

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032819\
 Data File : BF113384.D
 Acq On : 28 Mar 2019 20:03
 Operator : JU/SJ
 Sample : K2121-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-9

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-BF032519.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	4.887	473	476	490	rBV	68260	99120	1.68%	0.247%
2	5.316	545	549	573	rBV	1869765	2085967	35.26%	5.190%
3	6.346	720	724	741	rBV	1347902	1494391	25.26%	3.718%
4	6.475	741	746	749	rBV	3820600	3469688	58.64%	8.632%
5	6.698	781	784	797	rBV	1091055	989765	16.73%	2.462%
6	6.857	807	811	821	rBV	3473891	3156810	53.36%	7.854%
7	7.263	876	880	896	rBV	2502804	2766603	46.76%	6.883%
8	7.981	999	1002	1019	rBV	1222329	1291176	21.82%	3.212%
9	9.057	1181	1185	1201	rBV	4632658	4969949	84.00%	12.365%
10	9.734	1296	1300	1315	rVB	1524853	1539660	26.02%	3.831%
11	10.522	1429	1434	1450	rBV	3225196	3535770	59.76%	8.797%
12	11.210	1547	1551	1570	rVB	1773025	1753394	29.64%	4.362%
13	11.751	1639	1643	1661	rBV	641385	803016	13.57%	1.998%
14	12.457	1758	1763	1772	rBV8	22636	65835	1.11%	0.164%
15	12.533	1772	1776	1789	rBV	713292	913619	15.44%	2.273%
16	12.792	1815	1820	1824	rBV	5039211	5916481	100.00%	14.720%
17	13.792	1982	1990	1993	rBV5	44442	120084	2.03%	0.299%
18	13.839	1993	1998	2006	rVB	1768641	1951949	32.99%	4.856%
19	14.010	2023	2027	2032	rVB	79264	76508	1.29%	0.190%
20	14.310	2075	2078	2082	rVB	147701	132730	2.24%	0.330%
21	14.604	2124	2128	2134	rVB	227655	211952	3.58%	0.527%
22	14.916	2177	2181	2185	rBV	259942	266589	4.51%	0.663%
23	15.239	2231	2236	2250	rVB2	1090838	1844421	31.17%	4.589%
24	15.663	2302	2308	2313	rBV	246319	373326	6.31%	0.929%
25	16.121	2380	2386	2395	rVB2	138393	255599	4.32%	0.636%
26	16.657	2472	2477	2483	rVB	57086	109778	1.86%	0.273%

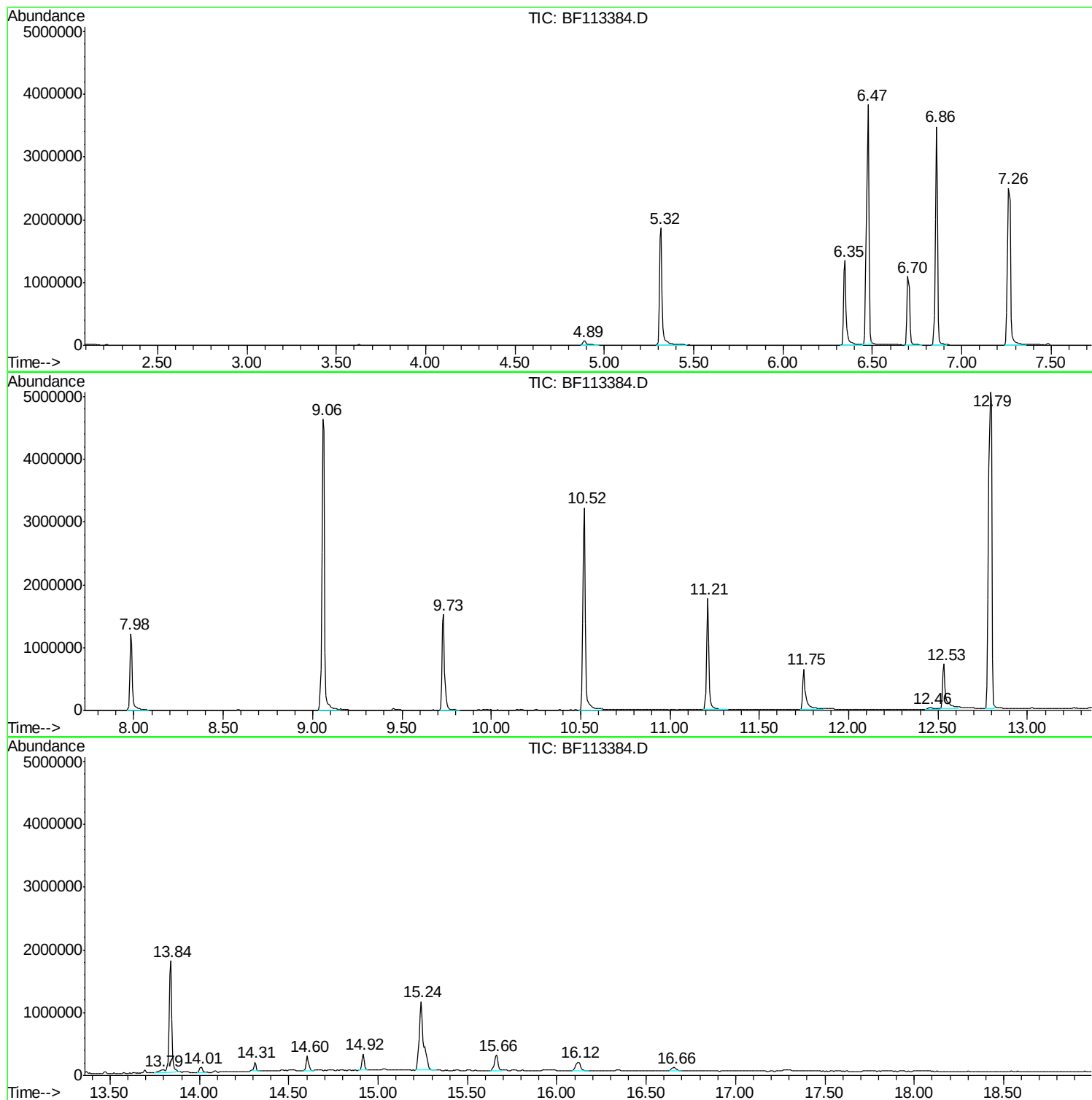
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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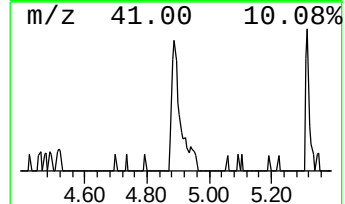
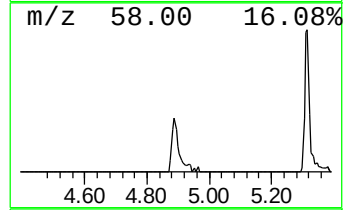
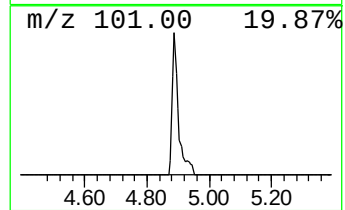
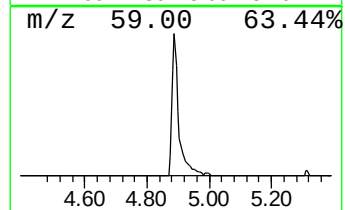
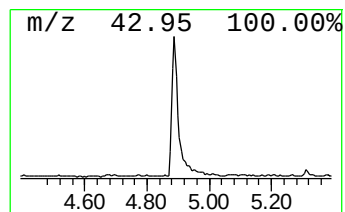
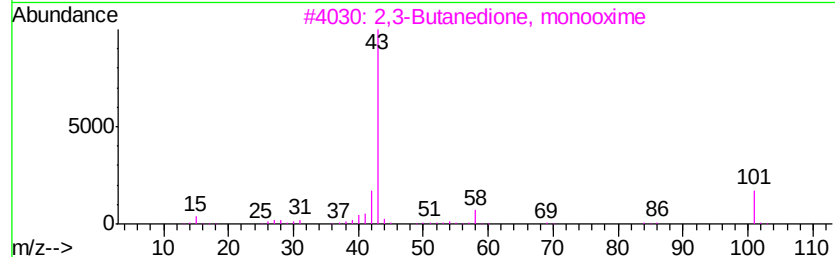
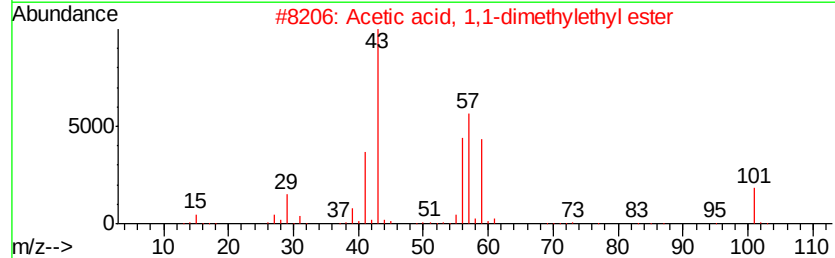
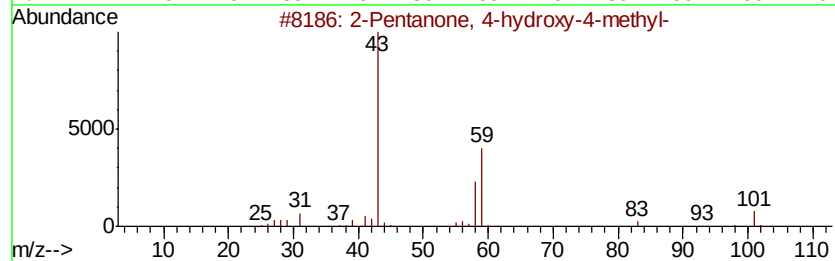
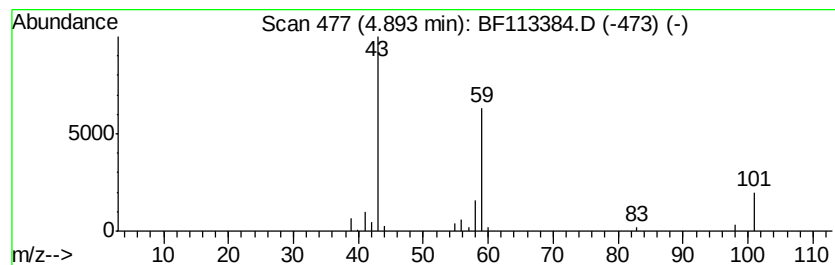
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.00 ng	99120	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		3-Hexanol	102	C6H14O	000623-37-0	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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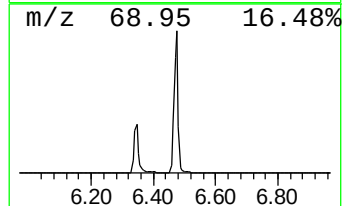
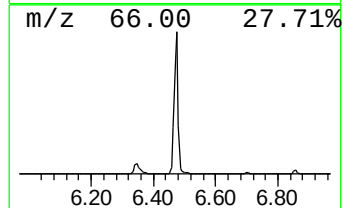
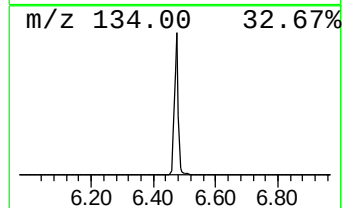
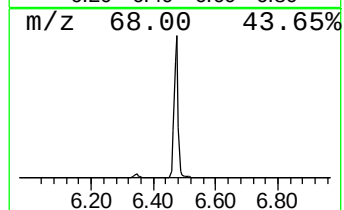
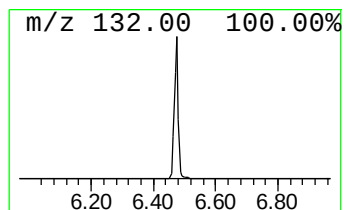
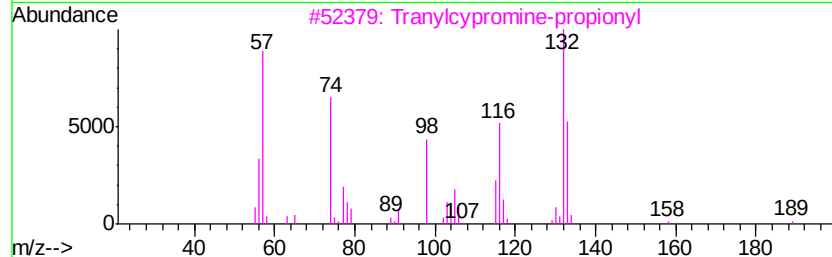
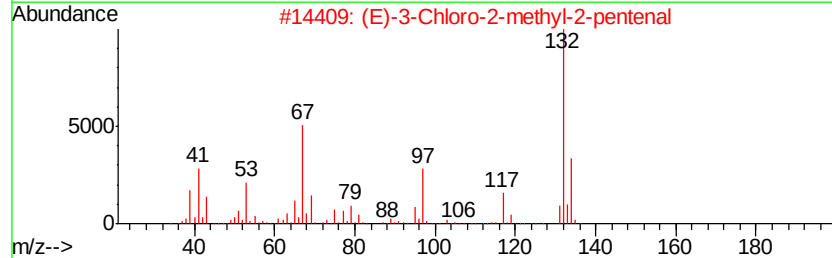
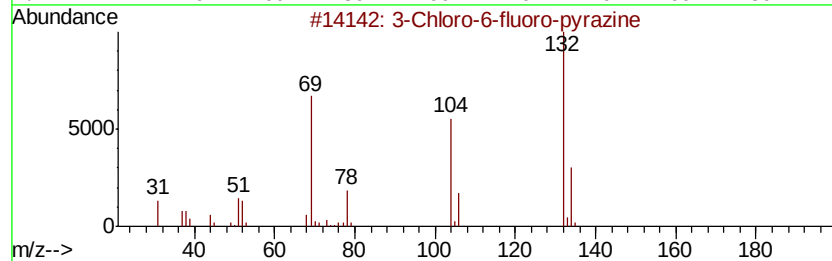
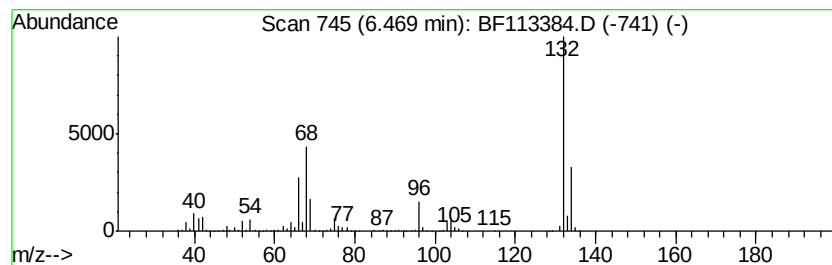
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	70.11 ng	3469690	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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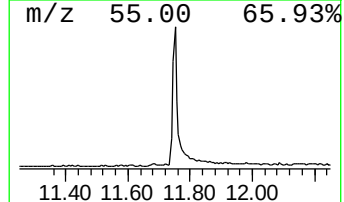
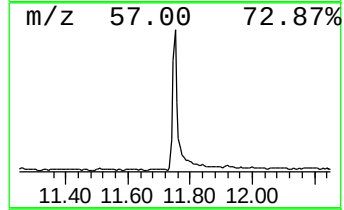
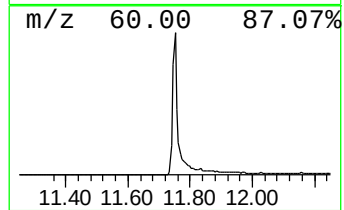
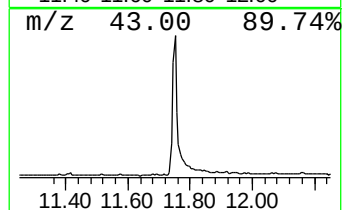
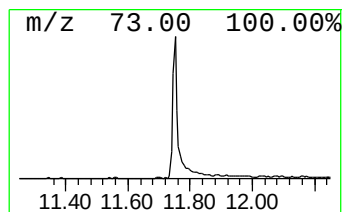
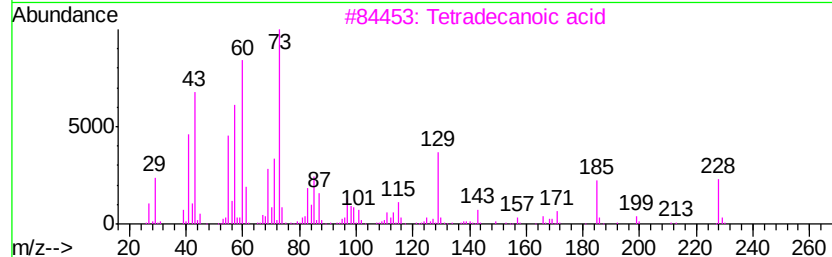
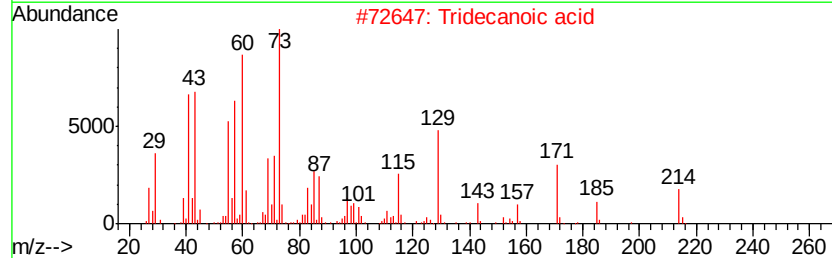
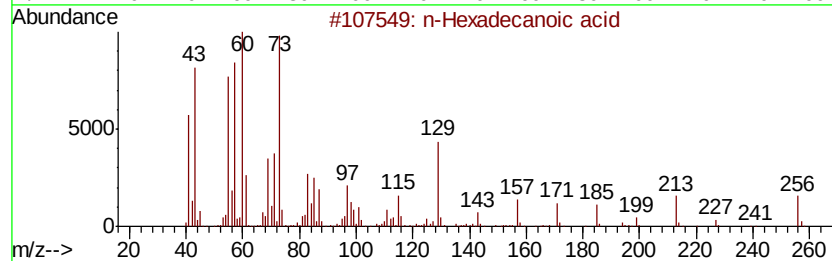
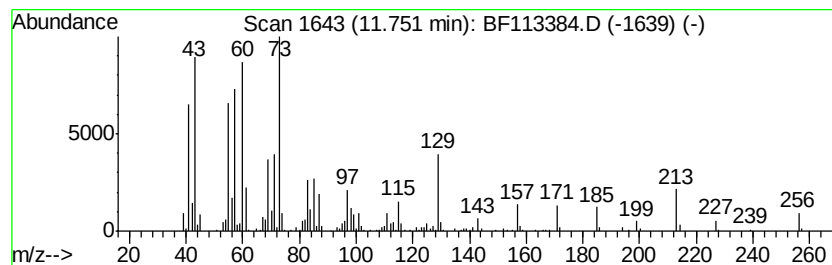
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	9.16 ng	803016	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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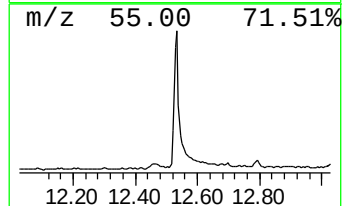
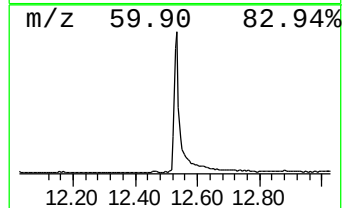
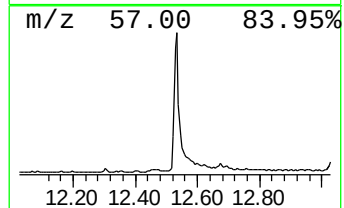
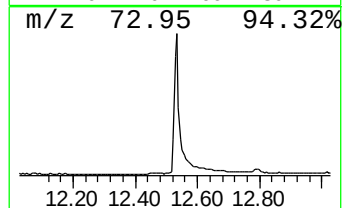
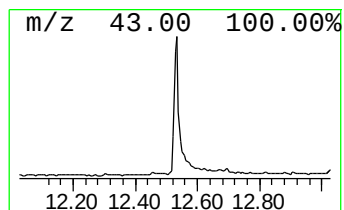
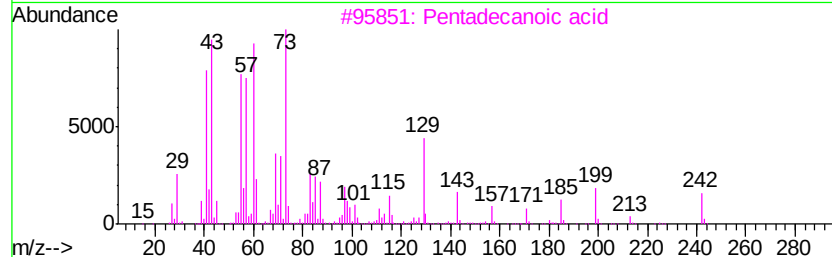
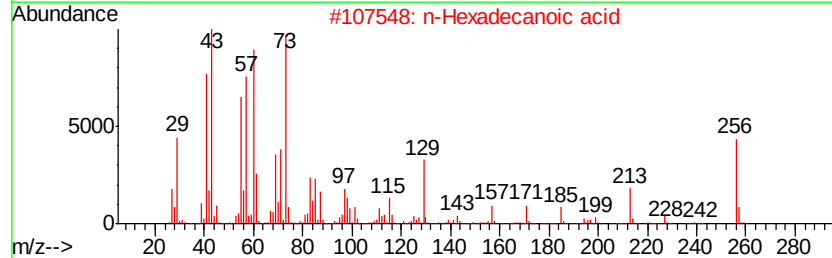
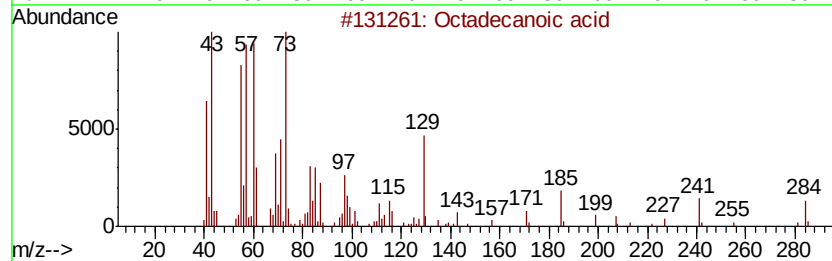
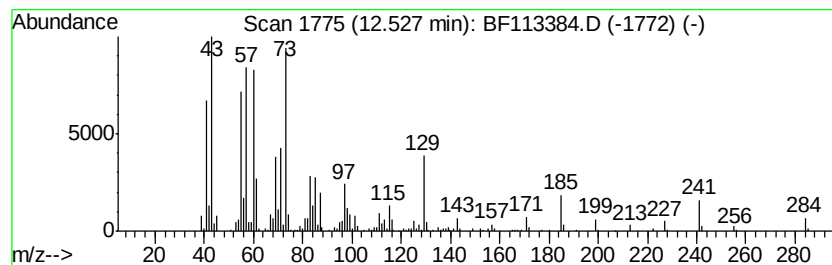
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	9.36 ng	913619	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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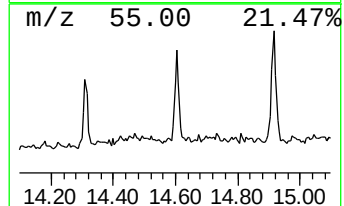
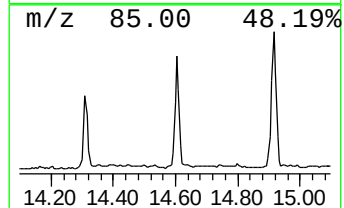
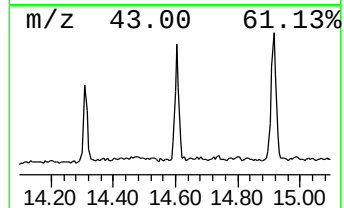
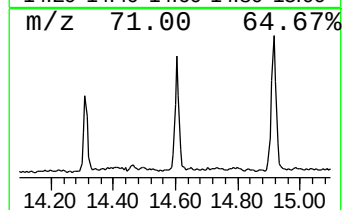
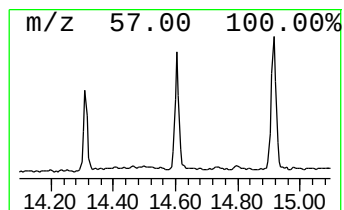
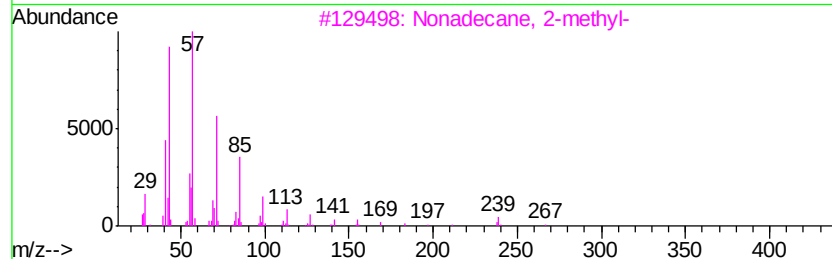
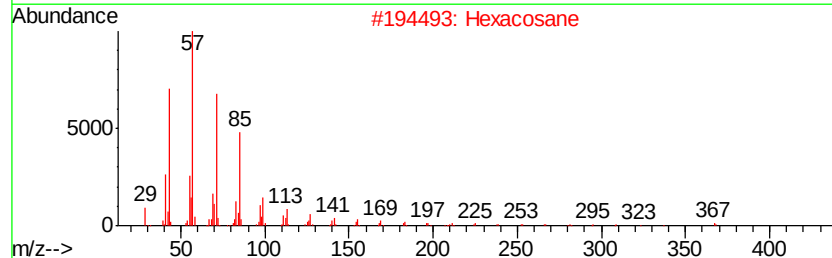
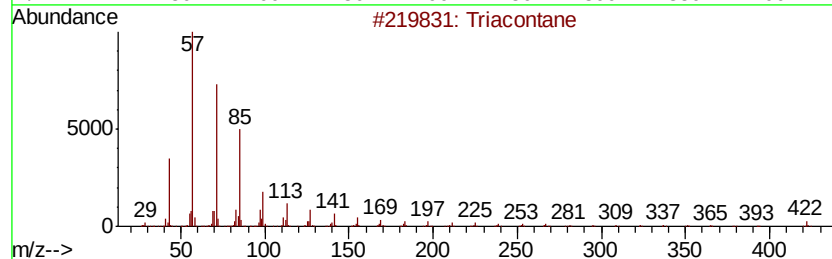
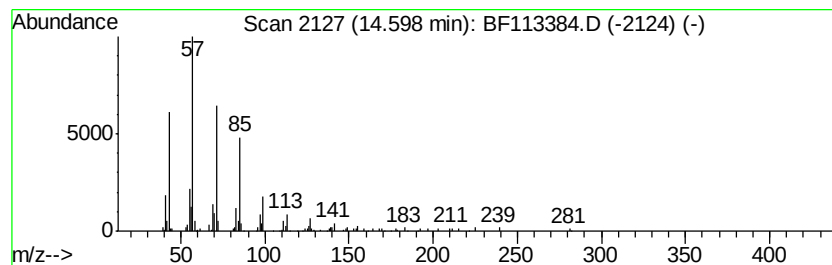
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Peak Number 6 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.30 ng	211952	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Heneicosane	296	C21H44	000629-94-7	90



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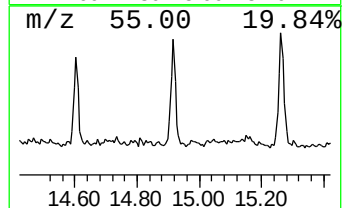
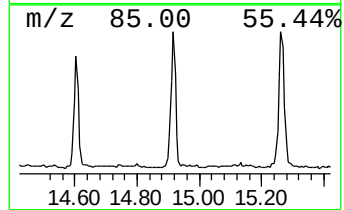
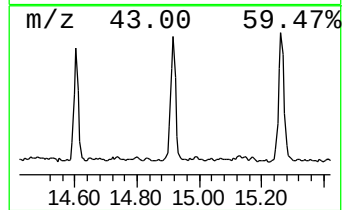
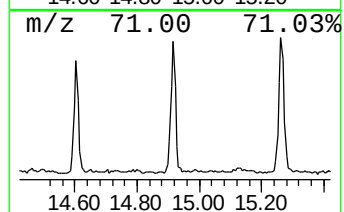
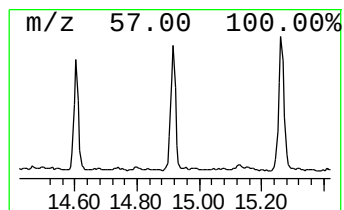
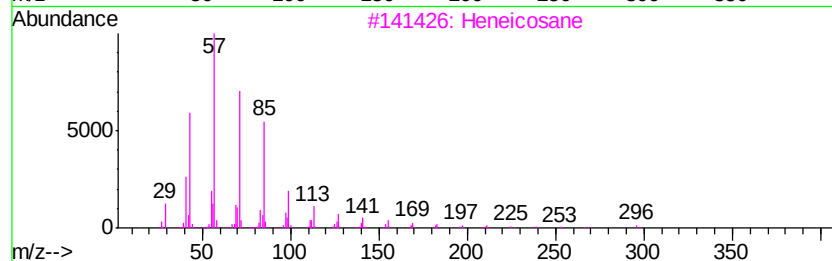
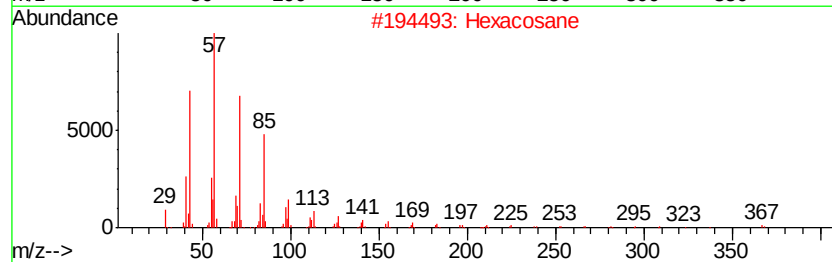
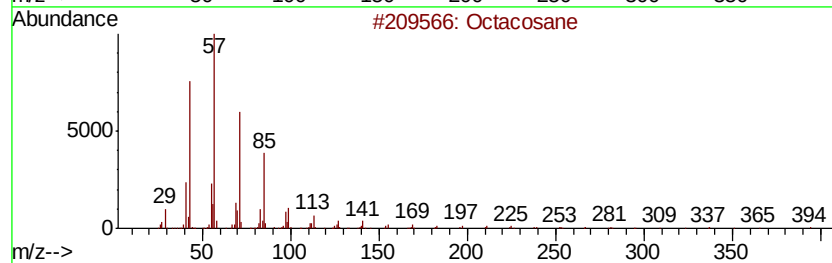
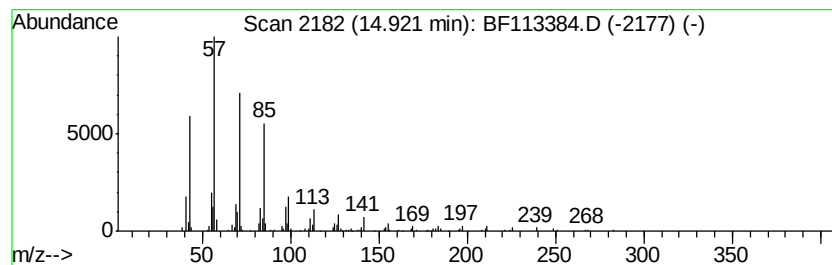
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.89 ng	266589	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032819\
Data File : BF113384.D
Acq On : 28 Mar 2019 20:03
Operator : JU/SJ
Sample : K2121-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

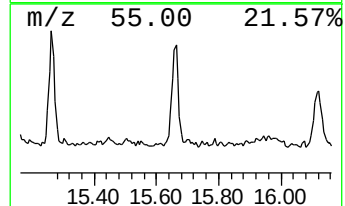
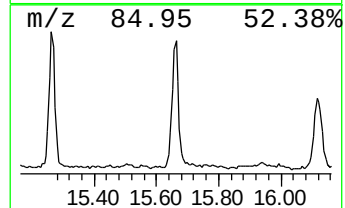
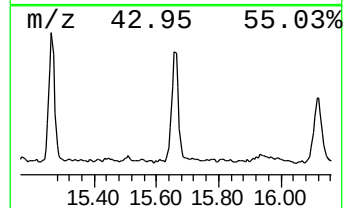
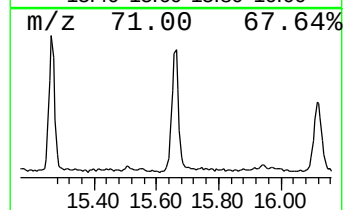
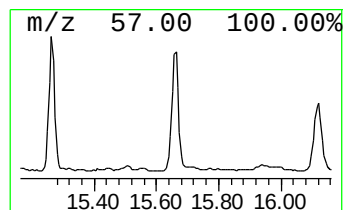
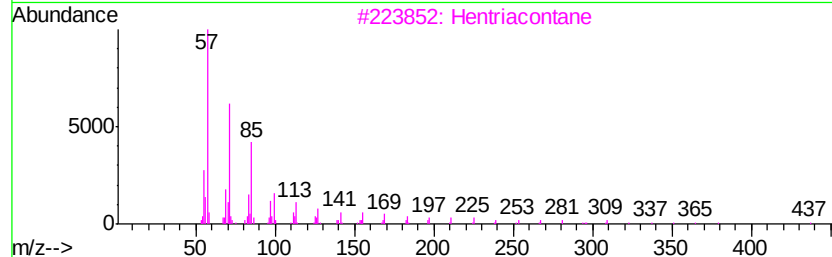
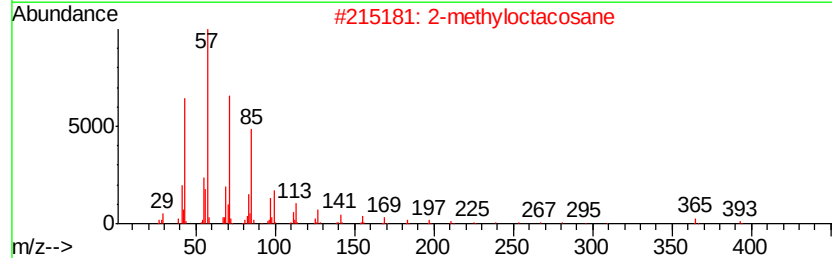
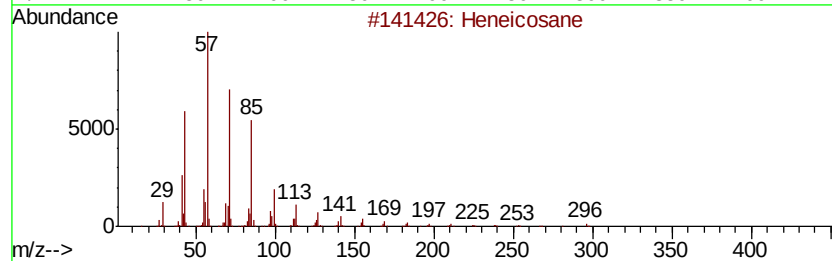
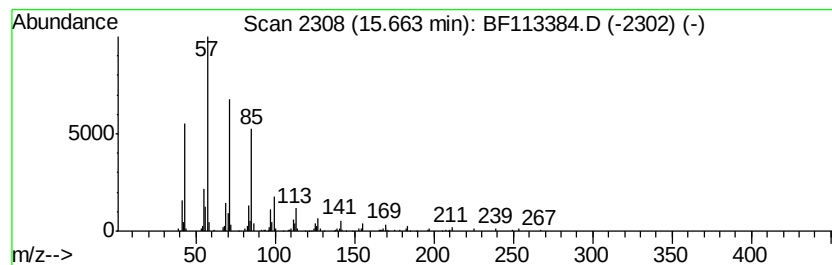
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	4.05 ng	373326	Perylene-d12	15.24

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	Triacontane		422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032819\
Data File : BF113384.D
Acq On : 28 Mar 2019 20:03
Operator : JU/SJ
Sample : K2121-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

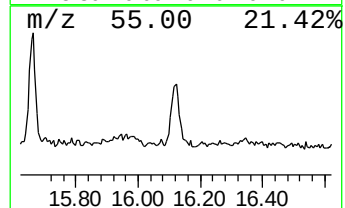
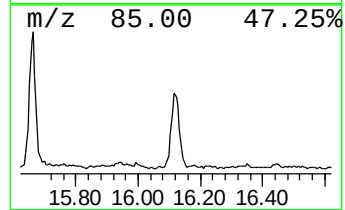
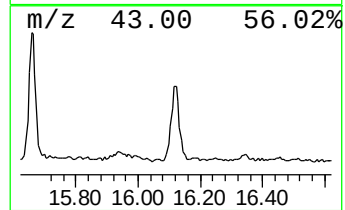
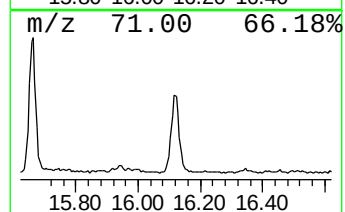
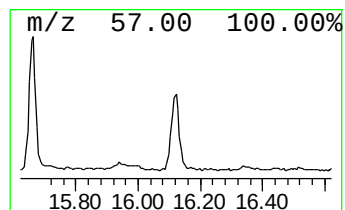
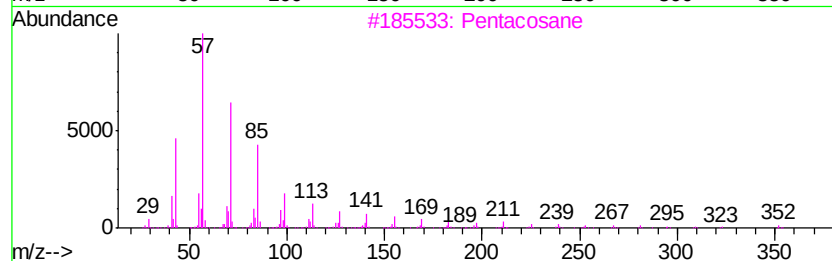
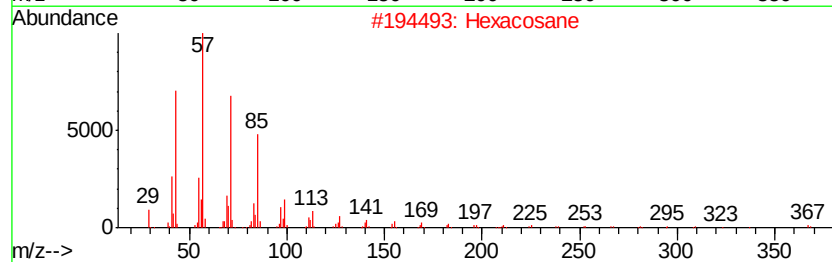
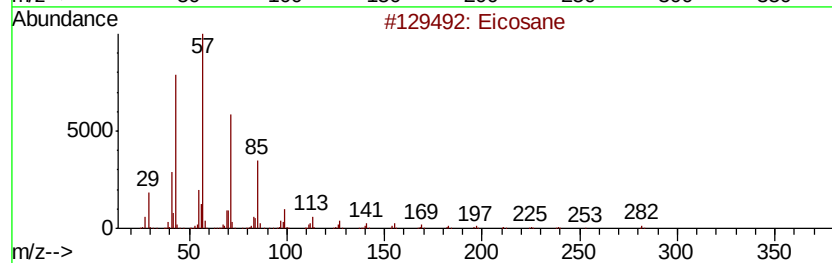
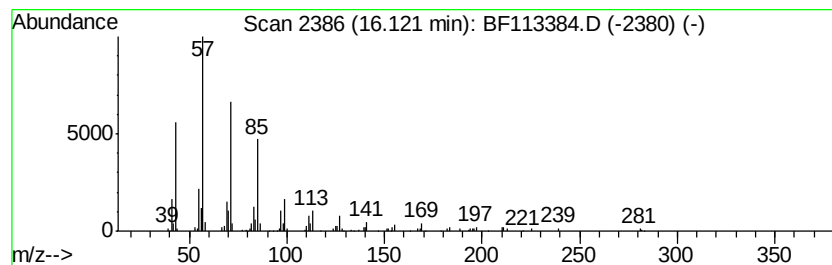
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.77 ng	255599	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Hexacosane		366	C26H54	000630-01-3	94
3	Pentacosane		352	C25H52	000629-99-2	91
4	Tetratetracontane		619	C44H90	007098-22-8	90
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032819\
Data File : BF113384.D
Acq On : 28 Mar 2019 20:03
Operator : JU/SJ
Sample : K2121-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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
2-Pentanone, 4-hy...	4.89	2.0	ng	99120	1	6.70	989765	20.0
unknown6.47	6.47	70.1	ng	3469690	1	6.70	989765	20.0
n-Hexadecanoic acid	11.75	9.2	ng	803016	4	11.21	1753390	20.0
Octadecanoic acid	12.53	9.4	ng	913619	5	13.84	1951950	20.0
triacontane	14.60	2.3	ng	211952	6	15.24	1844420	20.0
Octacosane	14.92	2.9	ng	266589	6	15.24	1844420	20.0
Heneicosane	15.66	4.0	ng	373326	6	15.24	1844420	20.0
Eicosane	16.12	2.8	ng	255599	6	15.24	1844420	20.0