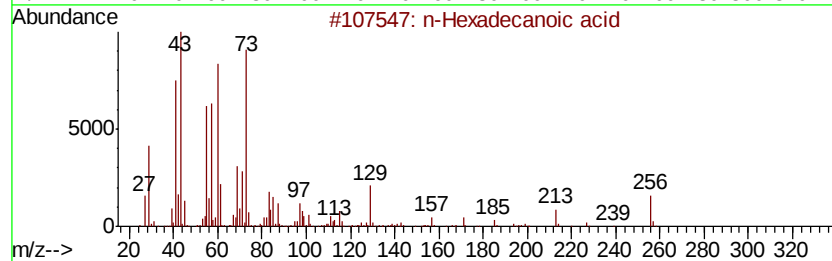
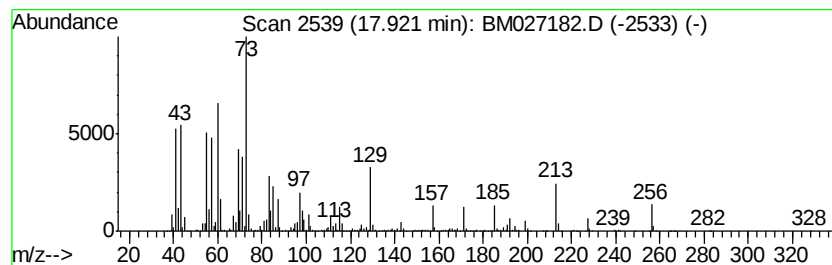
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	18.72 ng	1465540	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	58
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027182.D
Acq On : 21 Aug 2020 22:41
Operator : JU/CG
Sample : L3729-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-4-(3-4)

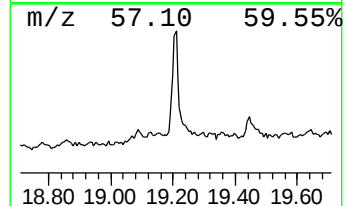
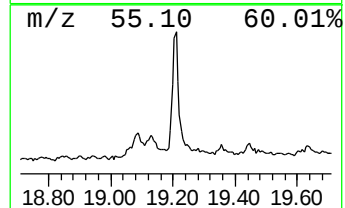
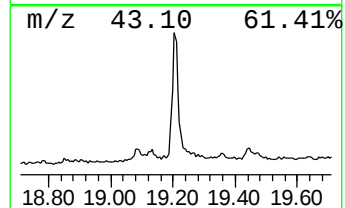
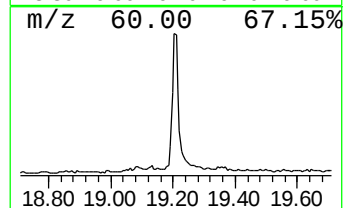
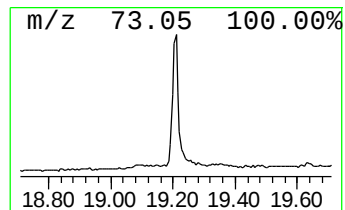
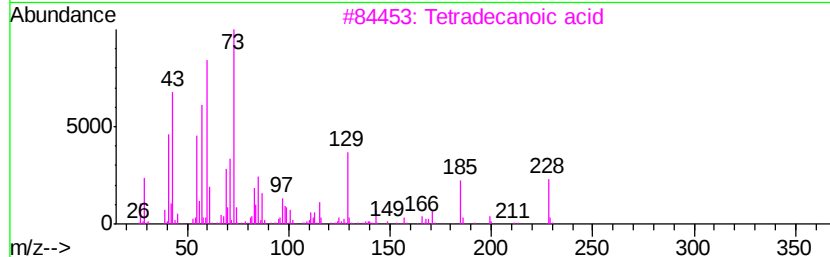
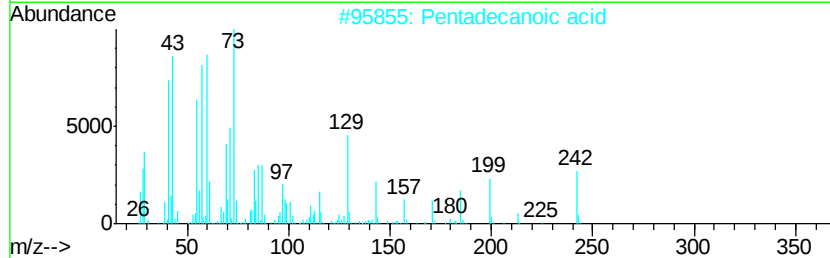
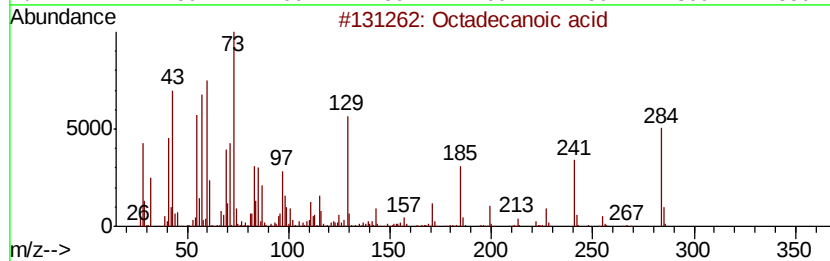
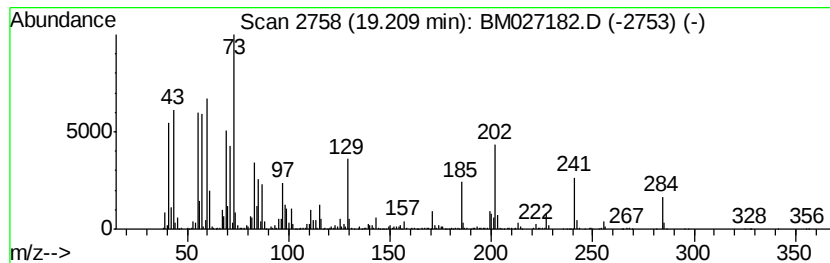
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.21	10.06 ng	1039600	Chrysene-d12	21.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027182.D
Acq On : 21 Aug 2020 22:41
Operator : JU/CG
Sample : L3729-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-4-(3-4)

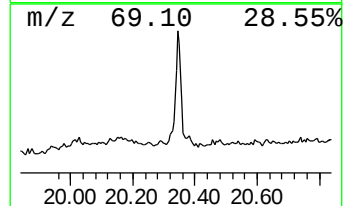
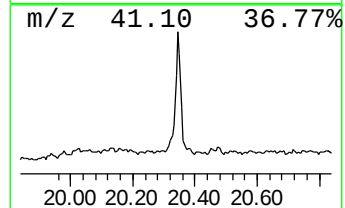
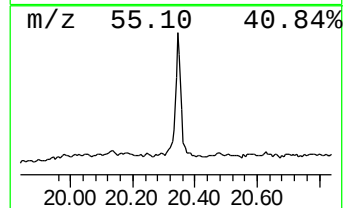
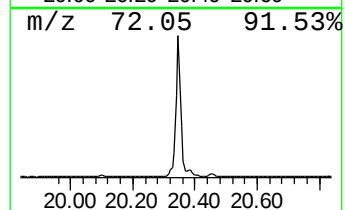
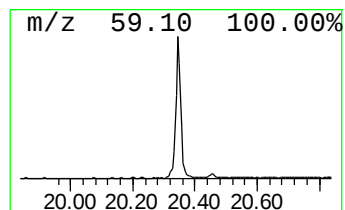
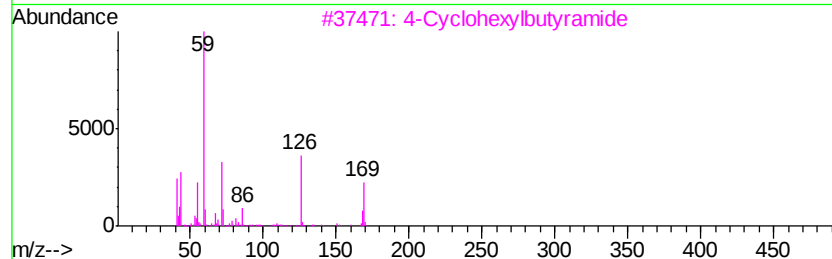
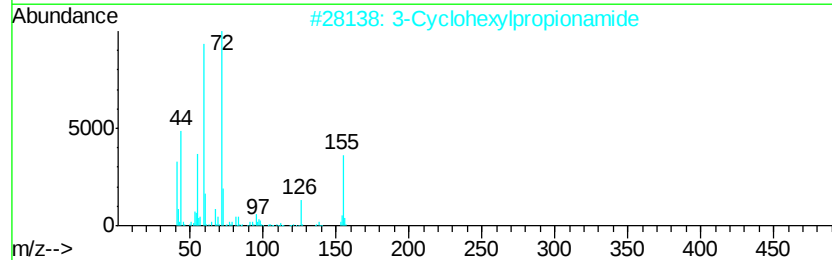
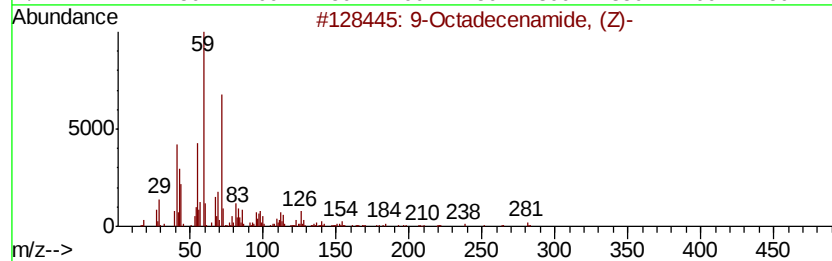
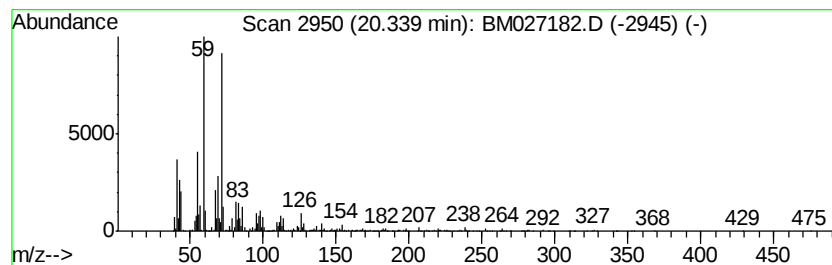
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.34	12.53 ng	1294740	Chrysene-d12	21.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	50
3		4-Cyclohexylbutyramide	169	C10H19NO	004441-62-7	38
4		Octanamide	143	C8H17NO	000629-01-6	38
5		Hexadecanamide	255	C16H33NO	000629-54-9	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
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Acq On : 21 Aug 2020 22:41
Operator : JU/CG
Sample : L3729-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

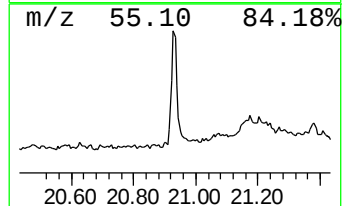
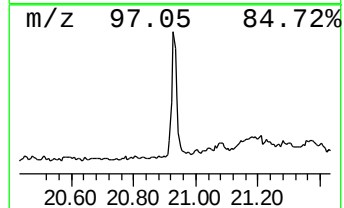
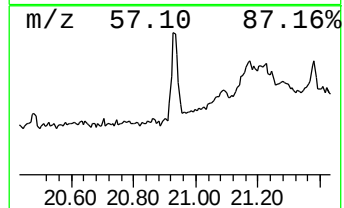
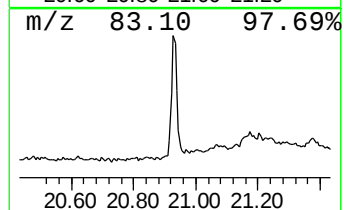
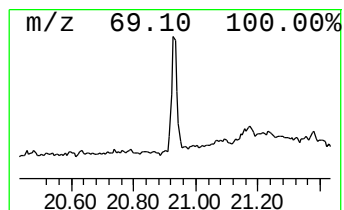
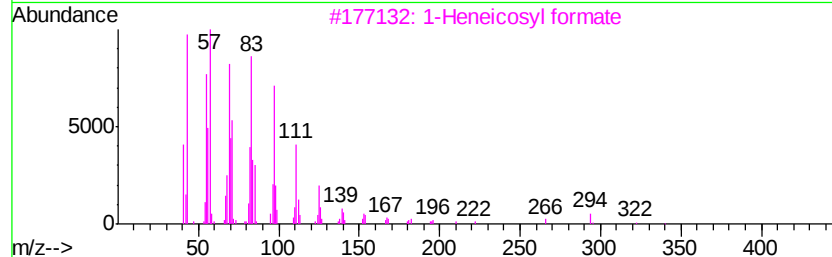
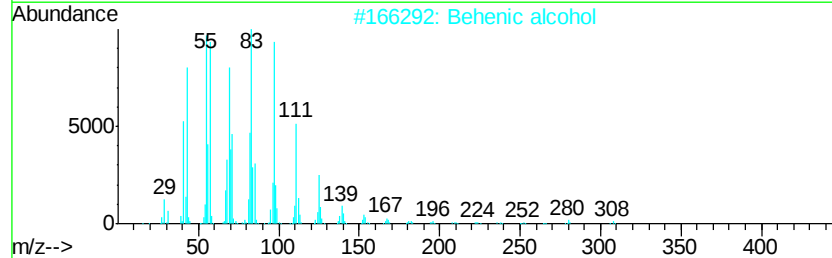
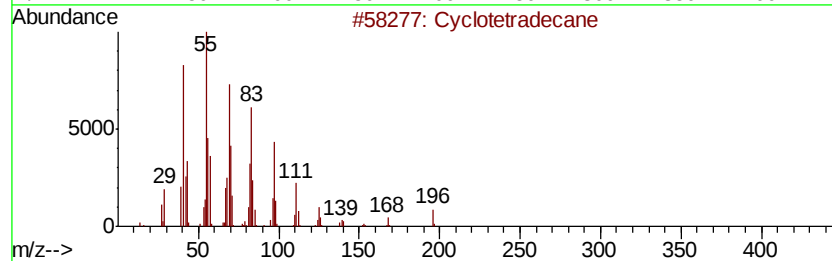
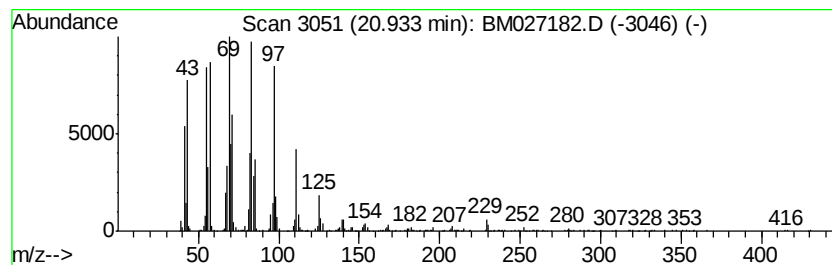
Instrument :
BNA_M
ClientSampleId :
COMP-4-(3-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.93	7.33 ng	757275	Chrysene-d12	21.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	98
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5	1-Hexadecanol	242	C16H34O	036653-82-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082120\
Data File : BM027182.D
Acq On : 21 Aug 2020 22:41
Operator : JU/CG
Sample : L3729-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-4-(3-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.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
Dodecanoic acid	14.70	5.8 ng		385594	3	14.25	1330760	20.0
1-Octanol, 5,7,7-...	16.20	3.2 ng		247486	4	16.99	1565400	20.0
unknown16.24	16.24	10.4 ng		815562	4	16.99	1565400	20.0
Pentafluoropropio...	16.29	5.8 ng		453909	4	16.99	1565400	20.0
Tetradecanoic acid	16.43	2.1 ng		166608	4	16.99	1565400	20.0
n-Hexadecanoic acid	17.92	18.7 ng		1465540	4	16.99	1565400	20.0
Octadecanoic acid	19.21	10.1 ng		1039600	5	21.19	2066640	20.0
9-Octadecenamide,...	20.34	12.5 ng		1294740	5	21.19	2066640	20.0
Cyclotetradecane	20.93	7.3 ng		757275	5	21.19	2066640	20.0