

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100819\
 Data File : BF117342.D
 Acq On : 8 Oct 2019 16:05
 Operator : JU
 Sample : K5239-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STONE-COMP

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_F\METHODS\8270-BF091319.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	5.422	564	567	592	rBV	669578	791817	62.03%	6.481%
2	6.445	737	741	759	rBV	751342	899025	70.43%	7.359%
3	6.575	759	763	772	rVV	1053607	931394	72.97%	7.624%
4	6.798	798	801	817	rVB	249546	229584	17.99%	1.879%
5	6.957	824	828	846	rBV	763298	729287	57.13%	5.970%
6	7.363	893	897	916	rBV	463813	555623	43.53%	4.548%
7	8.081	1016	1019	1030	rBV	257998	280292	21.96%	2.294%
8	9.157	1198	1202	1218	rBV	1133668	1153636	90.38%	9.443%
9	9.551	1266	1269	1276	rBV	59122	54494	4.27%	0.446%
10	9.833	1313	1317	1332	rBB	365214	350319	27.44%	2.868%
11	10.627	1448	1452	1461	rBV	541889	576555	45.17%	4.719%
12	11.322	1566	1570	1580	rBV	331500	356888	27.96%	2.921%
13	11.851	1654	1660	1673	rBV	378576	616546	48.30%	5.047%
14	12.498	1764	1770	1774	rBV3	14837	23505	1.84%	0.192%
15	12.545	1774	1778	1786	rBV6	19196	54005	4.23%	0.442%
16	12.633	1788	1793	1805	rBV	341316	507487	39.76%	4.154%
17	12.904	1835	1839	1842	rBV	1396211	1276453	100.00%	10.448%
18	13.133	1875	1878	1881	rBV5	11541	16604	1.30%	0.136%
19	13.468	1932	1935	1938	rBV4	20510	20547	1.61%	0.168%
20	13.815	1988	1994	2004	rVB4	93674	205862	16.13%	1.685%
21	13.968	2016	2020	2028	rBV	323587	361521	28.32%	2.959%
22	14.115	2041	2045	2048	rBV	101443	99575	7.80%	0.815%
23	14.421	2093	2097	2101	rBV	175709	174420	13.66%	1.428%
24	14.721	2144	2148	2151	rBV	249401	247163	19.36%	2.023%
25	14.792	2158	2160	2163	rVB2	19713	16692	1.31%	0.137%
26	15.051	2199	2204	2210	rBV	397585	436749	34.22%	3.575%
27	15.421	2261	2267	2277	rVB2	364718	616965	48.33%	5.050%
28	15.833	2332	2337	2345	rVB	197244	311080	24.37%	2.546%
29	16.321	2414	2420	2428	rVB2	100599	178002	13.95%	1.457%
30	16.886	2512	2516	2524	rVB4	35115	76465	5.99%	0.626%
31	17.556	2626	2630	2637	rVB8	12775	27450	2.15%	0.225%
32	18.274	2743	2752	2757	rBV8	12972	40645	3.18%	0.333%

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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_F\METHODS\8270-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

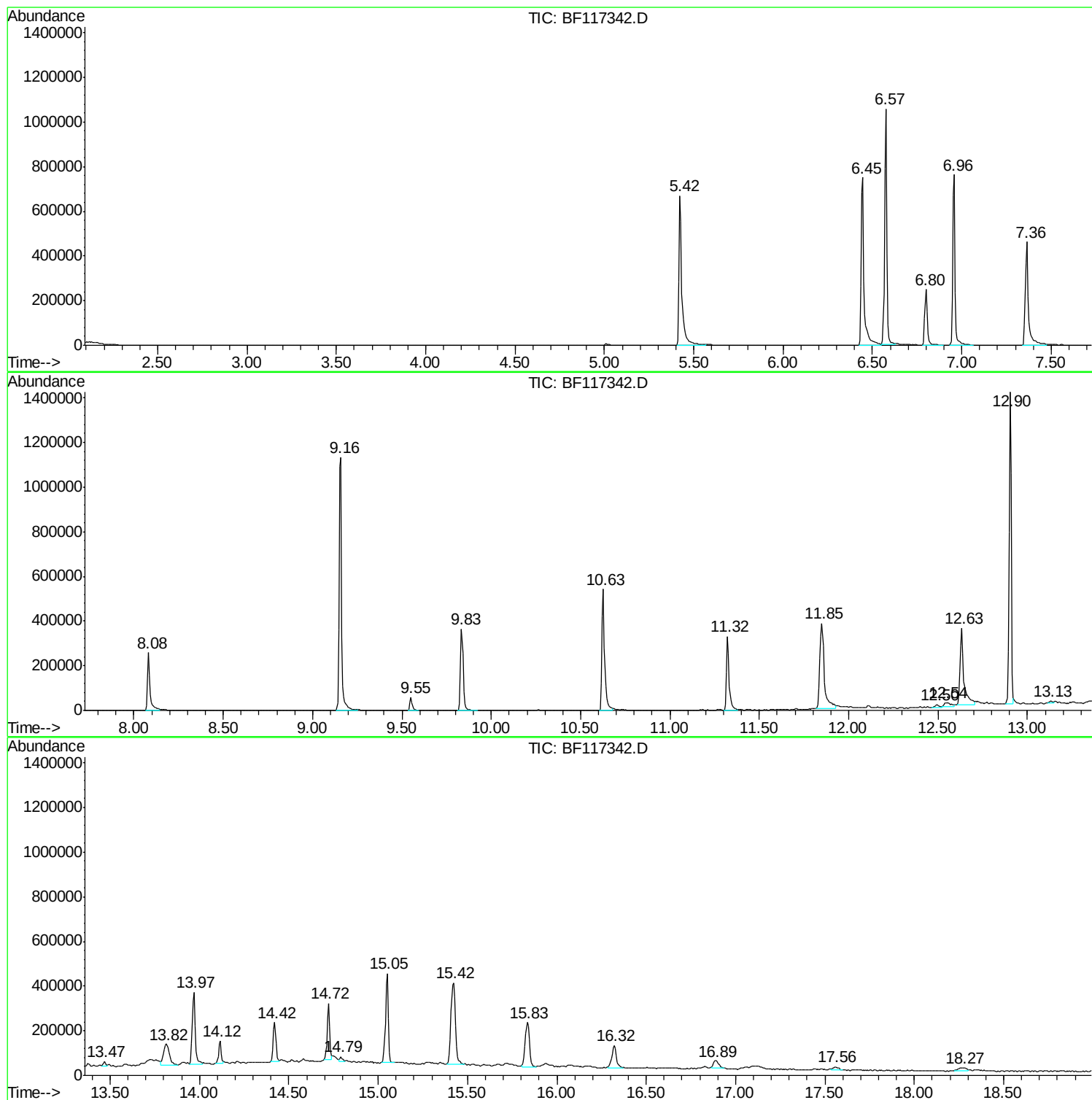
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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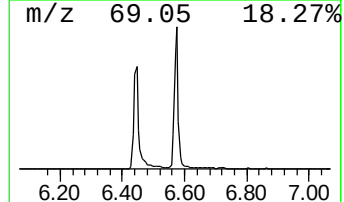
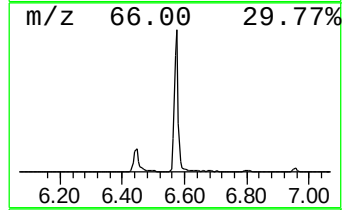
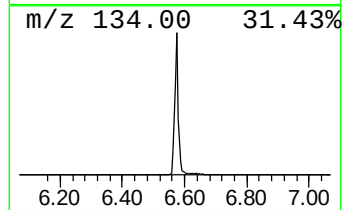
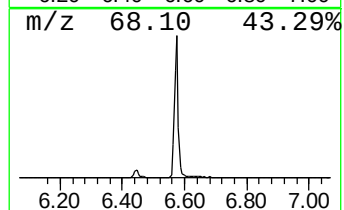
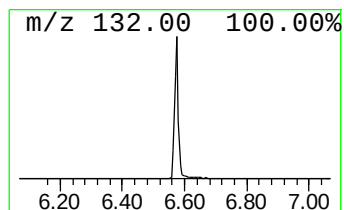
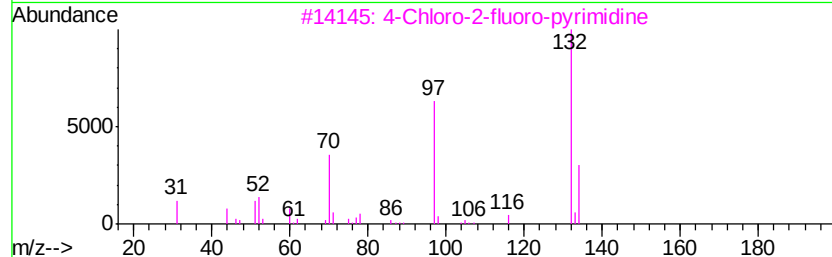
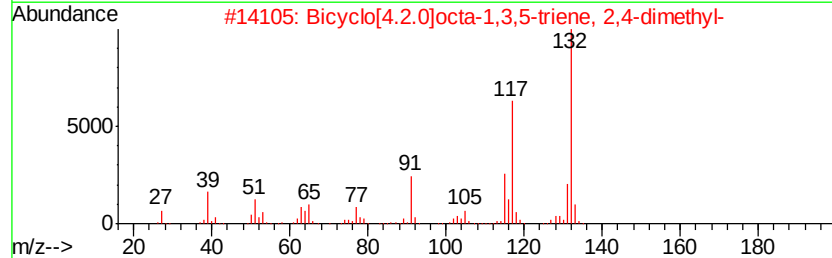
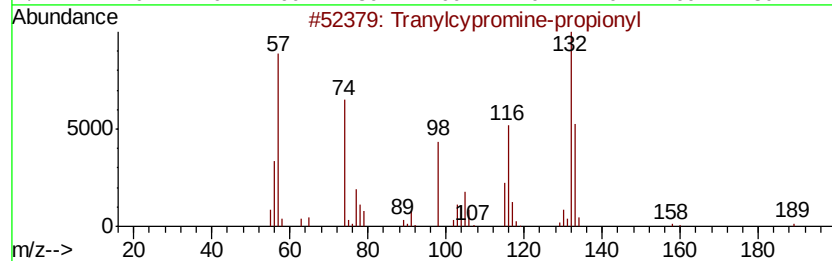
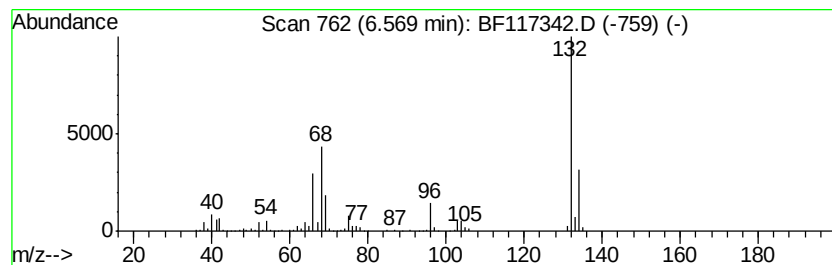
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	81.14 ng	931394	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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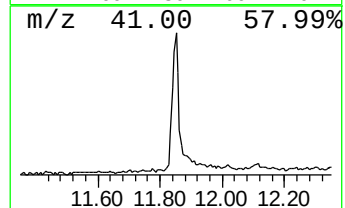
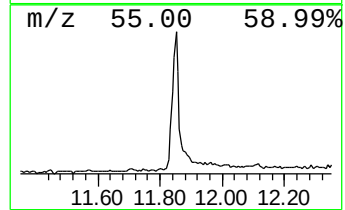
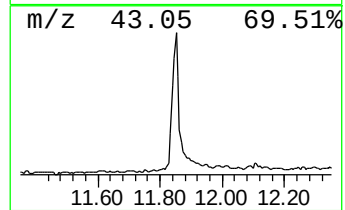
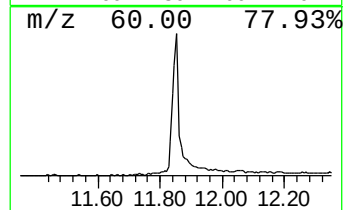
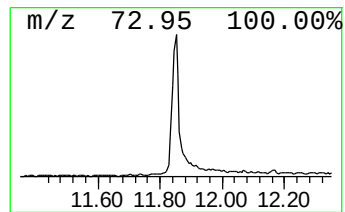
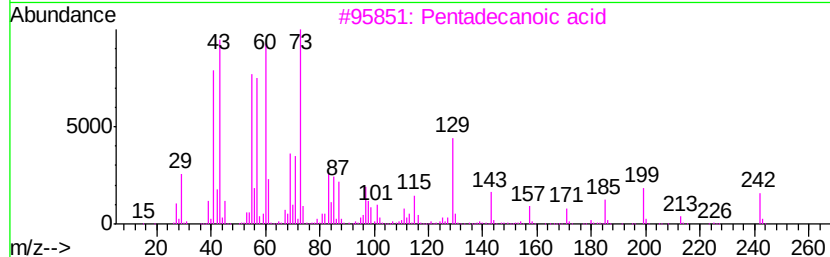
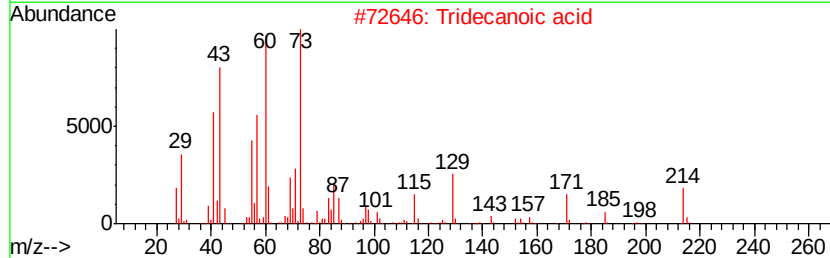
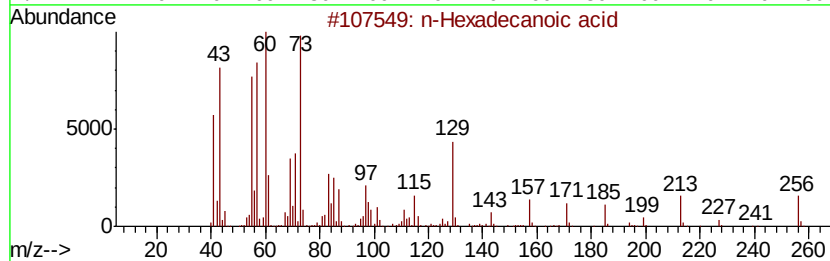
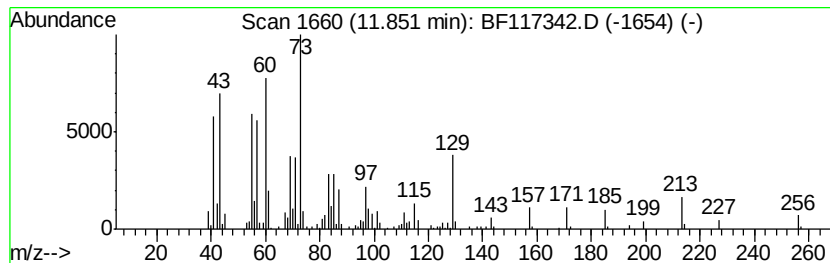
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	34.55 ng	616546	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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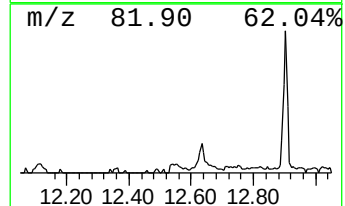
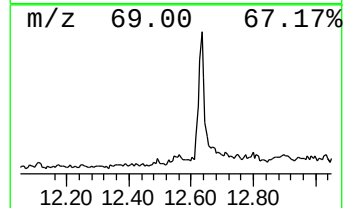
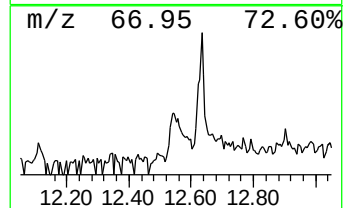
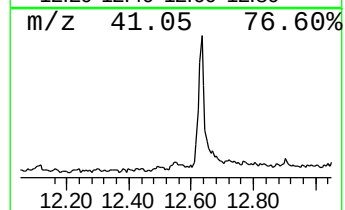
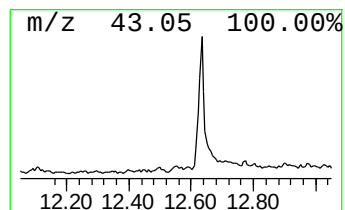
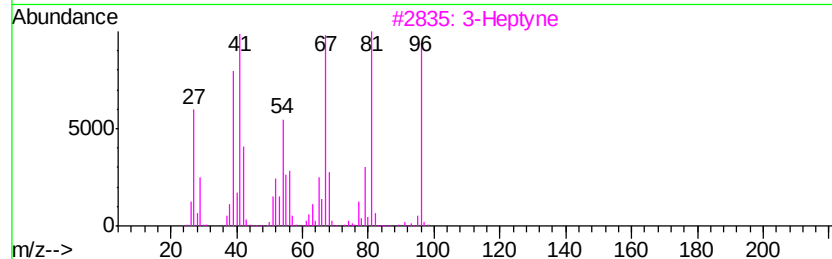
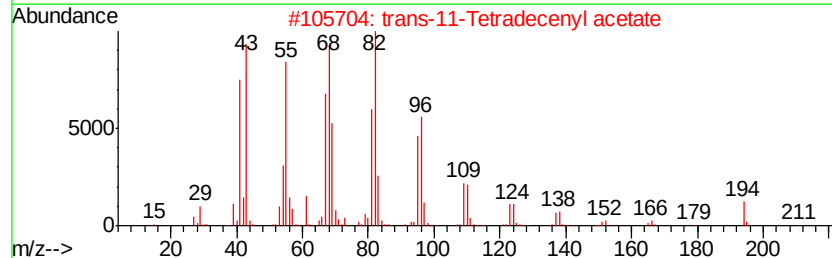
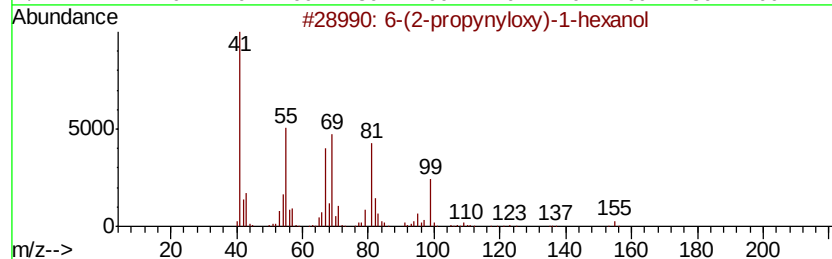
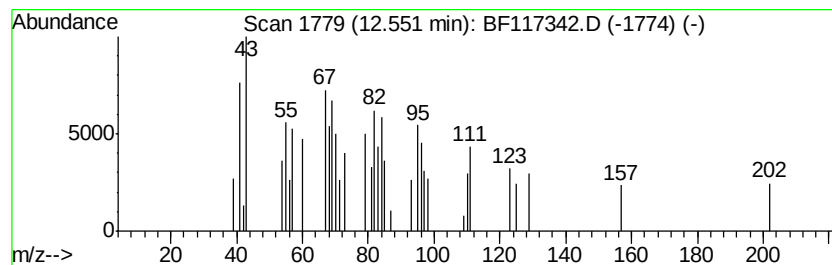
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.55 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.55	3.03 ng	54005	Phenanthrene-d10		11.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(2-propynyloxy)-1-hexanol			156	C9H16O2	058757-86-1	43
2	trans-11-Tetradecenyl acetate			254	C16H30O2	033189-72-9	38
3	3-Heptyne			96	C7H12	002586-89-2	30
4	6-Dodecyne			166	C12H22	006975-99-1	27
5	13-Tetradecene-11-yn-1-ol			208	C14H24O	1000131-00-4	27



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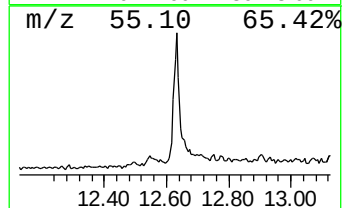
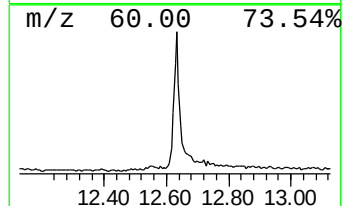
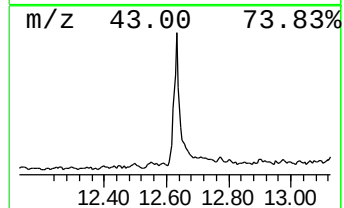
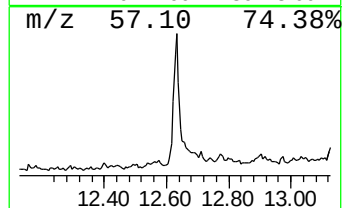
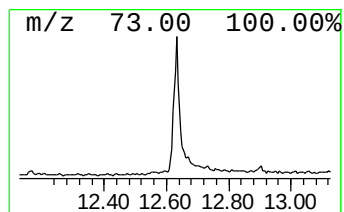
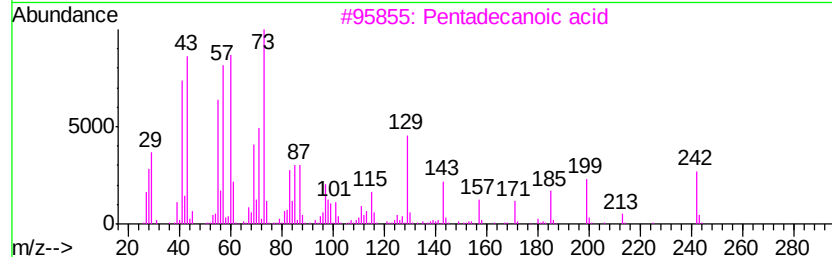
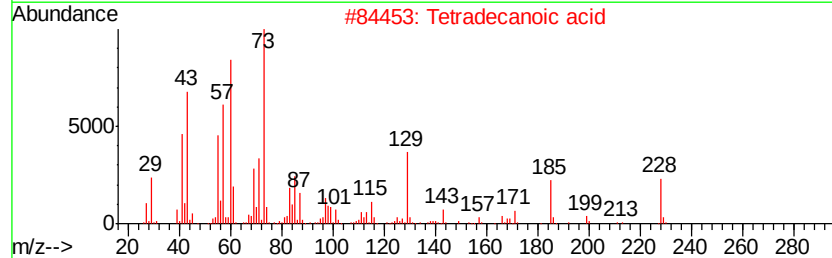
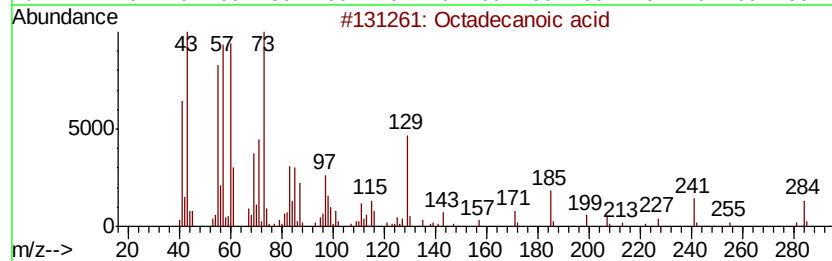
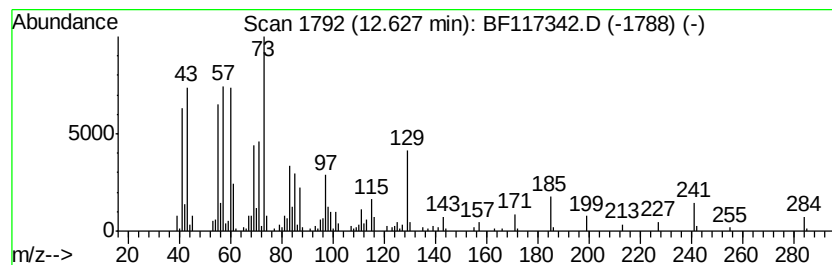
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	28.44 ng	507487	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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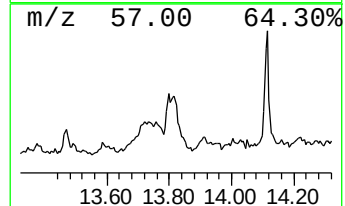
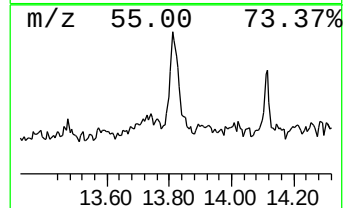
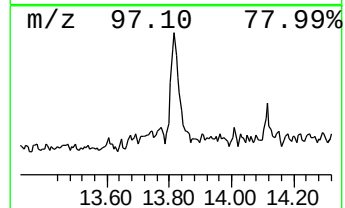
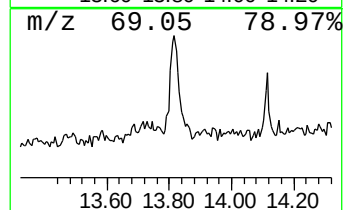
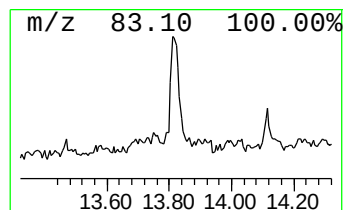
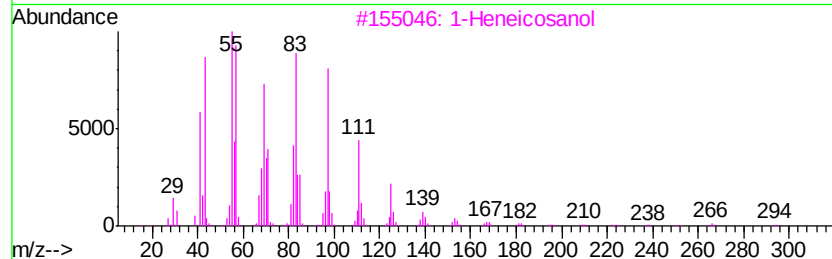
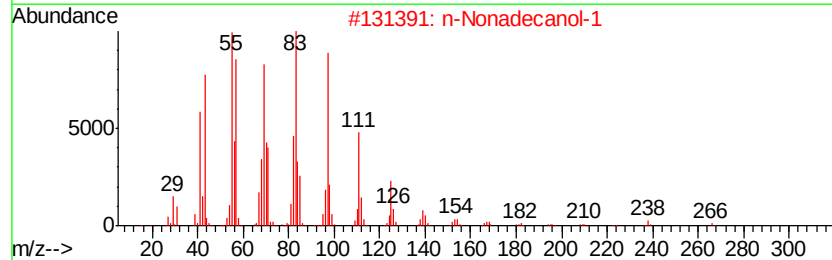
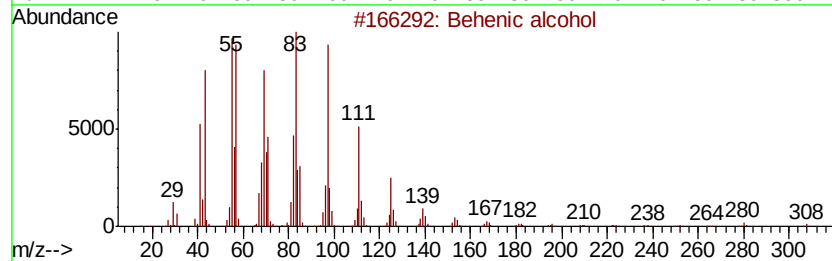
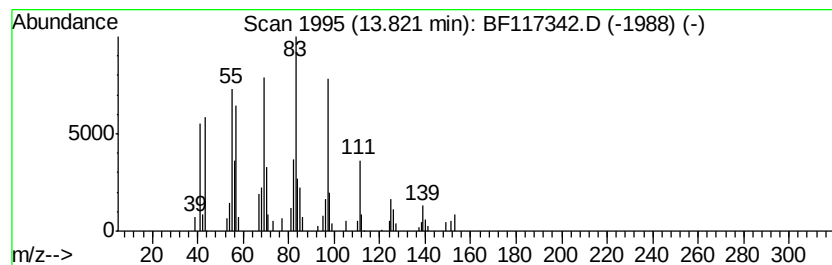
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	11.39 ng	205862	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	93
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	76
4		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	70
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	68



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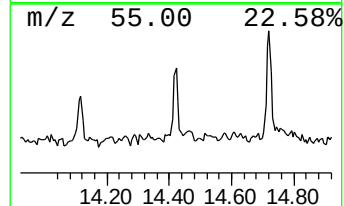
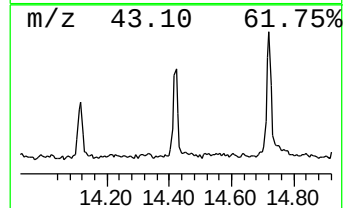
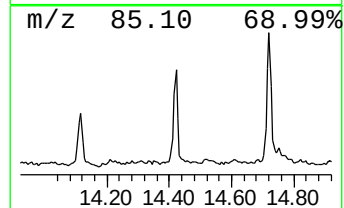
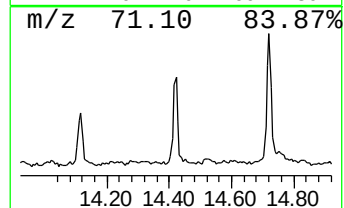
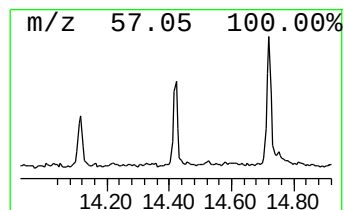
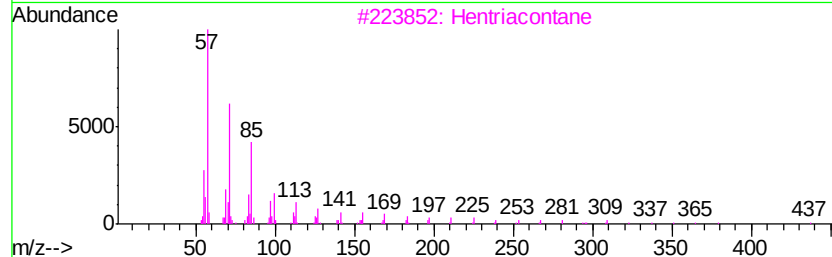
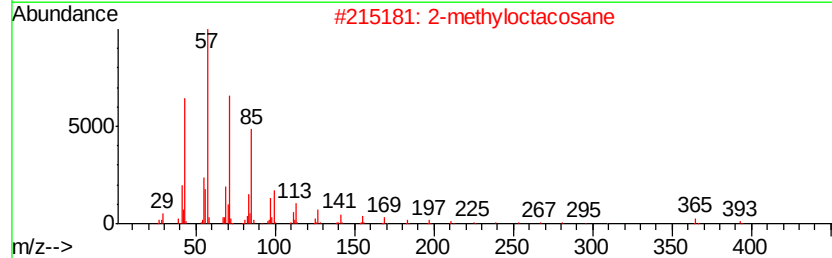
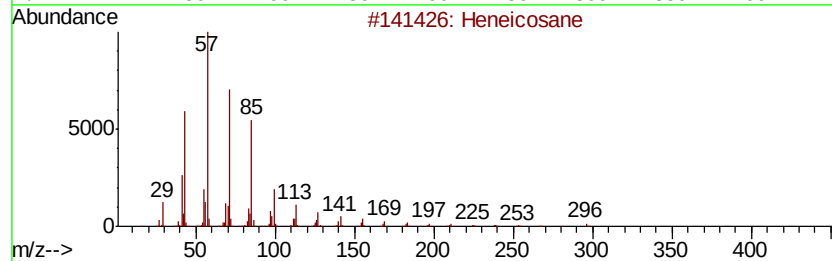
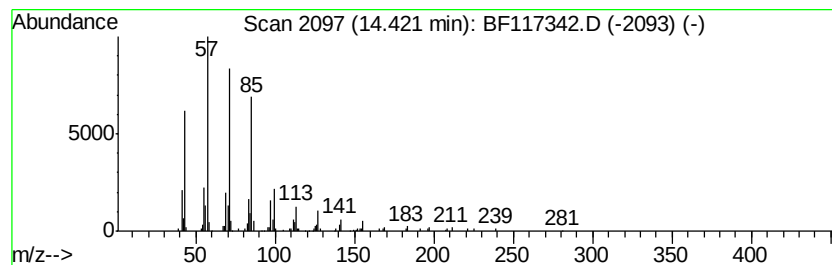
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	9.65 ng	174420	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Hentriacontane		437	C31H64	000630-04-6	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Hexacosane		366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100819\
Data File : BF117342.D
Acq On : 8 Oct 2019 16:05
Operator : JU
Sample : K5239-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

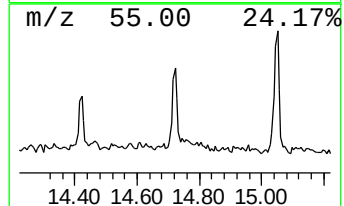
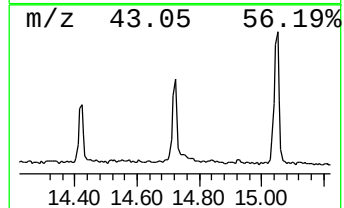
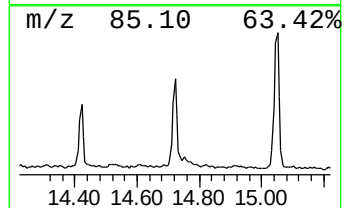
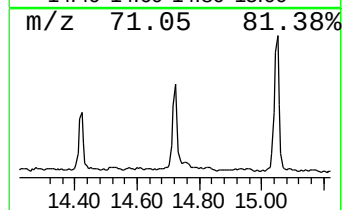
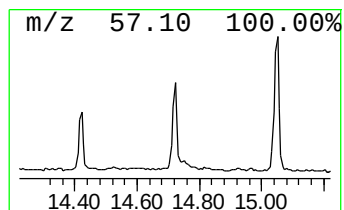
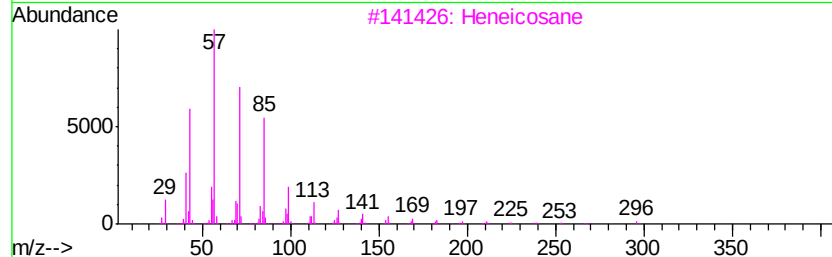
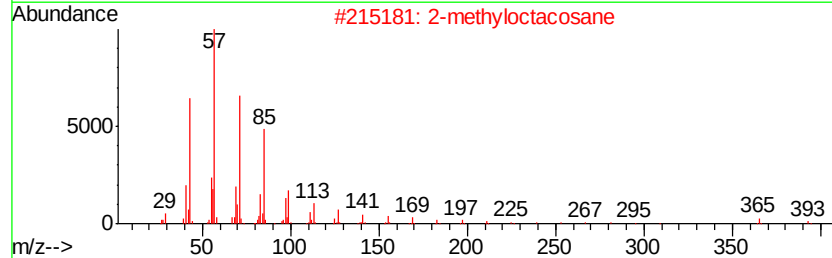
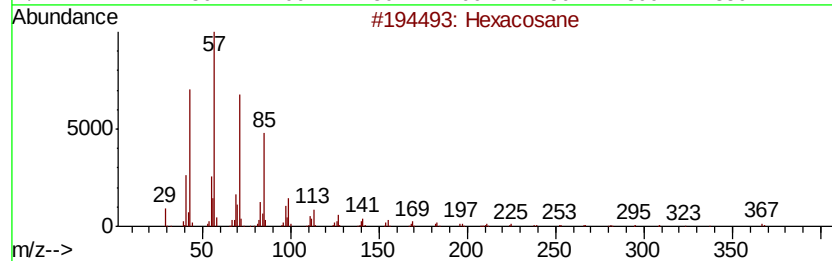
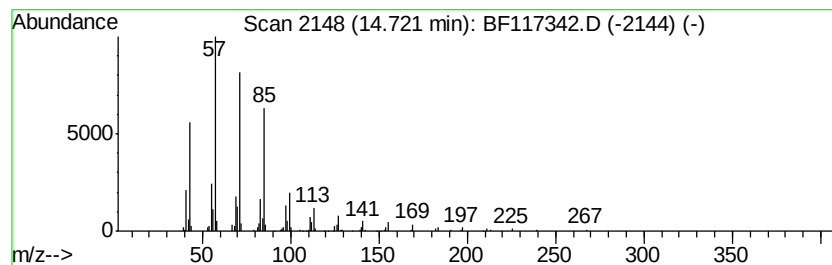
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ClientSampleId :
STONE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	8.01 ng	247163	Perylene-d12	15.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	91
2	2-methyloctacosane	408 C29H60	1000376-72-8	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Heptacosane	380 C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100819\
Data File : BF117342.D
Acq On : 8 Oct 2019 16:05
Operator : JU
Sample : K5239-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-COMP

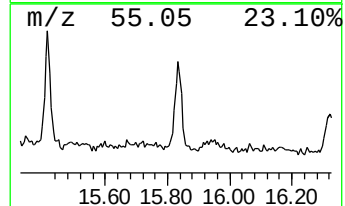
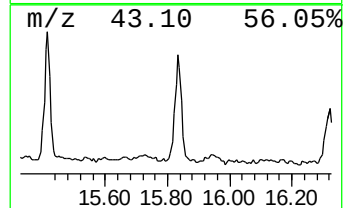
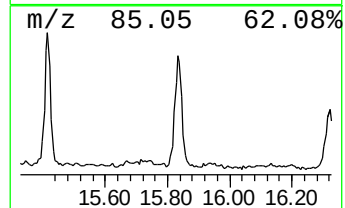
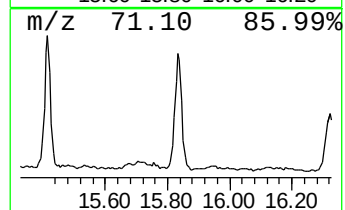
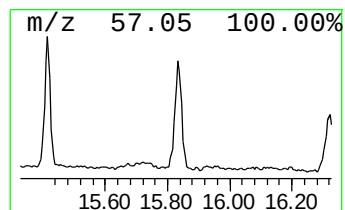
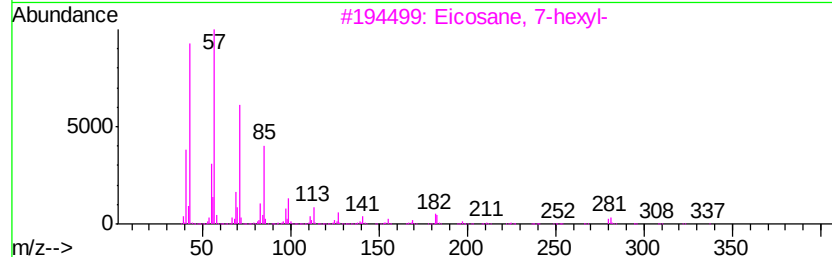
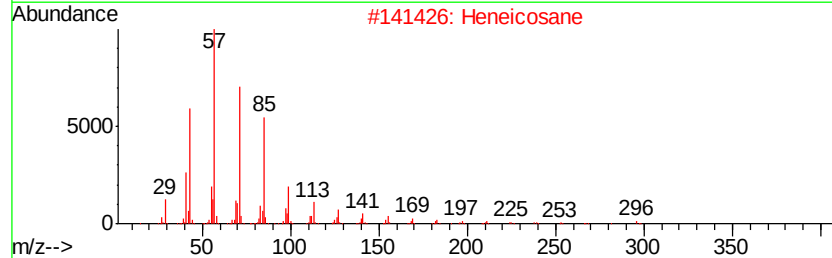
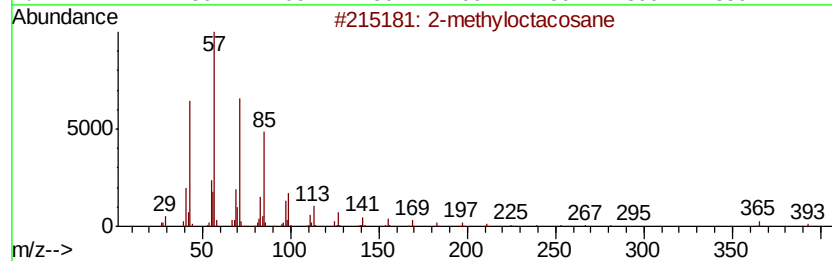
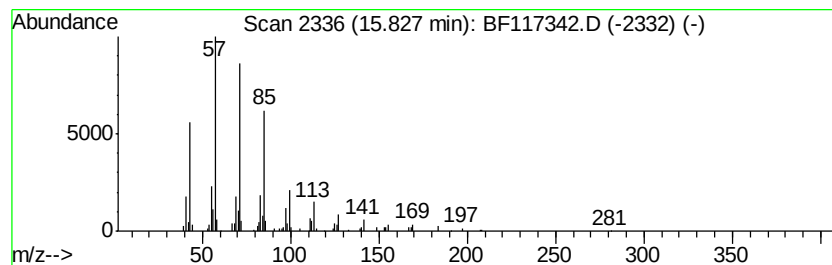
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	10.08 ng	311080	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
5		triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100819\
Data File : BF117342.D
Acq On : 8 Oct 2019 16:05
Operator : JU
Sample : K5239-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-COMP

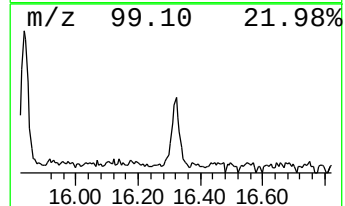
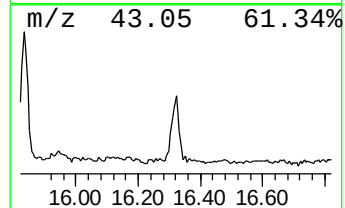
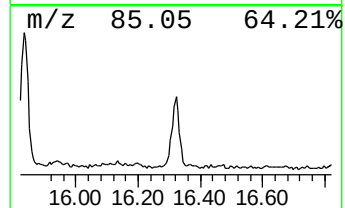
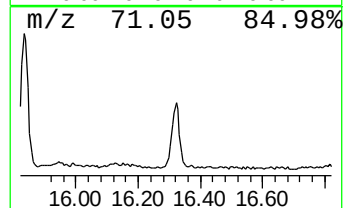
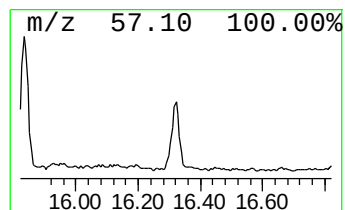
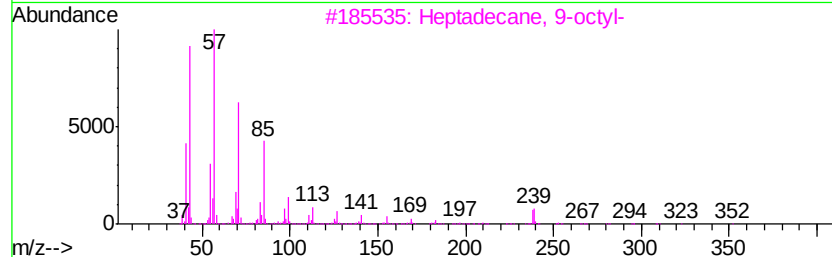
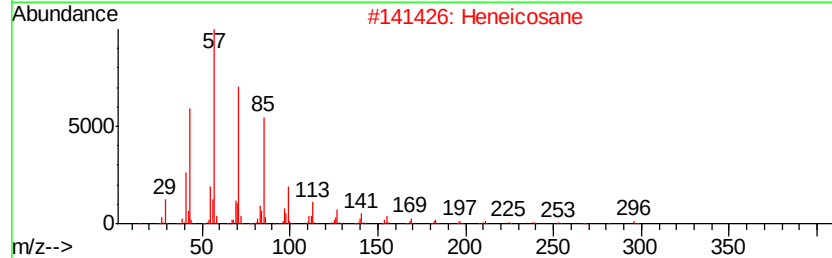
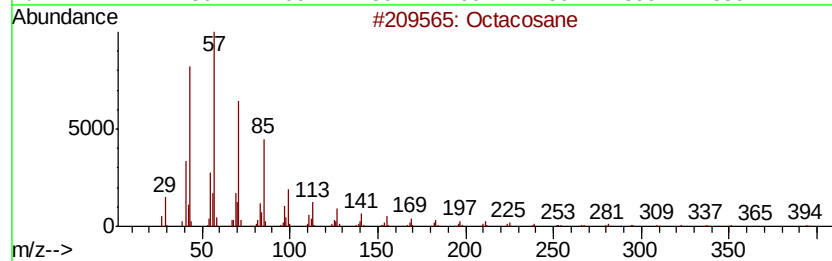
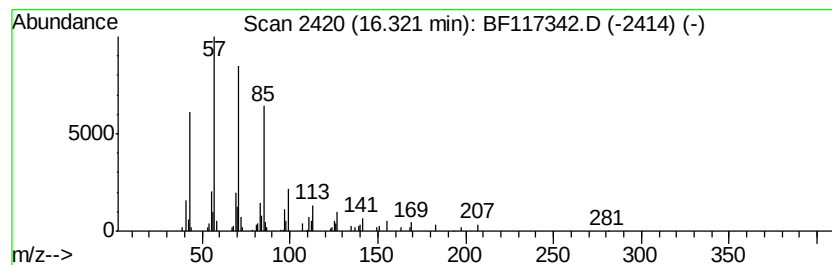
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	5.77 ng	178002	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100819\
Data File : BF117342.D
Acq On : 8 Oct 2019 16:05
Operator : JU
Sample : K5239-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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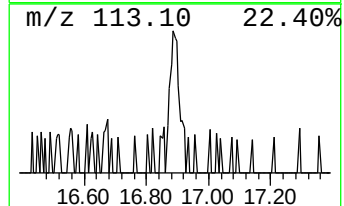
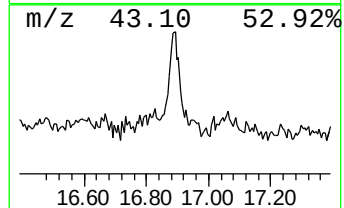
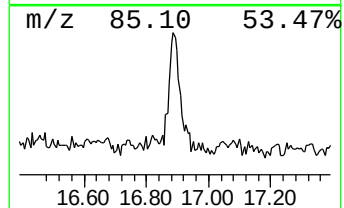
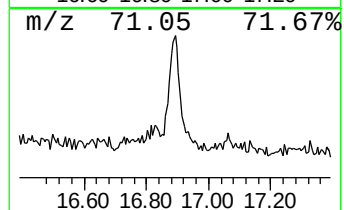
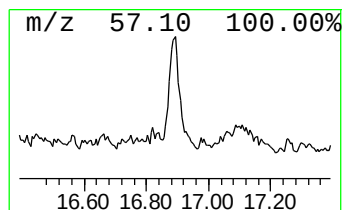
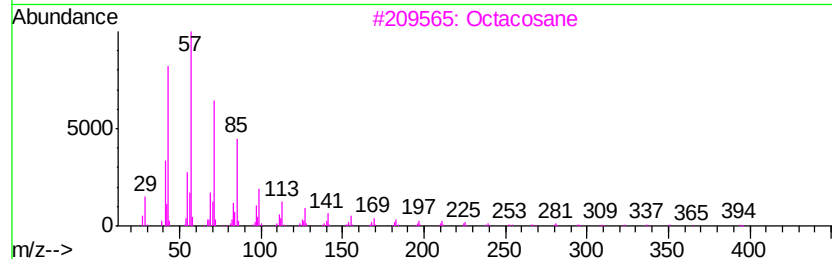
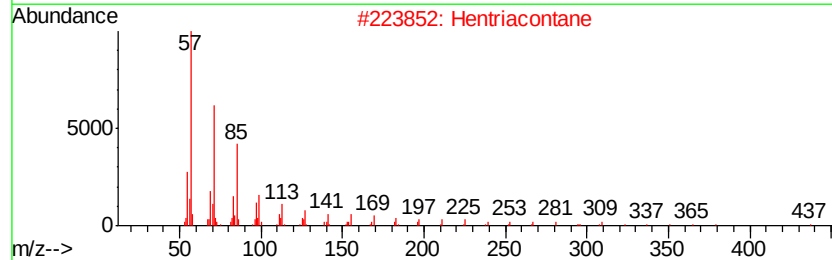
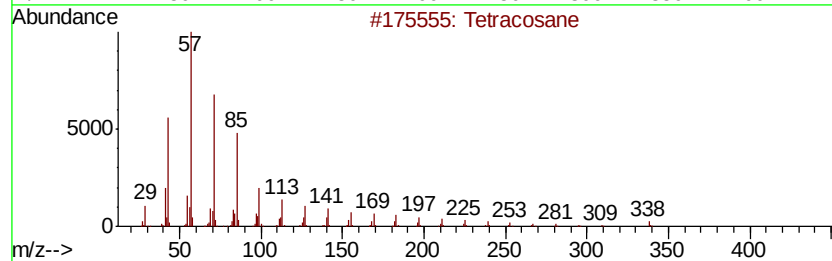
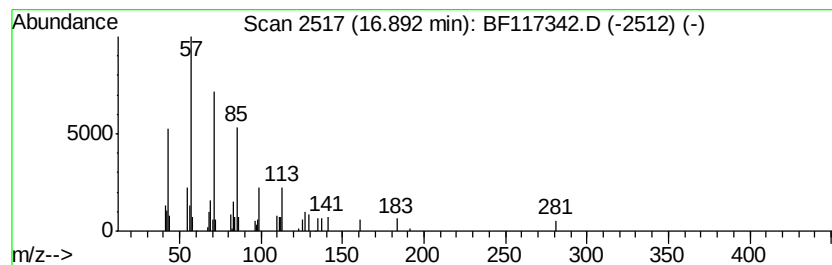
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.48 ng	76465	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	72
2		Hentriacontane	437	C31H64	000630-04-6	72
3		Octacosane	394	C28H58	000630-02-4	72
4		2-Bromotetradecane	276	C14H29Br	074036-95-6	64
5		Octadecane	254	C18H38	000593-45-3	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100819\
Data File : BF117342.D
Acq On : 8 Oct 2019 16:05
Operator : JU
Sample : K5239-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STONE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown6.57	6.57	81.1	ng	931394	1	6.80	229584	20.0
n-Hexadecanoic acid	11.85	34.5	ng	616546	4	11.32	356888	20.0
unknown12.55	12.55	3.0	ng	54005	4	11.32	356888	20.0
Octadecanoic acid	12.63	28.4	ng	507487	4	11.32	356888	20.0
Behenic alcohol	13.82	11.4	ng	205862	5	13.97	361521	20.0
Heneicosane	14.42	9.7	ng	174420	5	13.97	361521	20.0
Hexacosane	14.72	8.0	ng	247163	6	15.43	616965	20.0
2-methyloctacosane	15.83	10.1	ng	311080	6	15.43	616965	20.0
Octacosane	16.32	5.8	ng	178002	6	15.43	616965	20.0
Tetracosane	16.89	2.5	ng	76465	6	15.43	616965	20.0