

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
 Data File : BF117935.D
 Acq On : 22 Nov 2019 23:08
 Operator : JU
 Sample : K5839-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-NW-02

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-BF111319.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	2.216	16	22	29	rVB	496888	641641	11.52%	1.358%
2	4.010	323	327	335	rVB	63528	88924	1.60%	0.188%
3	5.122	509	516	527	rVB	741045	988978	17.75%	2.093%
4	5.522	576	584	587	rBV	3692999	3537048	63.49%	7.485%
5	6.528	749	755	759	rBV	3523322	3743532	67.19%	7.922%
6	6.669	775	779	783	rBV	4039922	4011987	72.01%	8.491%
7	6.904	815	819	822	rBV	1355828	1155336	20.74%	2.445%
8	7.063	841	846	849	rBV	3436759	3276685	58.81%	6.934%
9	7.240	873	876	880	rVB	74010	65055	1.17%	0.138%
10	7.463	909	914	917	rBV	2441653	2517310	45.18%	5.327%
11	7.604	934	938	943	rVB	76142	68560	1.23%	0.145%
12	8.192	1032	1038	1041	rBV	1571321	1542618	27.69%	3.265%
13	9.269	1216	1221	1224	rBV	5285777	4980959	89.40%	10.541%
14	9.663	1283	1288	1291	rBV	486816	407986	7.32%	0.863%
15	9.951	1332	1337	1341	rBV	2129589	1923944	34.53%	4.072%
16	10.745	1466	1472	1475	rBV	3556065	3374606	60.57%	7.142%
17	11.445	1587	1591	1594	rBV	2462529	2028396	36.41%	4.293%
18	11.969	1676	1680	1694	rBV	672118	647924	11.63%	1.371%
19	12.657	1794	1797	1798	rBV	89559	72141	1.29%	0.153%
20	12.674	1798	1800	1810	rVV	168698	210266	3.77%	0.445%
21	12.757	1810	1814	1822	rVV	385147	411233	7.38%	0.870%
22	13.039	1857	1862	1865	rBV	5829278	5571339	100.00%	11.791%
23	13.263	1893	1900	1910	rVB	44594	60343	1.08%	0.128%
24	13.604	1950	1958	1962	rBV2	68609	73430	1.32%	0.155%
25	13.933	2010	2014	2030	rBV2	430894	699511	12.56%	1.480%
26	14.092	2037	2041	2045	rBV	1905878	1662669	29.84%	3.519%
27	14.251	2065	2068	2076	rVB	195721	175591	3.15%	0.372%
28	14.557	2116	2120	2132	rBV	289357	357362	6.41%	0.756%
29	14.874	2170	2174	2180	rVB	315755	301172	5.41%	0.637%
30	14.951	2184	2187	2192	rVB	82356	86391	1.55%	0.183%
31	15.027	2196	2200	2207	rVB	64954	74899	1.34%	0.159%
32	15.227	2229	2234	2237	rBV	297887	329105	5.91%	0.696%
33	15.592	2291	2296	2300	rBV	1046846	1383532	24.83%	2.928%
34	15.621	2300	2301	2310	rVB	207793	229601	4.12%	0.486%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.833	2331	2337	2342	rBV4	33361	58724	1.05%	0.124%
36	16.080	2373	2379	2385	rBV	152065	226982	4.07%	0.480%
37	16.157	2385	2392	2397	rBV8	32192	89945	1.61%	0.190%
38	16.610	2463	2469	2476	rBV	62936	109076	1.96%	0.231%
39	16.909	2514	2520	2525	rBV7	31169	67838	1.22%	0.144%

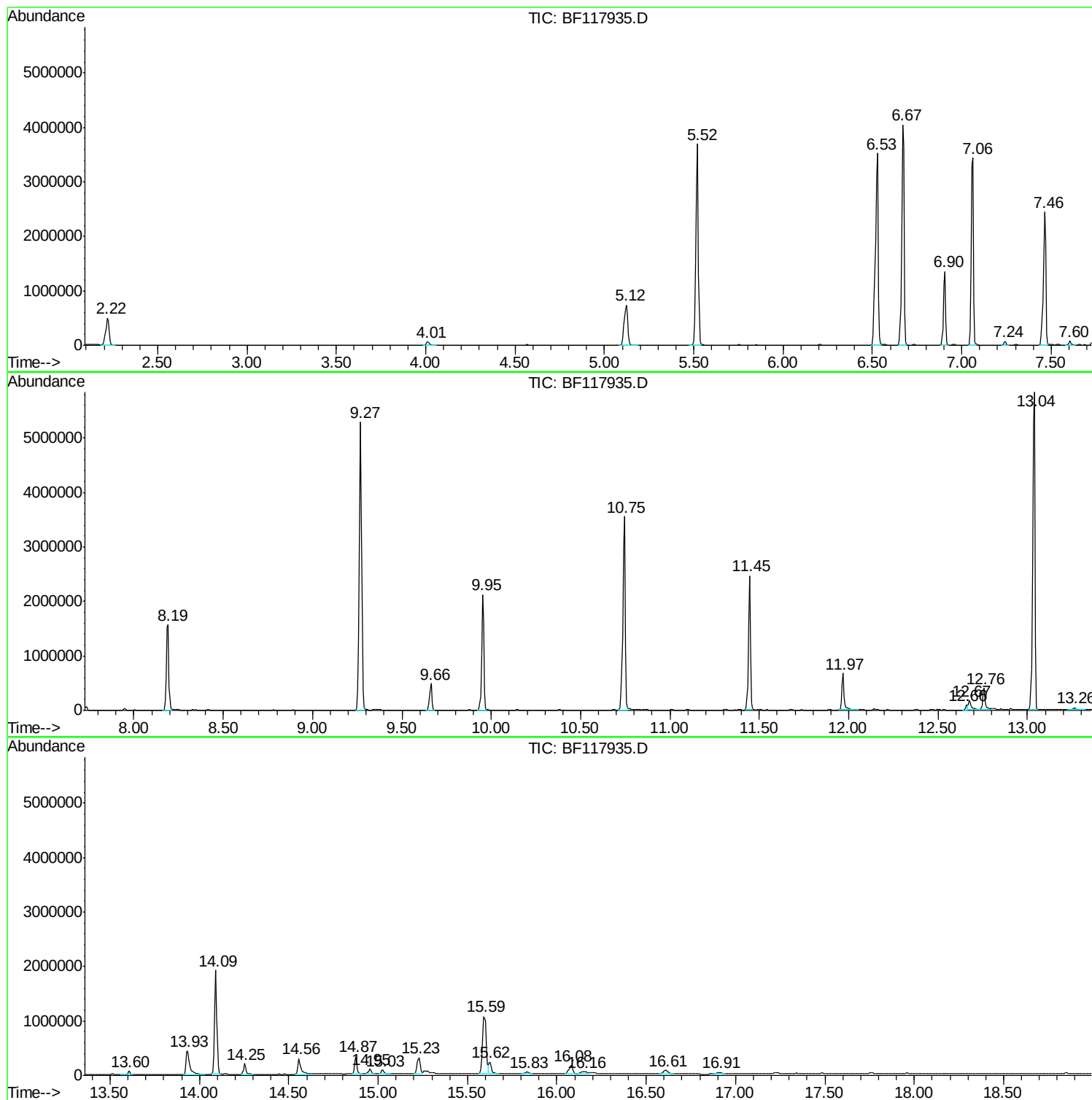
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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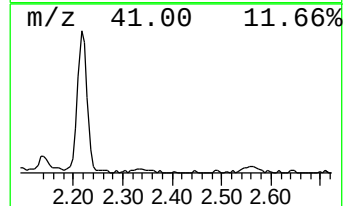
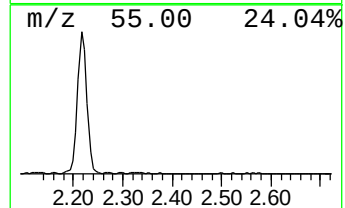
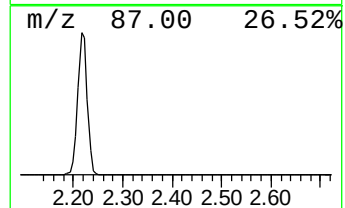
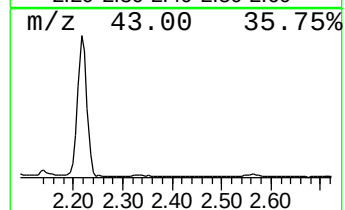
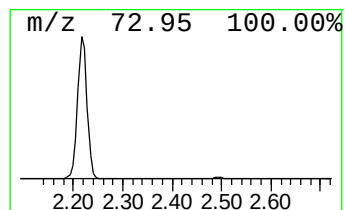
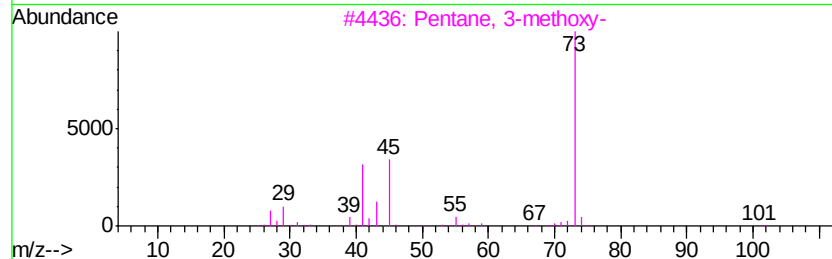
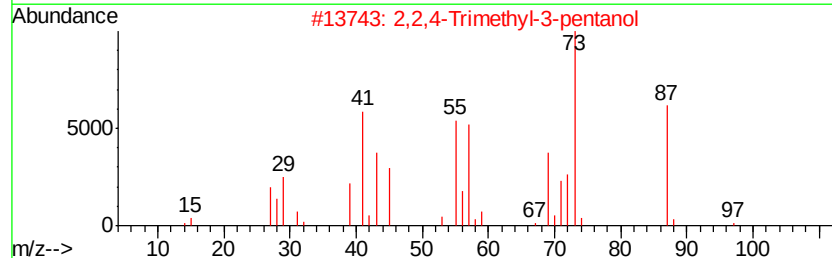
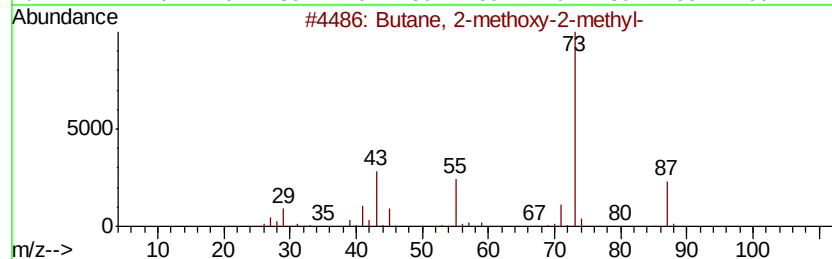
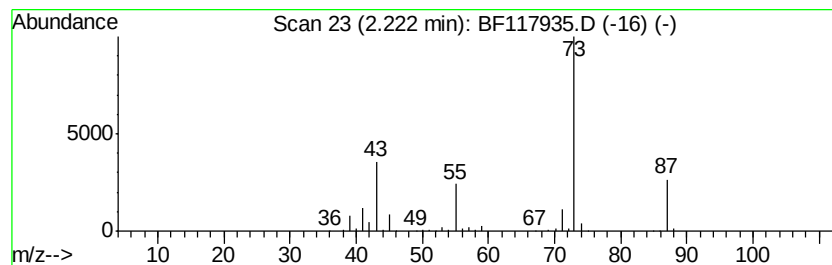
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	11.11 ng	641641	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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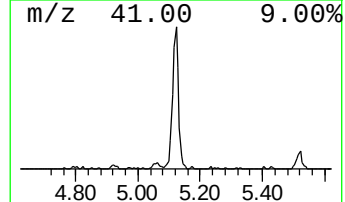
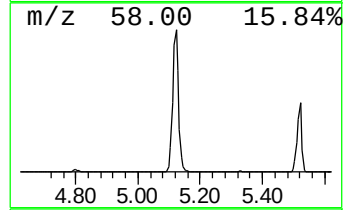
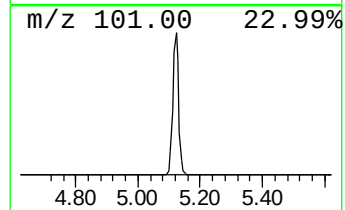
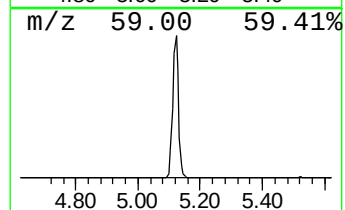
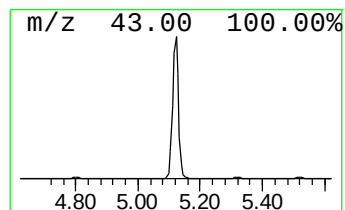
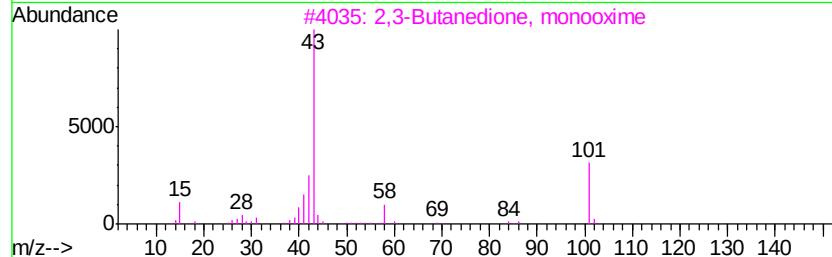
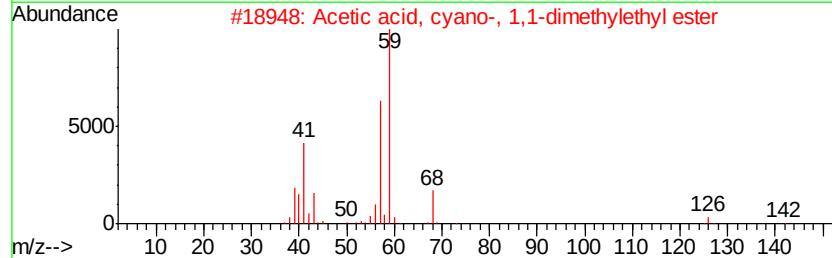
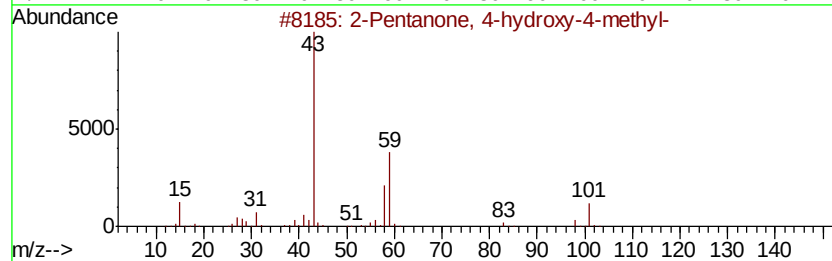
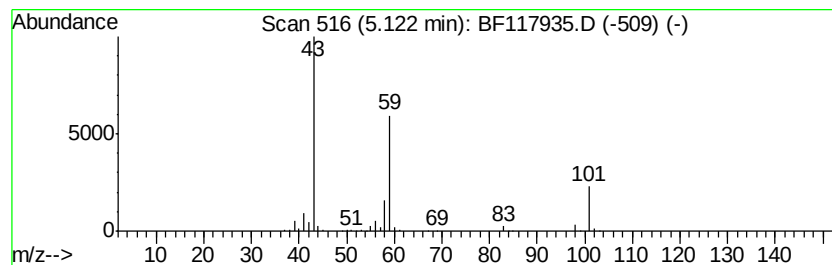
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	17.12 ng	988978	1,4-Dichlorobenzene-d4	6.90

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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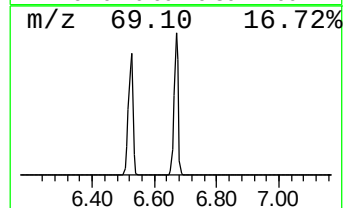
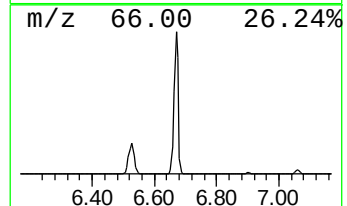
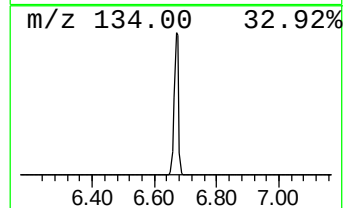
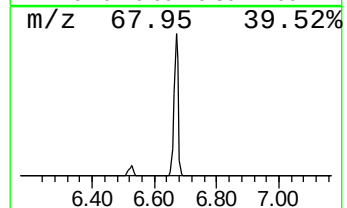
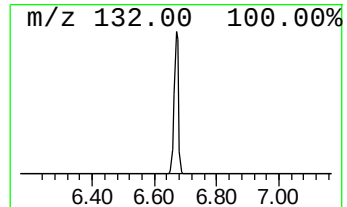
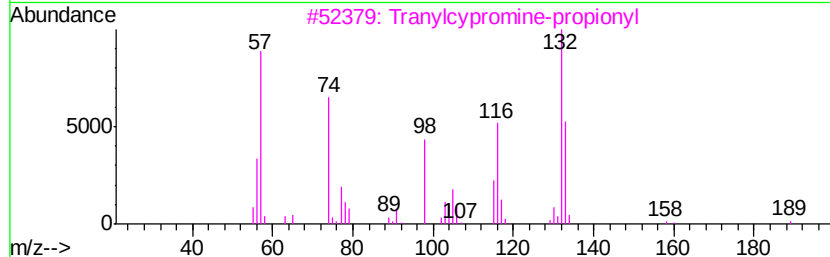
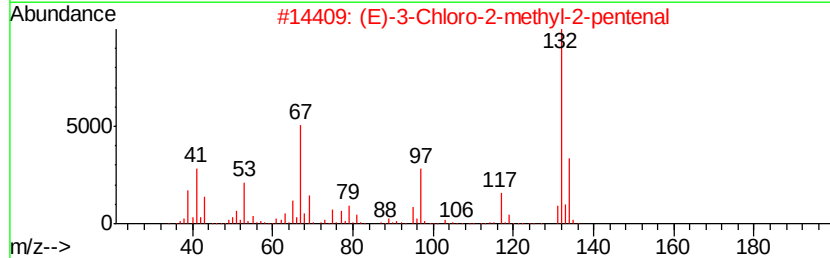
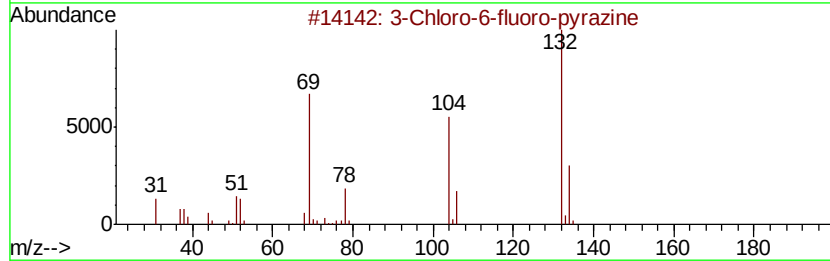
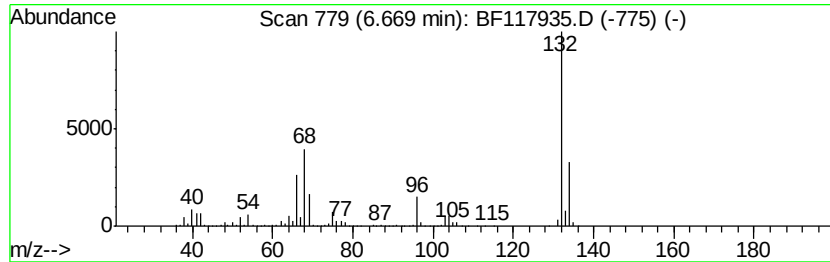
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	69.45 ng	4011990	1,4-Dichlorobenzene-d4	6.90

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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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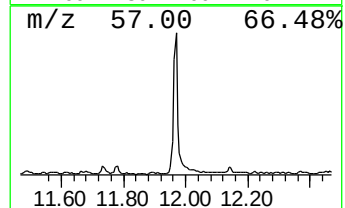
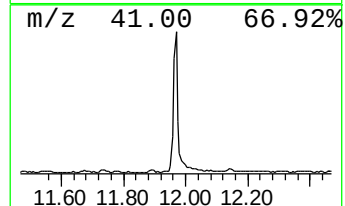
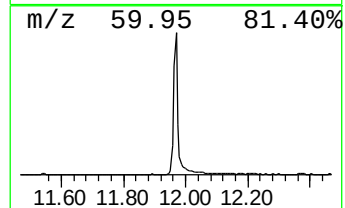
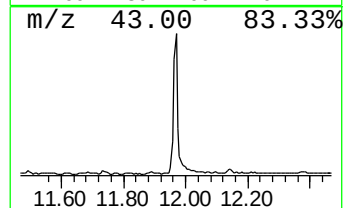
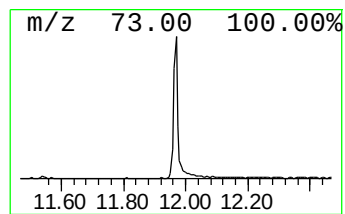
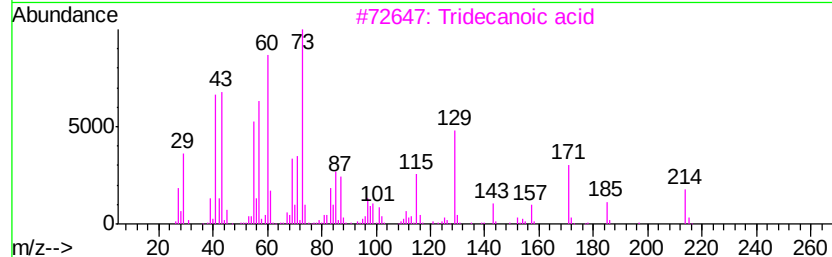
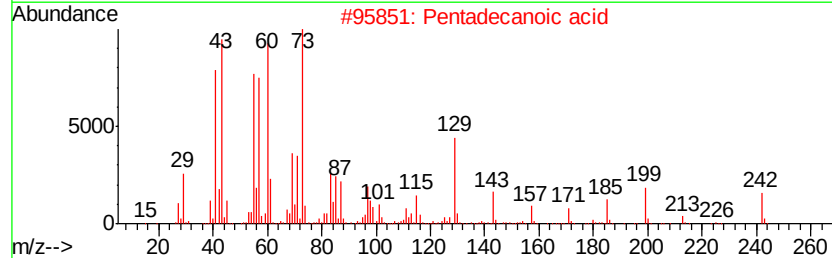
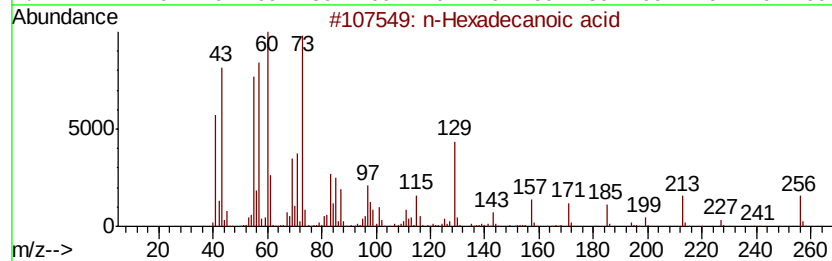
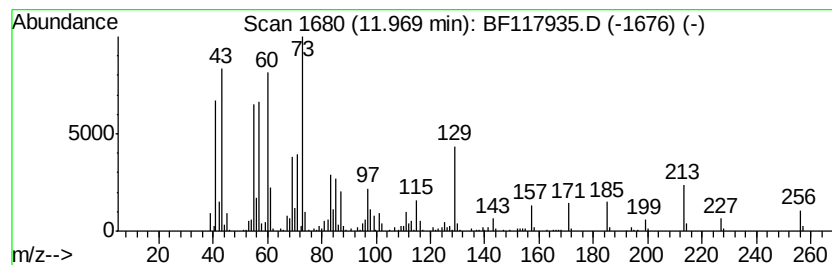
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	6.39 ng	647924	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	80



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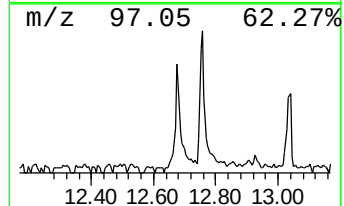
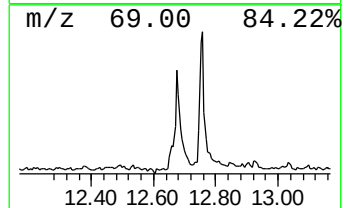
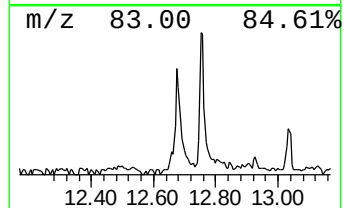
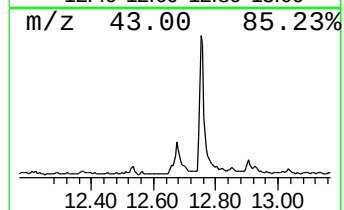
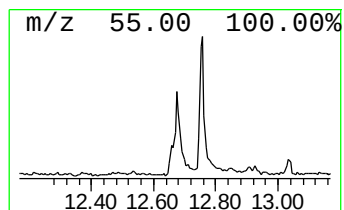
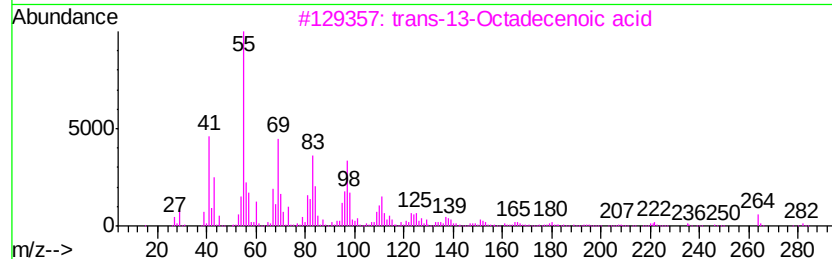
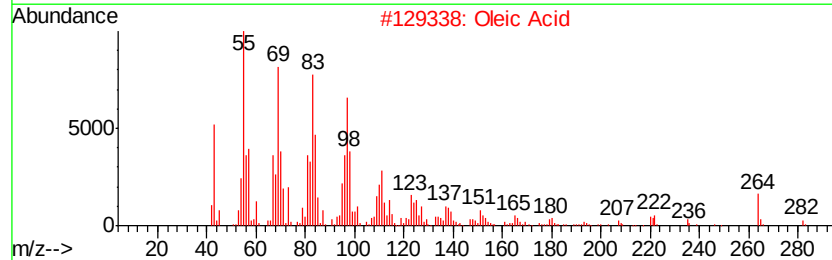
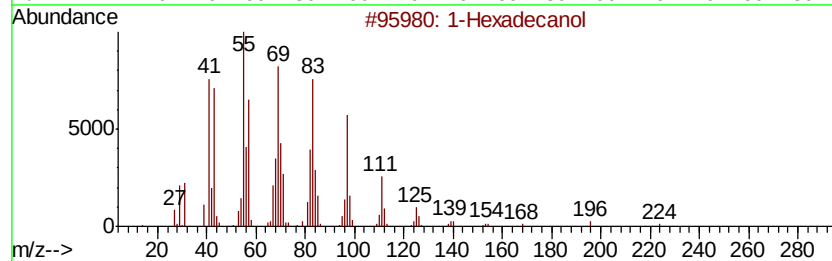
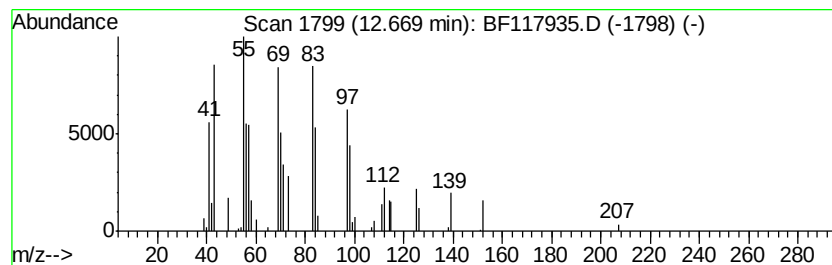
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexadecanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.67	2.07 ng	210266	Phenanthrene-d10		11.45		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	81
2			Oleic Acid	282	C18H34O2	000112-80-1	80
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	64
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	58
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	58



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Data File : BF117935.D
Acq On : 22 Nov 2019 23:08
Operator : JU
Sample : K5839-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-NW-02

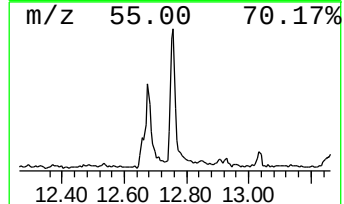
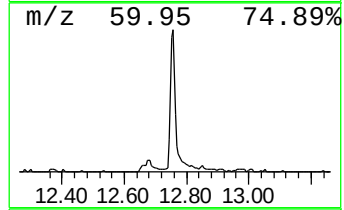
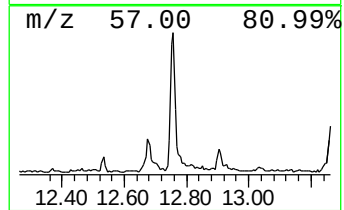
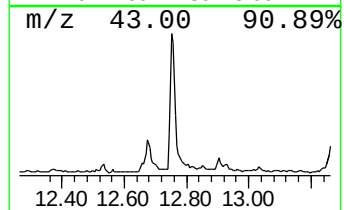
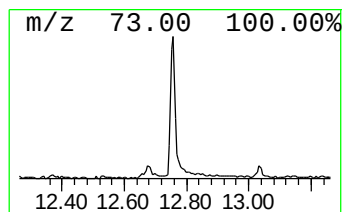
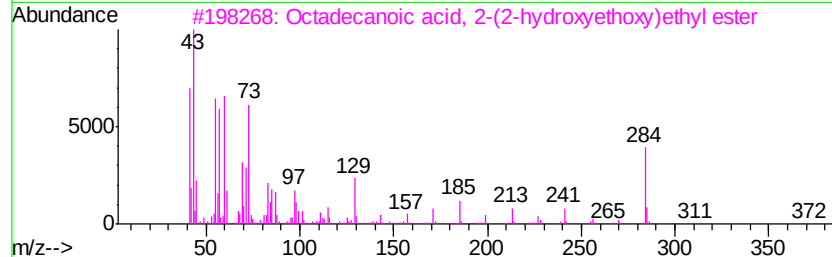
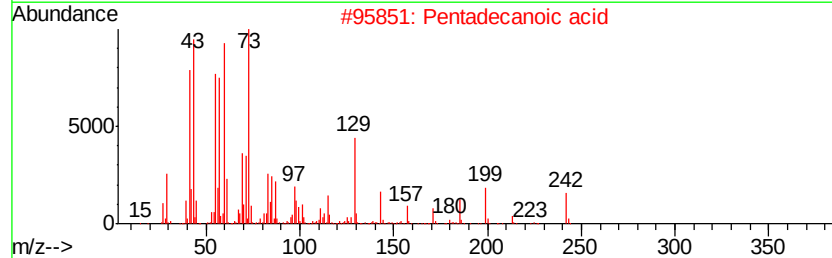
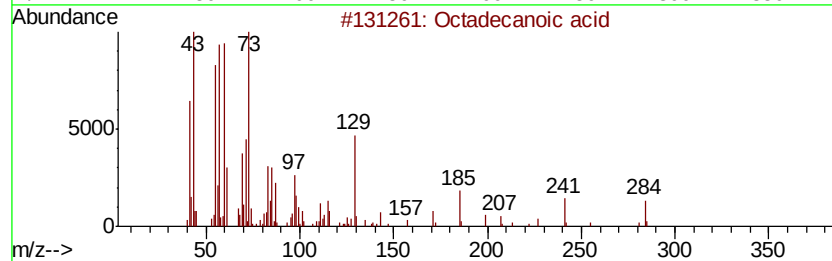
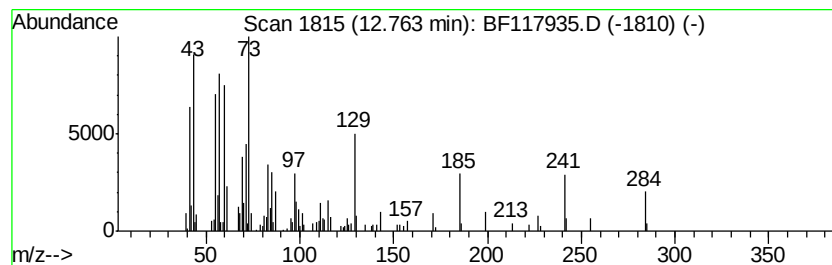
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	4.05 ng	411233	Phenanthrene-d10	11.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
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Acq On : 22 Nov 2019 23:08
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Misc :
ALS Vial : 12 Sample Multiplier: 1

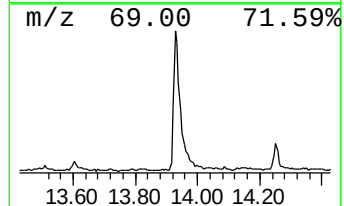
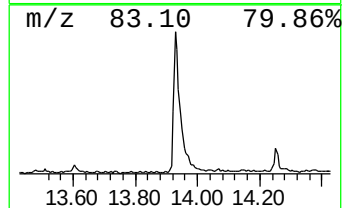
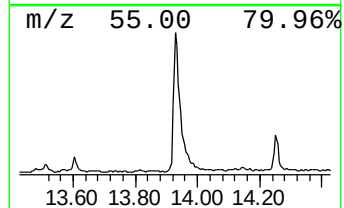
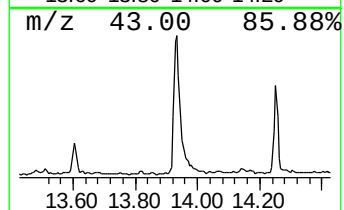
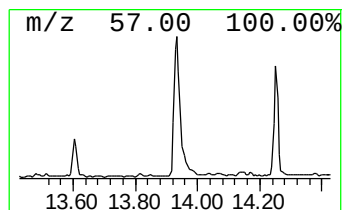
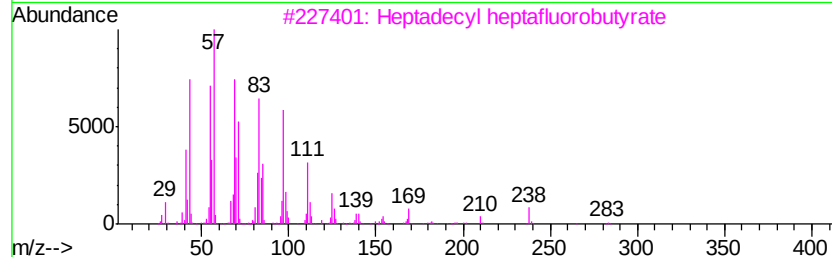
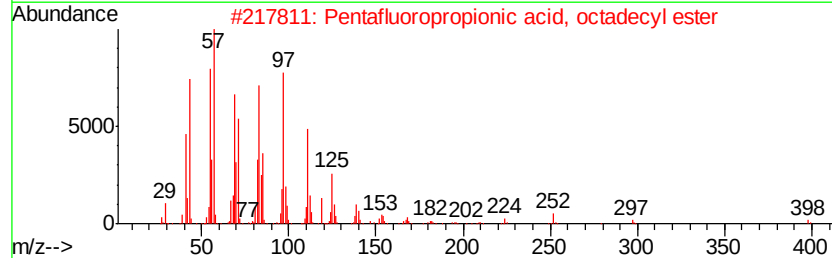
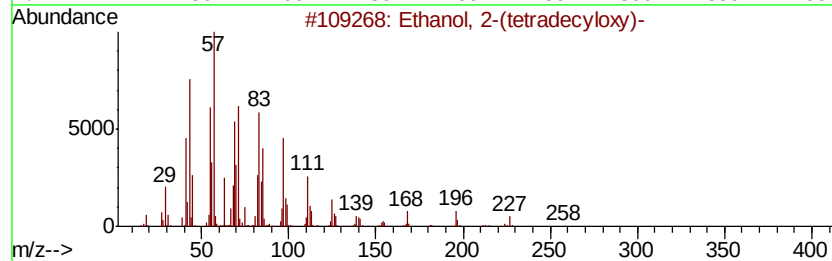
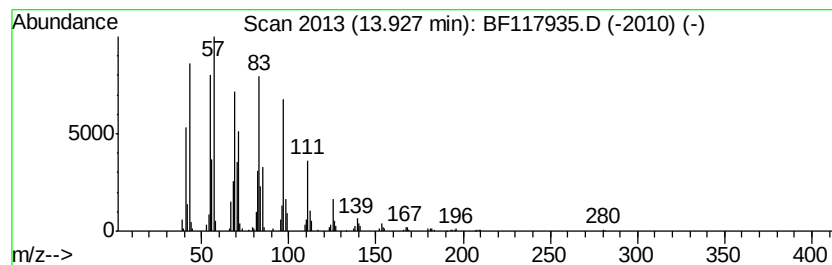
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.93	8.41 ng	699511	Chrysene-d12	14.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3		Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	87
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
 Data File : BF117935.D
 Acq On : 22 Nov 2019 23:08
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 Sample : K5839-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

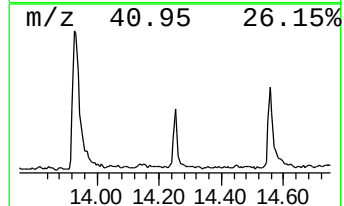
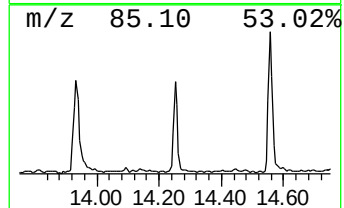
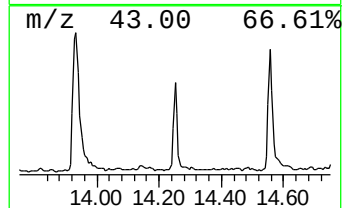
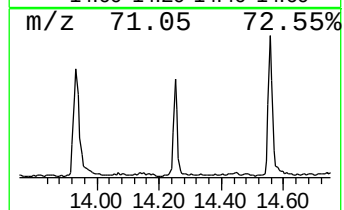
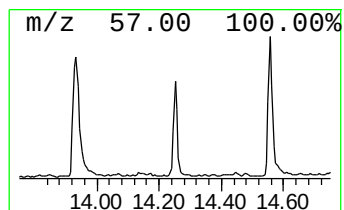
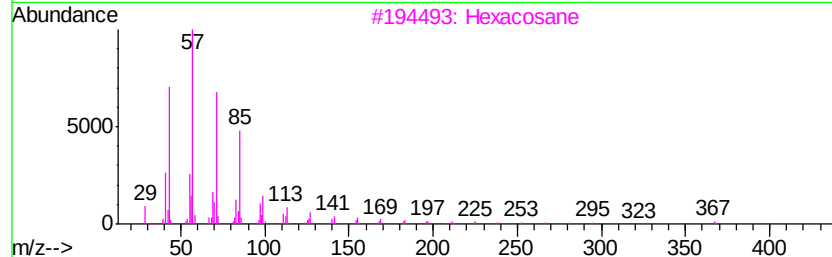
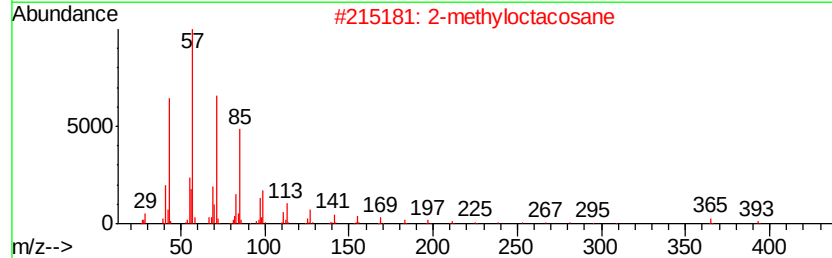
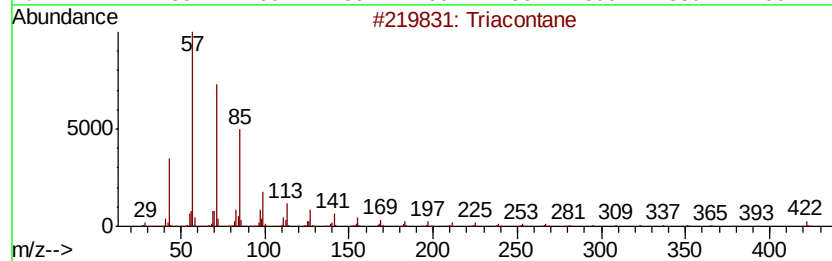
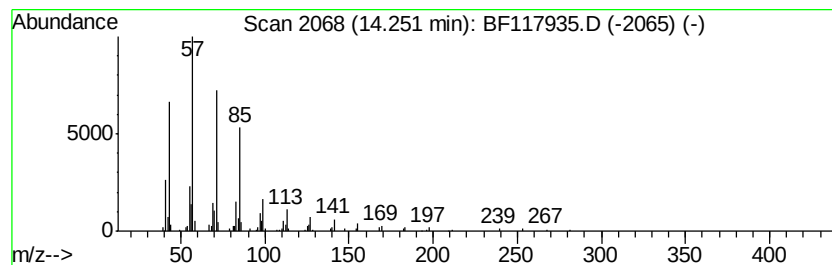
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Triacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.11 ng	175591	Chrysene-d12	14.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triacontane	422 C30H62	000638-68-6 91
2		2-methyloctacosane	408 C29H60	1000376-72-8 91
3		Hexacosane	366 C26H54	000630-01-3 91
4		Heneicosane	296 C21H44	000629-94-7 91
5		Eicosane, 2-methyl-	296 C21H44	001560-84-5 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117935.D
Acq On : 22 Nov 2019 23:08
Operator : JU
Sample : K5839-03
Misc :
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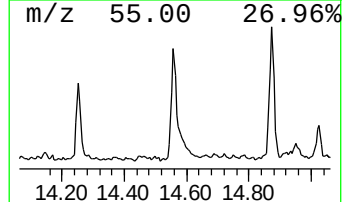
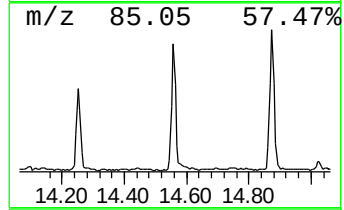
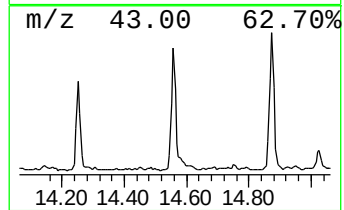
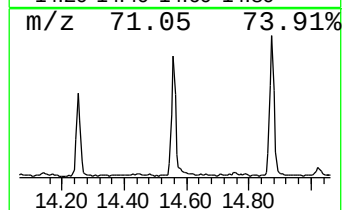
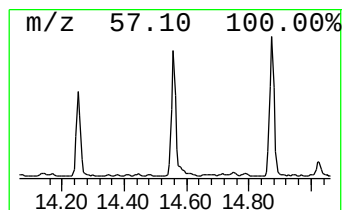
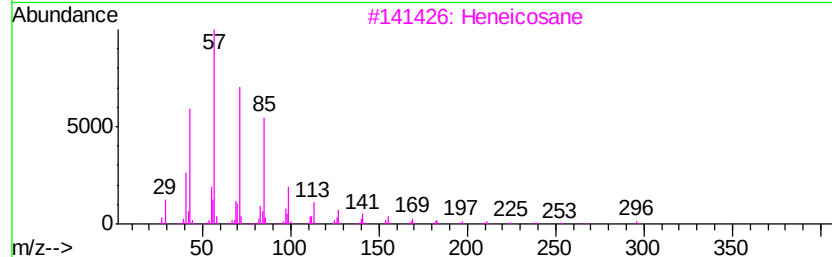
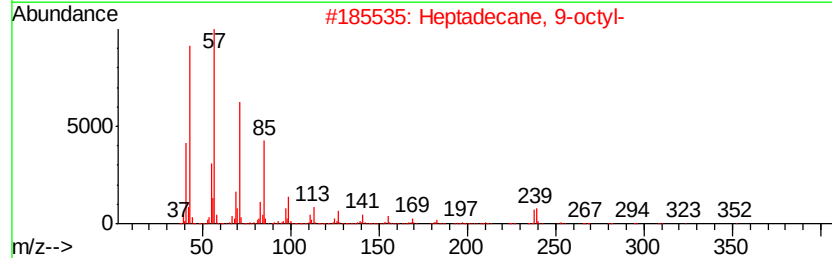
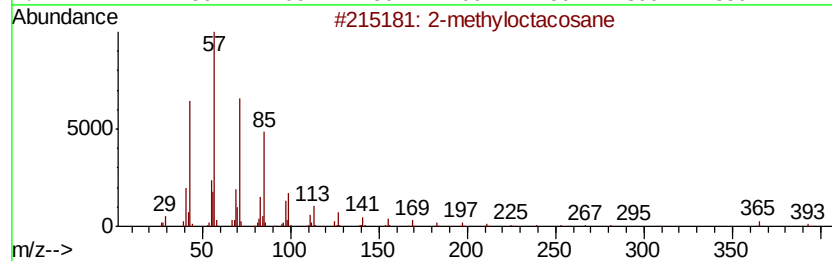
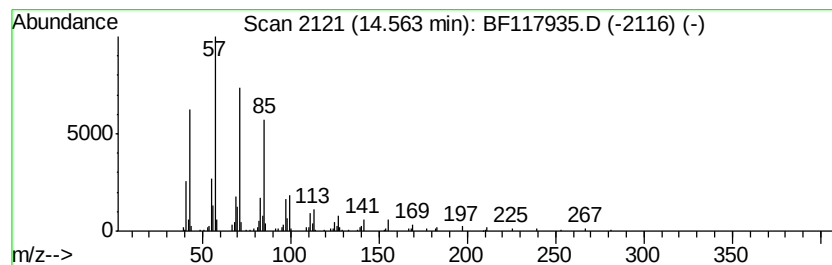
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	4.30 ng	357362	Chrysene-d12	14.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-methyloctacosane	408 C29H60	1000376-72-8	91
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Octacosane	394 C28H58	000630-02-4	91
5	Hexacosane	366 C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
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Misc :
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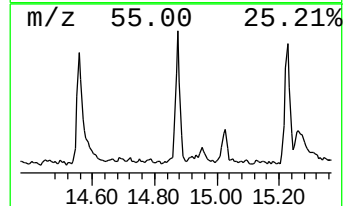
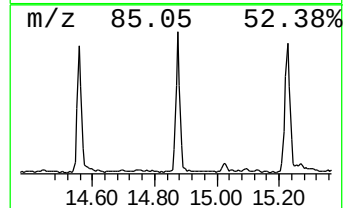
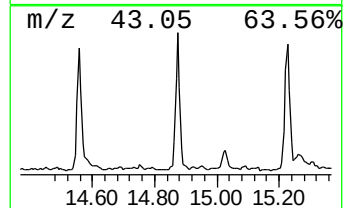
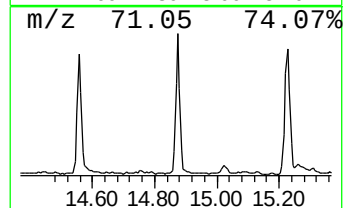
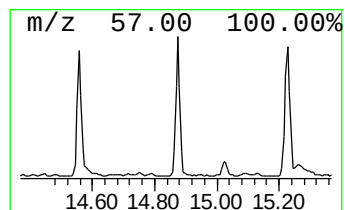
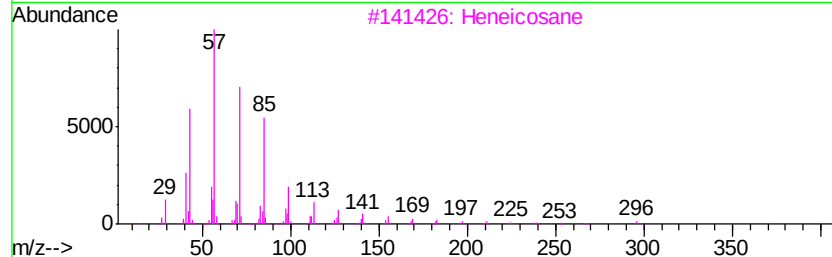
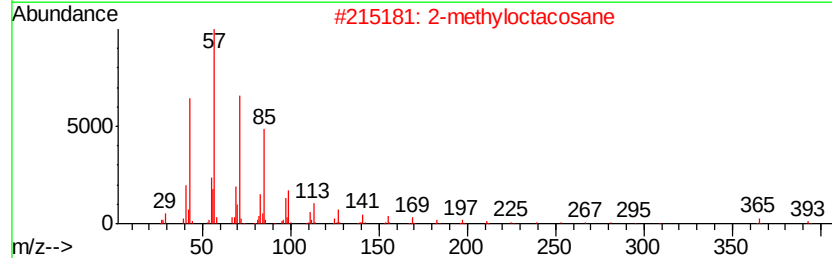
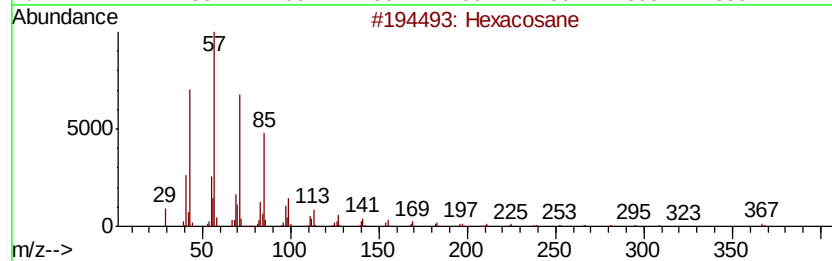
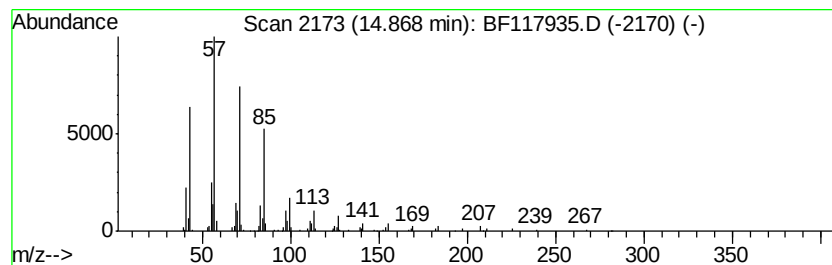
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.87	4.35 ng	301172	Perylene-d12		15.59	
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	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117935.D
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Misc :
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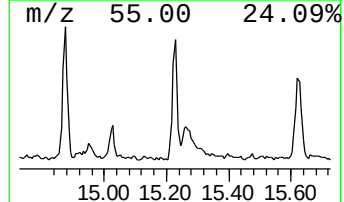
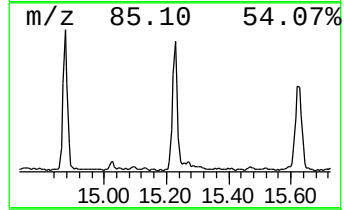
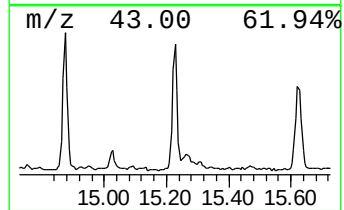
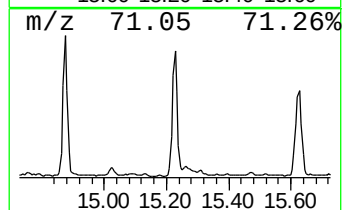
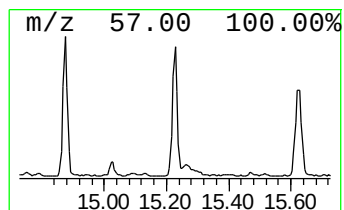
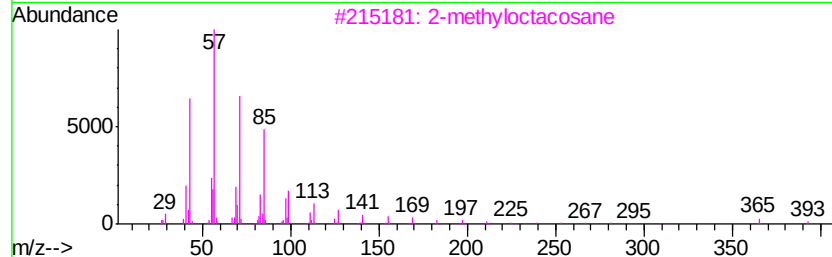
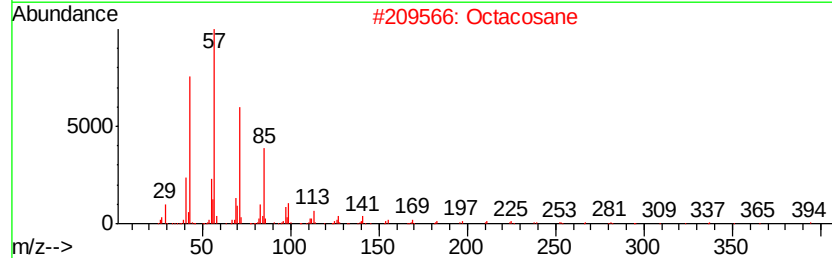
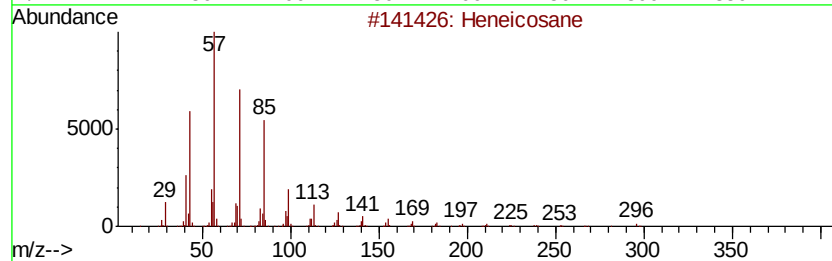
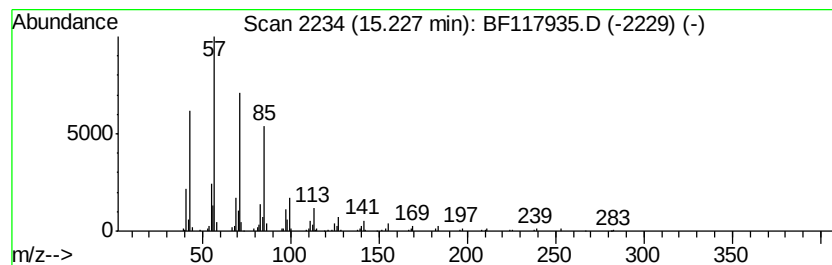
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	4.76 ng	329105	Perylene-d12	15.59
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Octacosane	394 C28H58	000630-02-4	91
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
5	Heptacosane	380 C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
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Acq On : 22 Nov 2019 23:08
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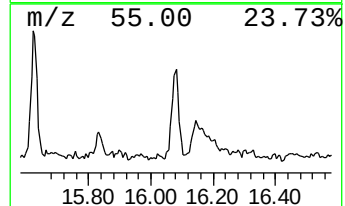
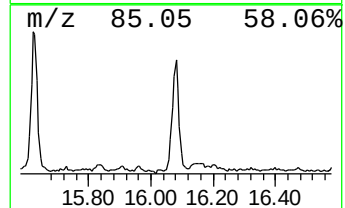
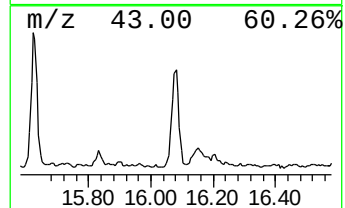
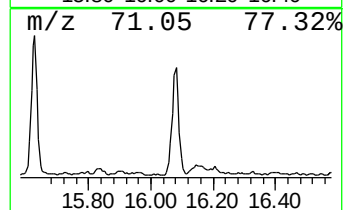
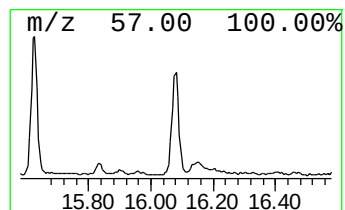
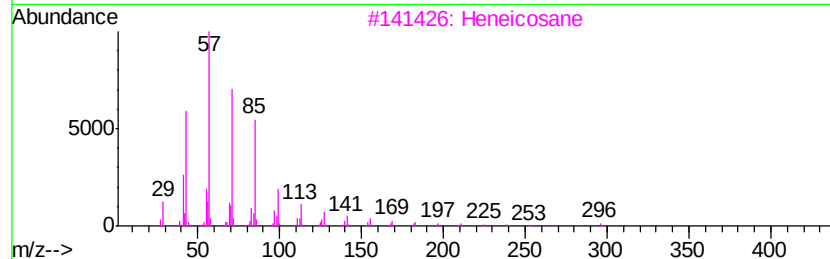
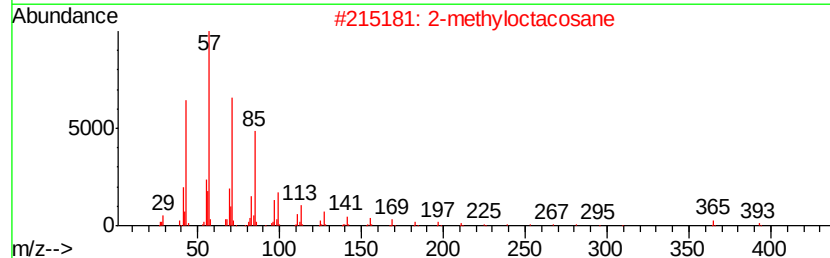
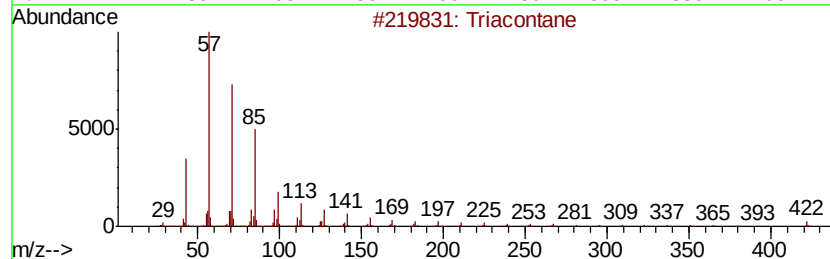
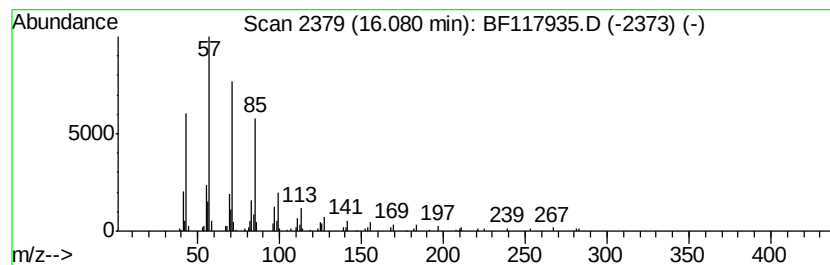
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptadecane, 9-octyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.28 ng	226982	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	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\BF112219\
Data File : BF117935.D
Acq On : 22 Nov 2019 23:08
Operator : JU
Sample : K5839-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-NW-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.22	11.1 ng		641641	1	6.90	1155340	20.0
2-Pentanone, 4-hy...	5.12	17.1 ng		988978	1	6.90	1155340	20.0
unknown6.67	6.67	69.5 ng		4011990	1	6.90	1155340	20.0
n-Hexadecanoic acid	11.97	6.4 ng		647924	4	11.45	2028400	20.0
1-Hexadecanol	12.67	2.1 ng		210266	4	11.45	2028400	20.0
Octadecanoic acid	12.76	4.0 ng		411233	4	11.45	2028400	20.0
Ethanol, 2-(tetra...	13.93	8.4 ng		699511	5	14.09	1662670	20.0
triacontane	14.25	2.1 ng		175591	5	14.09	1662670	20.0
2-methyloctacosane	14.56	4.3 ng		357362	5	14.09	1662670	20.0
Hexacosane	14.87	4.3 ng		301172	6	15.59	1383530	20.0
Heneicosane	15.23	4.8 ng		329105	6	15.59	1383530	20.0
Heptadecane, 9-oc...	16.08	3.3 ng		226982	6	15.59	1383530	20.0