

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072519\
 Data File : BF115762.D
 Acq On : 25 Jul 2019 16:53
 Operator : HP/JU
 Sample : K3990-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-B

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-BF071219.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	2.152	7	11	18	rVB	418573	571423	12.87%	1.199%
2	5.492	575	579	599	rBV	569830	1519202	34.22%	3.189%
3	5.628	599	602	613	rVB	183159	302751	6.82%	0.635%
4	6.016	662	668	675	rVB	75868	107205	2.41%	0.225%
5	6.498	745	750	753	rBV	2625984	2778670	62.59%	5.833%
6	6.639	770	774	778	rBV	3050814	2941487	66.25%	6.174%
7	6.687	780	782	792	rVB	50735	67291	1.52%	0.141%
8	6.869	810	813	818	rVB	981959	773596	17.42%	1.624%
9	7.028	836	840	843	rBV	2763464	2339806	52.70%	4.911%
10	7.428	903	908	911	rBV	1982209	1870288	42.13%	3.926%
11	8.151	1027	1031	1050	rBV	1105188	1035884	23.33%	2.174%
12	9.228	1209	1214	1217	rBV	3863549	3594985	80.97%	7.546%
13	9.616	1276	1280	1294	rBV	548688	492765	11.10%	1.034%
14	9.904	1325	1329	1342	rBV	1431166	1288664	29.03%	2.705%
15	10.692	1459	1463	1481	rBV	2402250	2580811	58.13%	5.417%
16	11.392	1578	1582	1590	rBV	1498056	1393362	31.38%	2.925%
17	11.916	1667	1671	1693	rBV	584769	729167	16.42%	1.531%
18	12.698	1800	1804	1817	rBV	252748	348724	7.85%	0.732%
19	12.974	1846	1851	1854	rBV	4262927	4439722	100.00%	9.319%
20	13.833	1993	1997	2000	rBV	75416	80321	1.81%	0.169%
21	13.874	2000	2004	2007	rVV	144469	128728	2.90%	0.270%
22	13.927	2007	2013	2026	rVV3	125351	483802	10.90%	1.016%
23	14.027	2026	2030	2040	rVB	1409385	1351669	30.44%	2.837%
24	14.163	2049	2053	2055	rBV	295418	275555	6.21%	0.578%
25	14.186	2055	2057	2066	rVB	423475	401271	9.04%	0.842%
26	14.474	2102	2106	2108	rBV	589263	684718	15.42%	1.437%
27	14.498	2108	2110	2120	rVB	922063	797756	17.97%	1.675%
28	14.804	2155	2162	2170	rBV	1710573	2495472	56.21%	5.238%
29	14.880	2171	2175	2178	rVB	46816	49629	1.12%	0.104%
30	15.139	2213	2219	2229	rBV	1901727	2988189	67.31%	6.272%
31	15.374	2253	2259	2265	rBV3	56342	112998	2.55%	0.237%
32	15.521	2275	2284	2299	rBV2	1928210	4237897	95.45%	8.896%
33	15.786	2324	2329	2334	rVV	58024	88658	2.00%	0.186%
34	15.839	2334	2338	2344	rVB2	29325	49642	1.12%	0.104%

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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-BF071219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.957	2350	2358	2369	rBV	1308139	2373349	53.46%	4.982%
36	16.268	2408	2411	2417	rVB	29222	45423	1.02%	0.095%
37	16.462	2436	2444	2463	rBV	649034	1310300	29.51%	2.750%
38	17.056	2537	2545	2553	rBV2	177278	393436	8.86%	0.826%
39	17.756	2660	2664	2675	rVB4	46928	116202	2.62%	0.244%

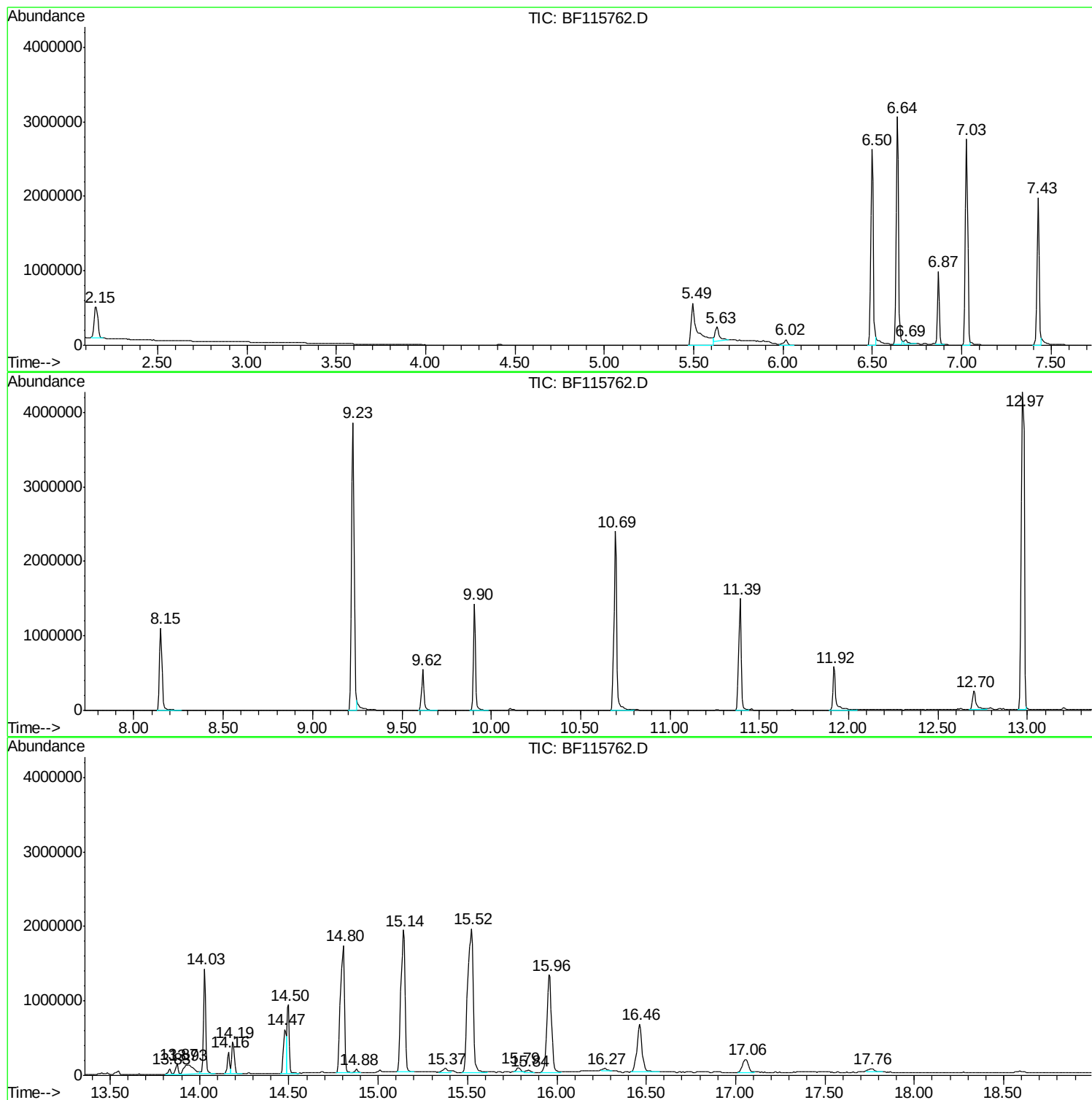
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BNA_F
ClientSampled :
TP-1-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.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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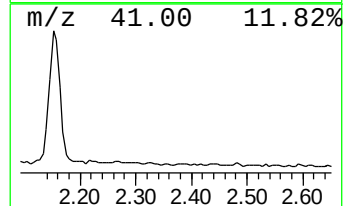
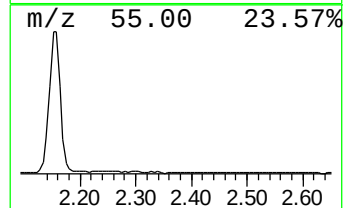
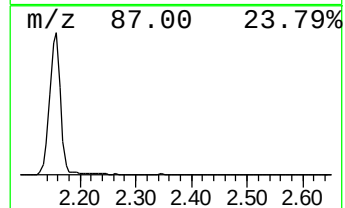
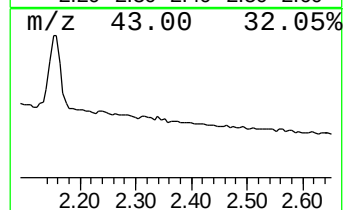
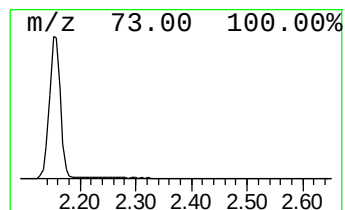
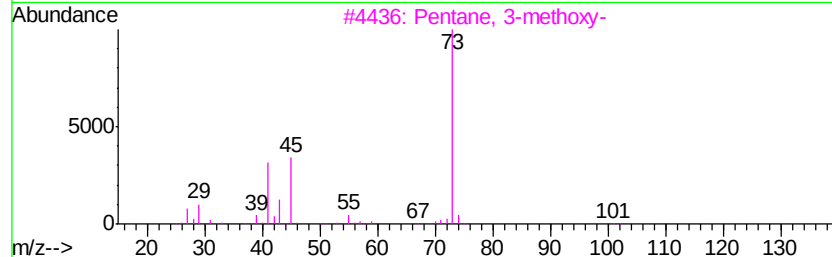
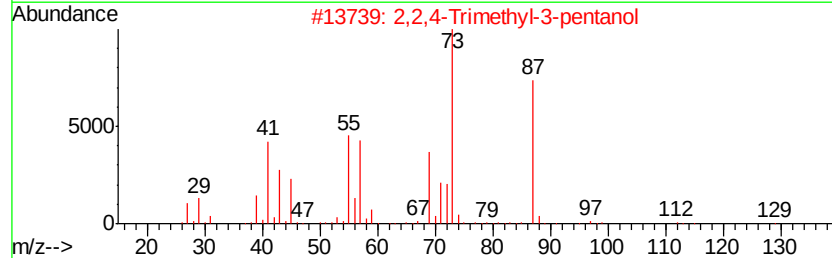
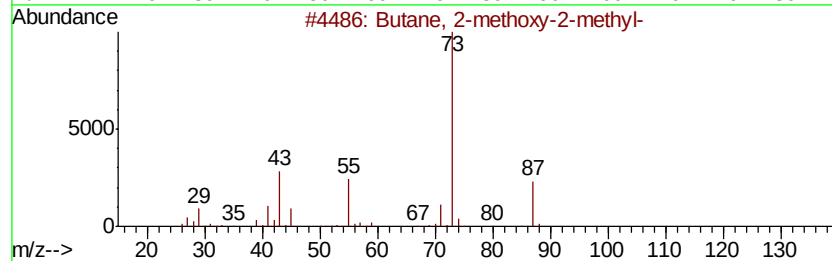
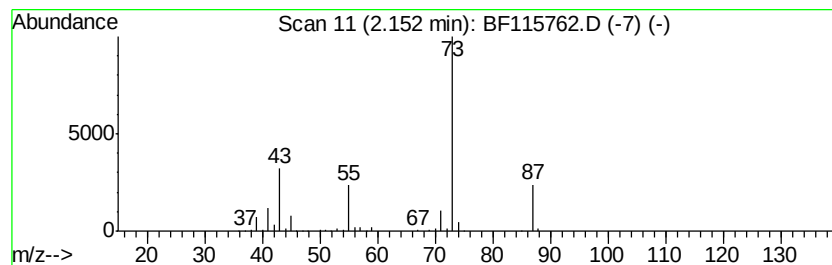
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	14.77 ng	571423	1,4-Dichlorobenzene-d4	6.87

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	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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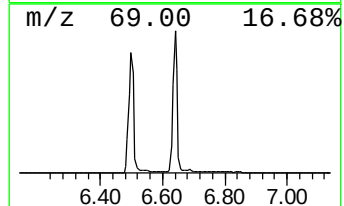
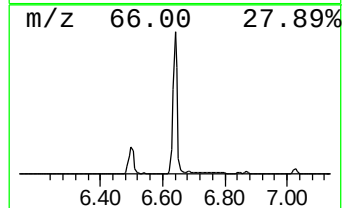
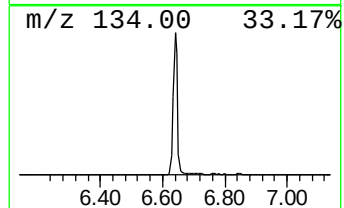
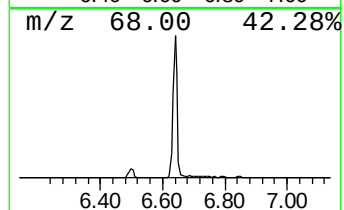
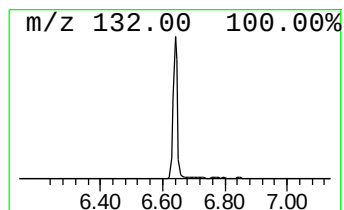
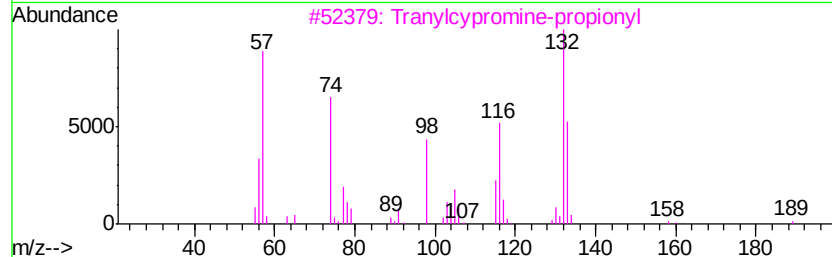
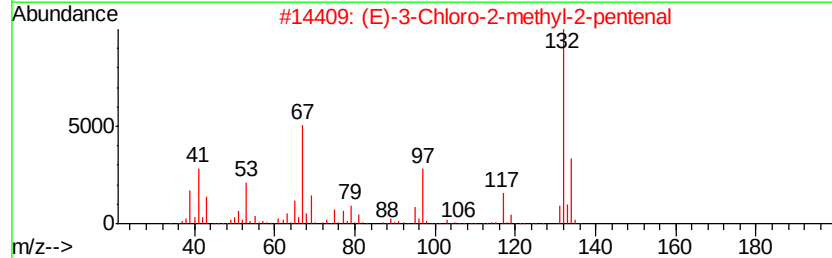
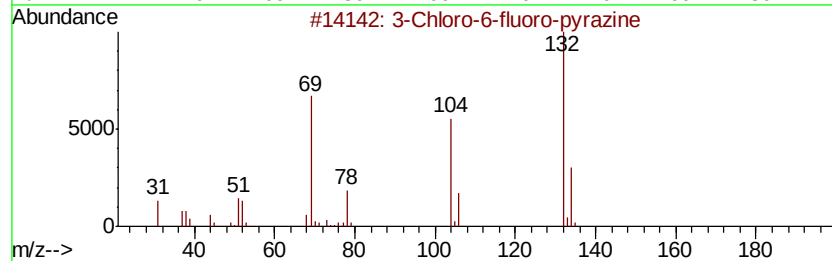
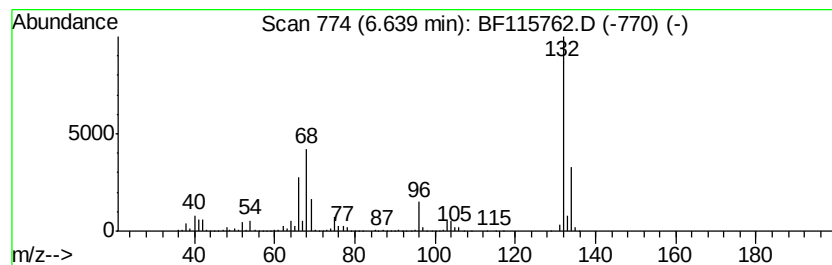
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	76.05 ng	2941490	1,4-Dichlorobenzene-d4	6.87

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
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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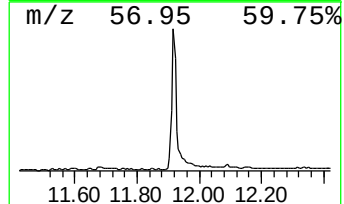
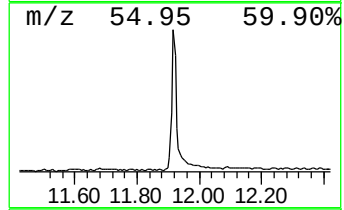
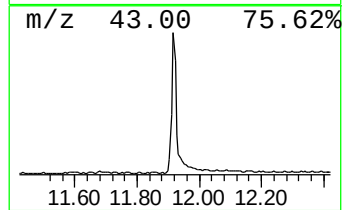
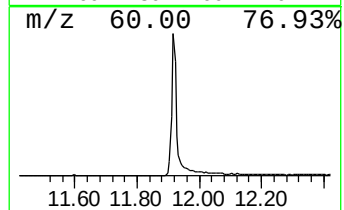
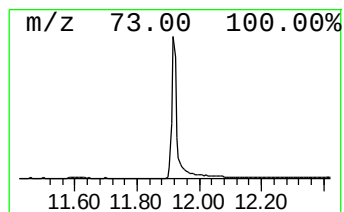
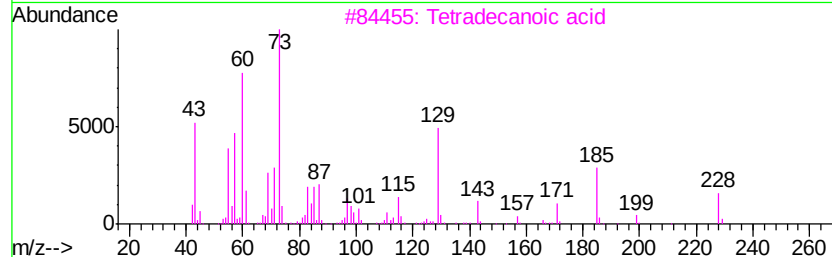
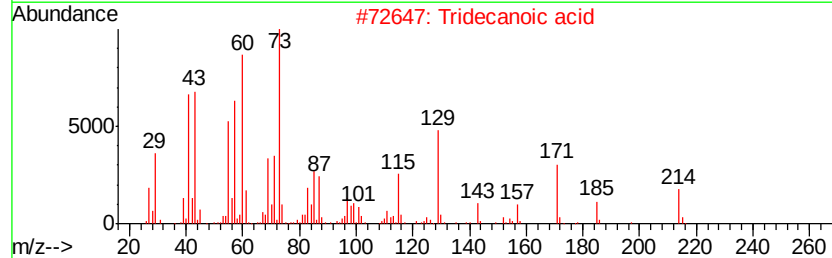
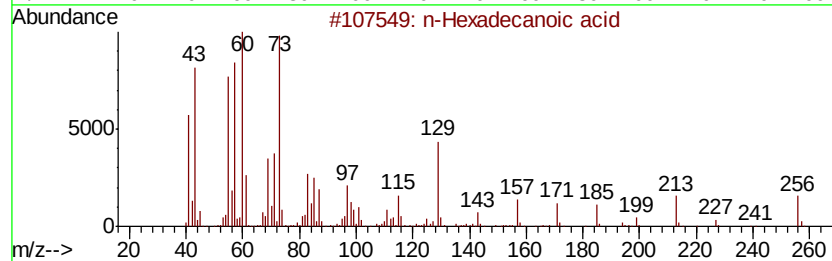
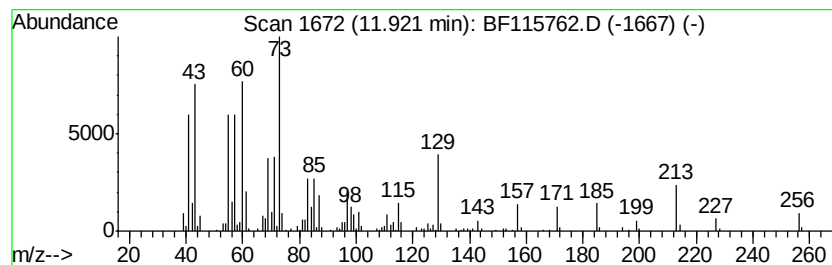
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	10.47 ng	729167	Phenanthrene-d10	11.39

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	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		Dodecanoic acid	200	C12H24O2	000143-07-7	25



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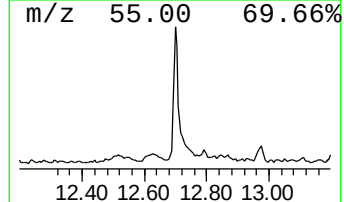
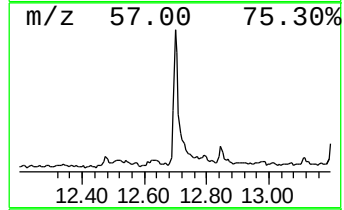
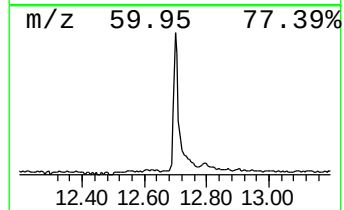
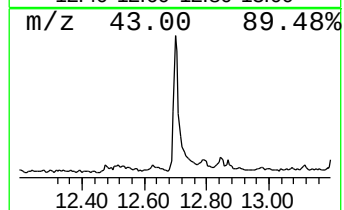
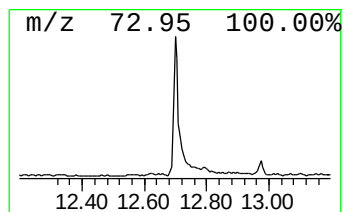
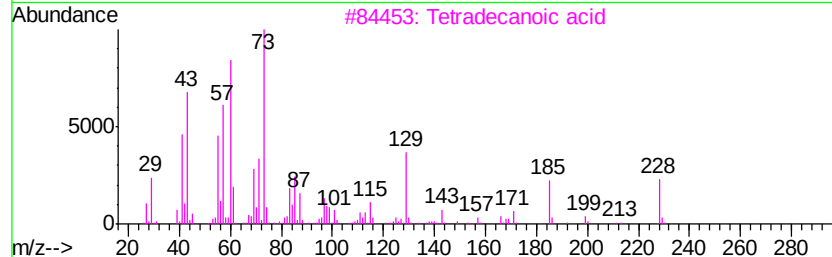
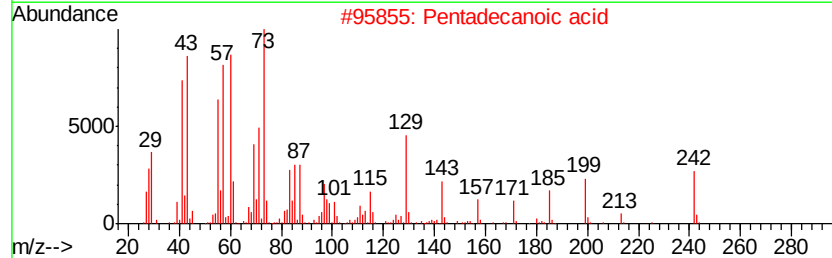
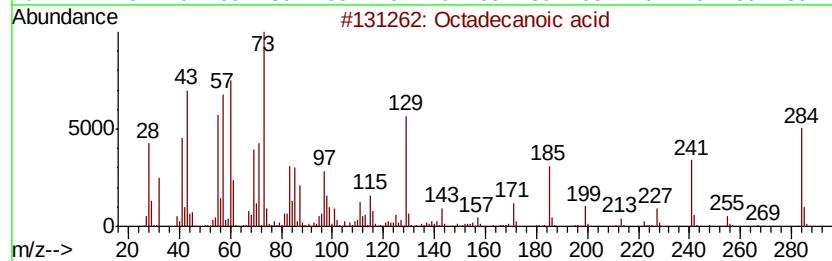
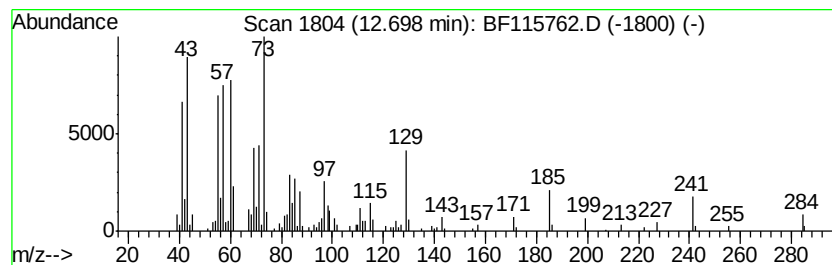
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	5.01 ng	348724	Phenanthrene-d10	11.39

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	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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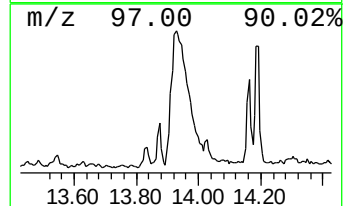
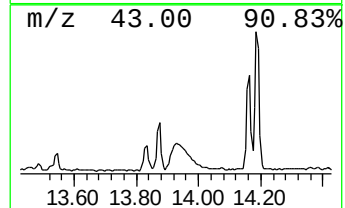
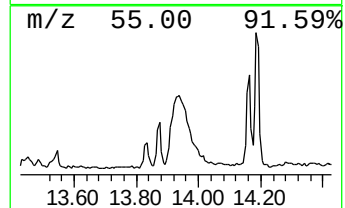
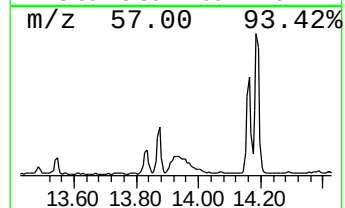
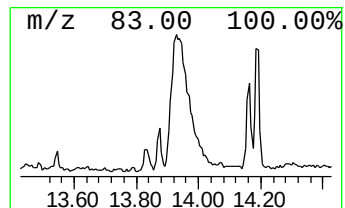
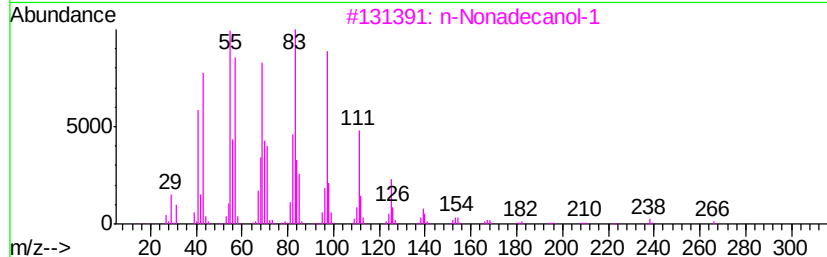
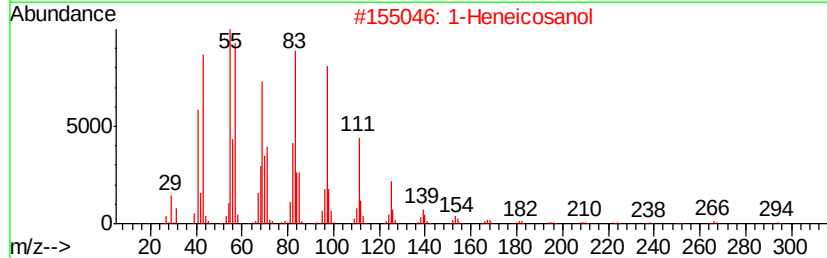
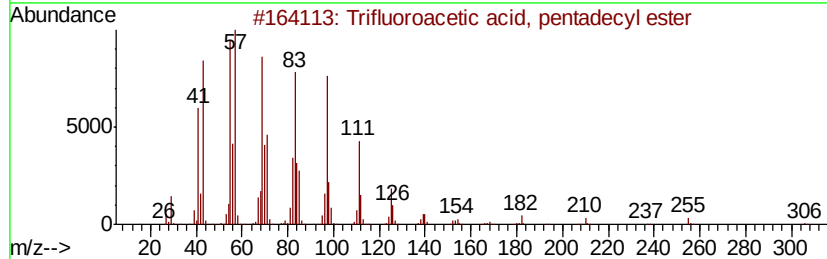
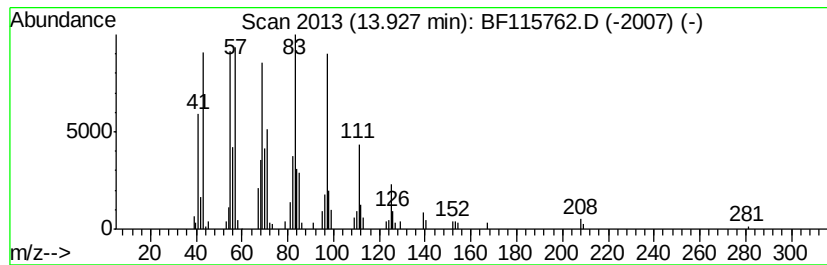
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.16 ng	483802	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	95



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Operator : HP/JU
Sample : K3990-02
Misc :
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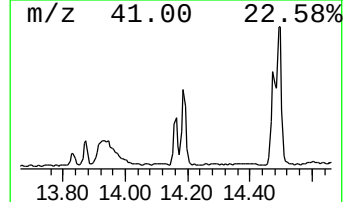
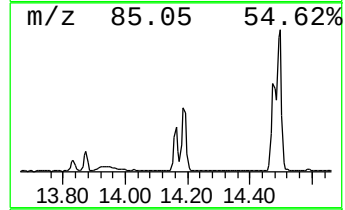
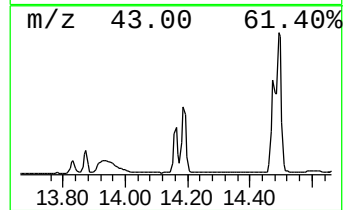
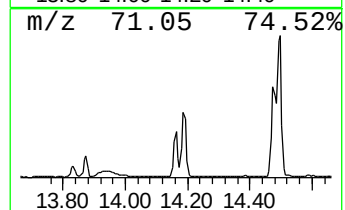
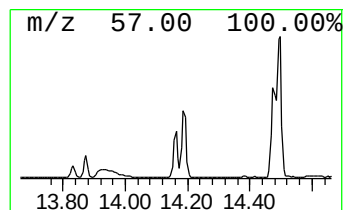
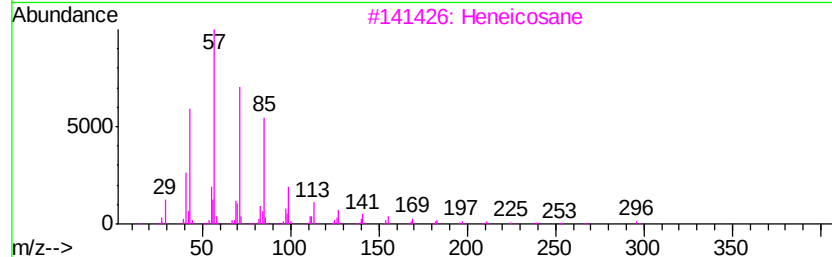
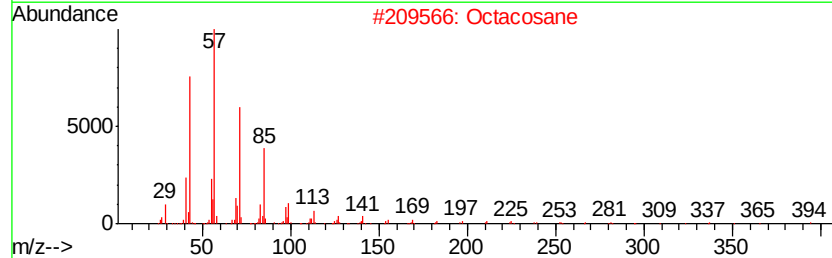
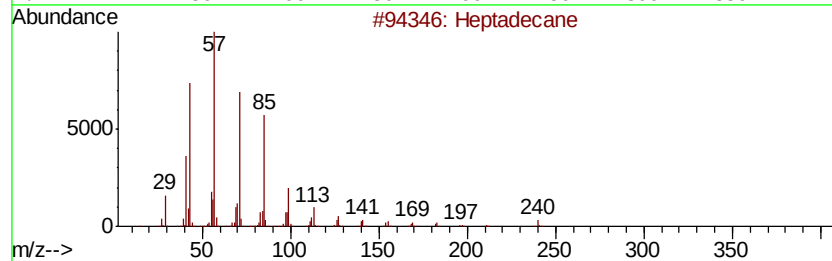
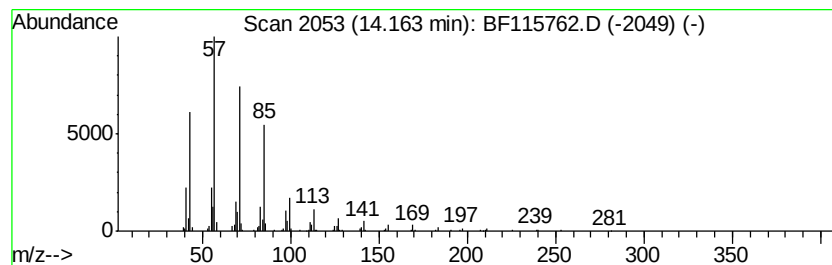
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ClientSampleId :
TP-1-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.16	4.08 ng	275555	Chrysene-d12		14.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
Data File : BF115762.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1-B

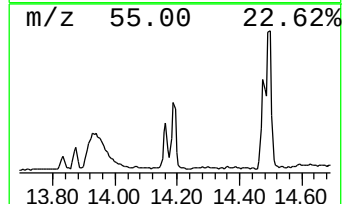
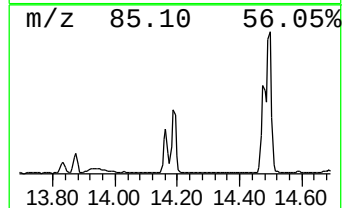
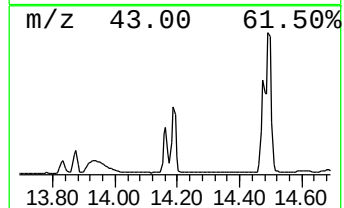
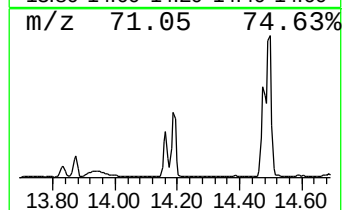
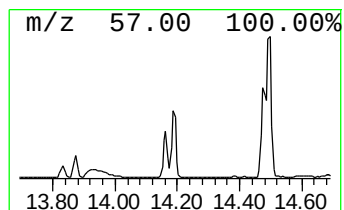
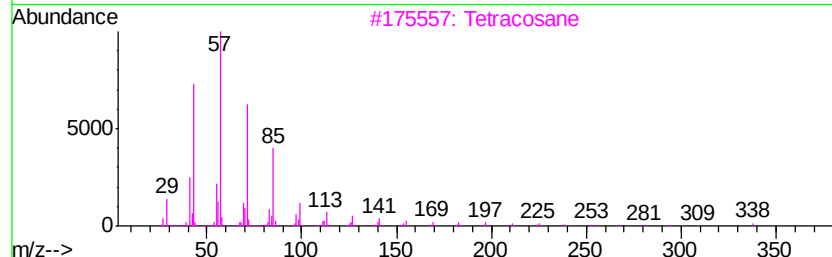
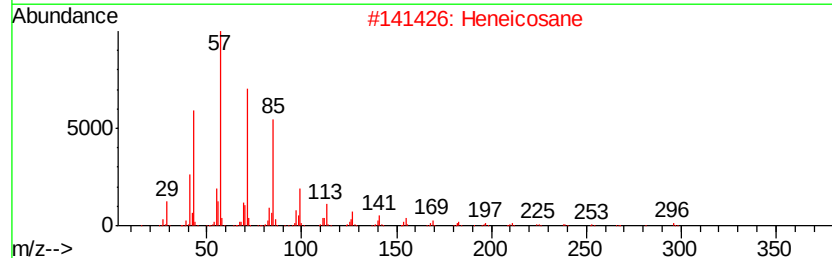
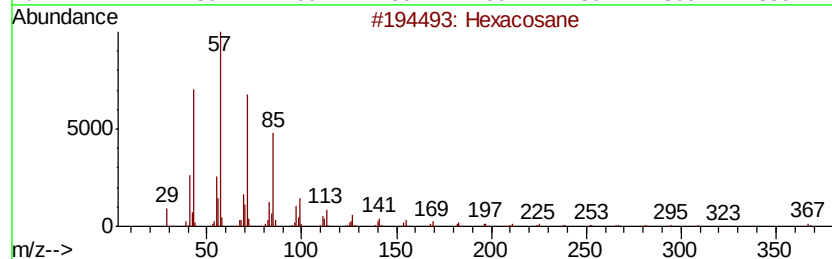
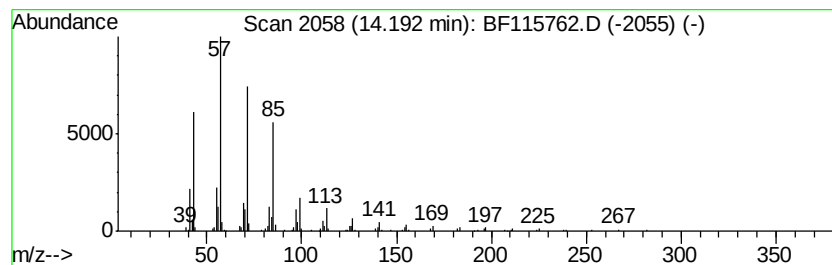
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	5.94 ng	401271	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexadecane	226	C16H34	000544-76-3	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
Data File : BF115762.D
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Sample : K3990-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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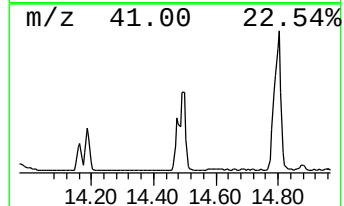
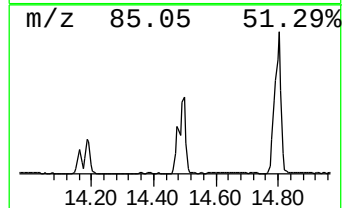
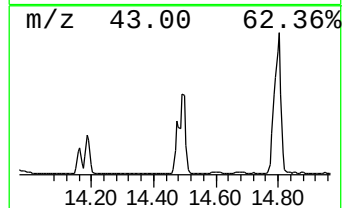
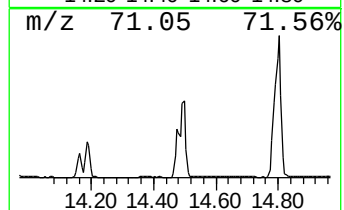
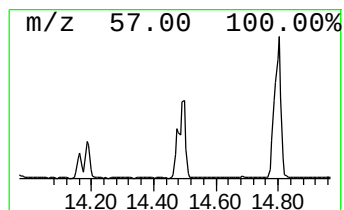
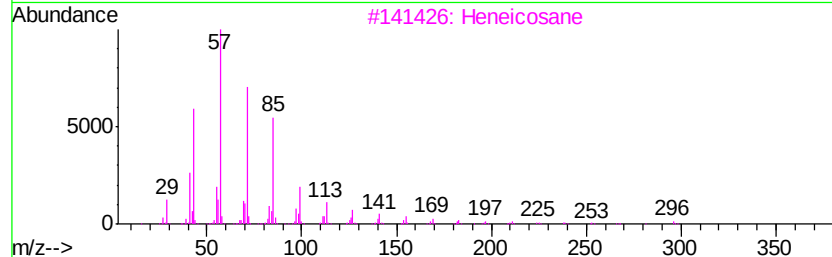
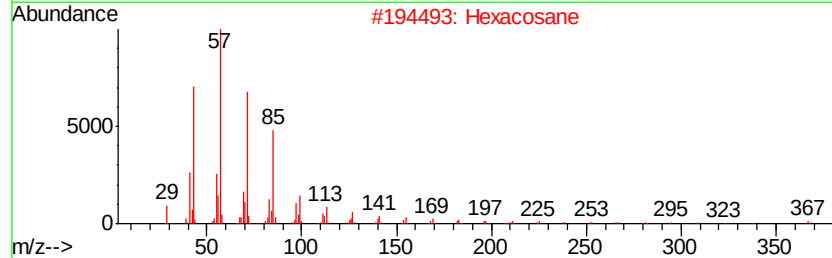
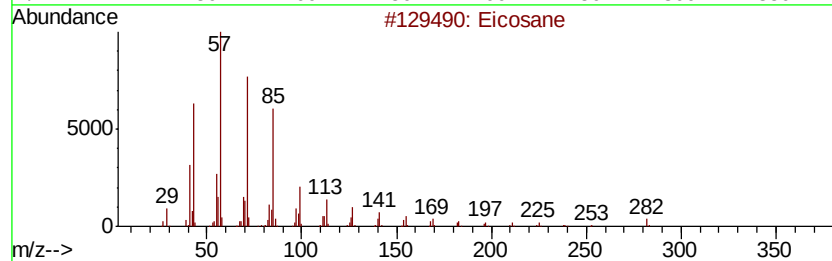
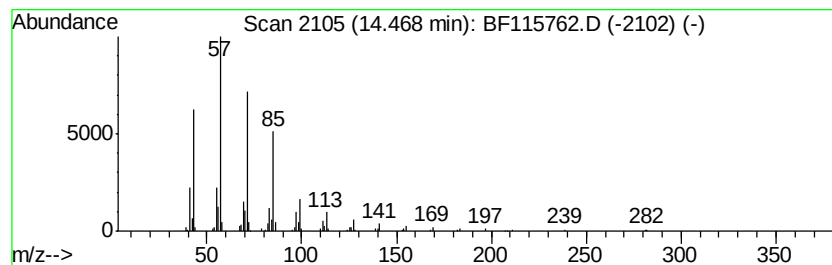
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	10.13 ng	684718	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
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Sample : K3990-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

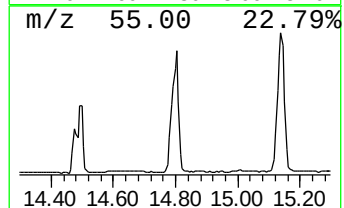
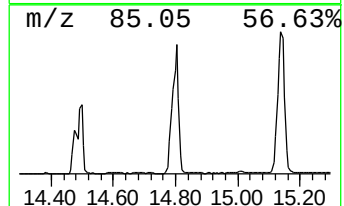
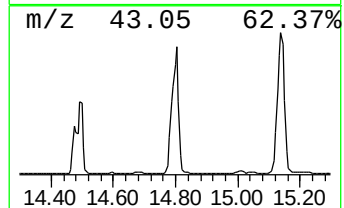
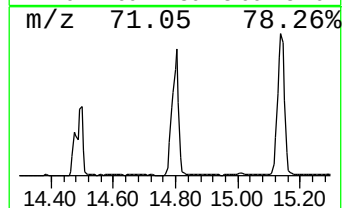
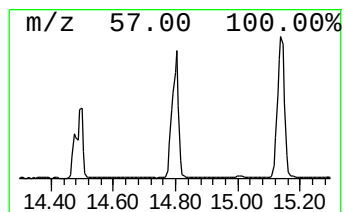
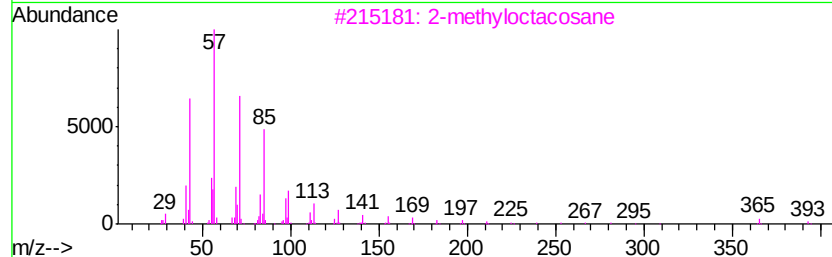
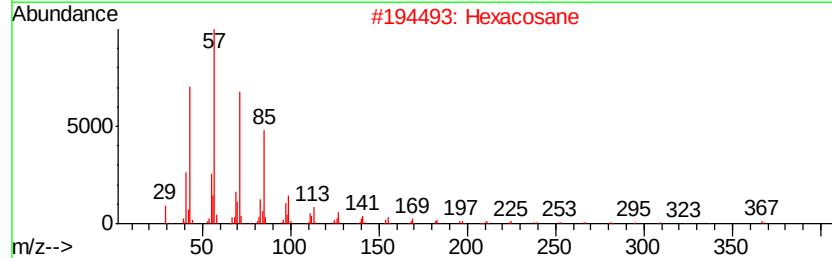
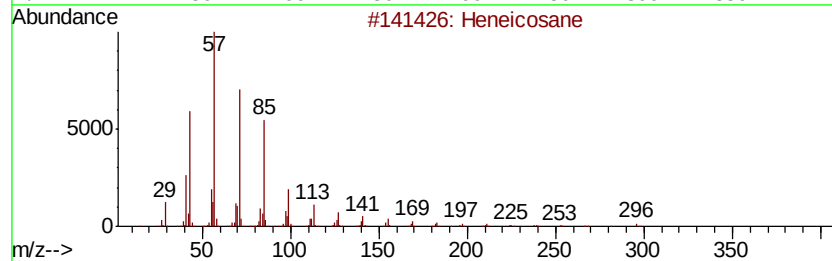
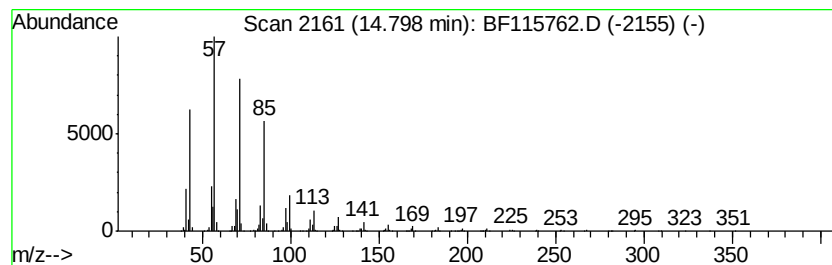
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	11.78 ng	2495470	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296	C21H44	000629-94-7 91
2	Hexacosane	366	C26H54	000630-01-3 91
3	2-methyloctacosane	408	C29H60	1000376-72-8 91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8 90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
Data File : BF115762.D
Acq On : 25 Jul 2019 16:53
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Sample : K3990-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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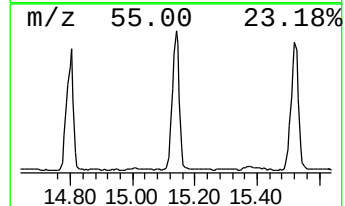
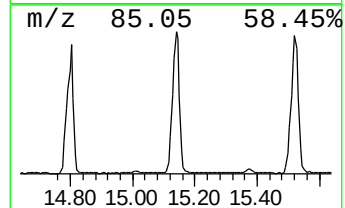
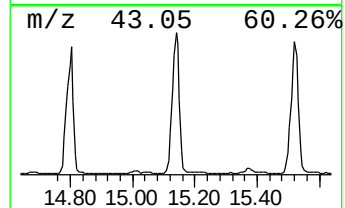
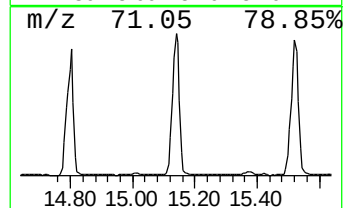
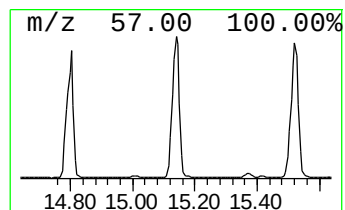
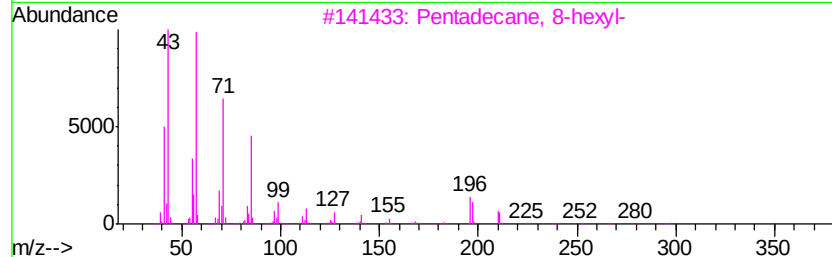
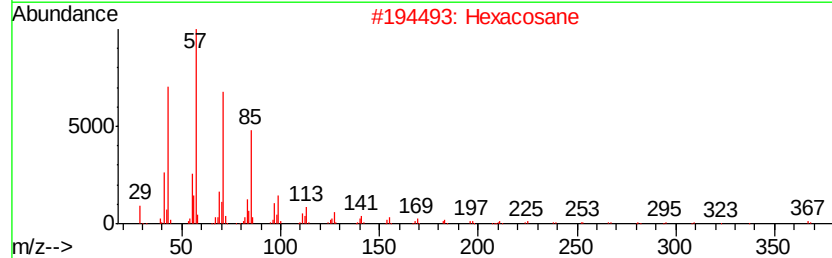
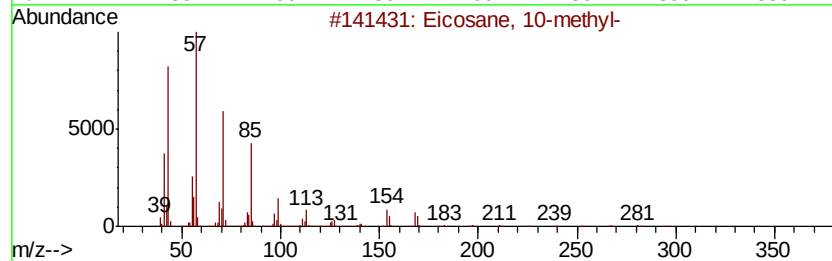
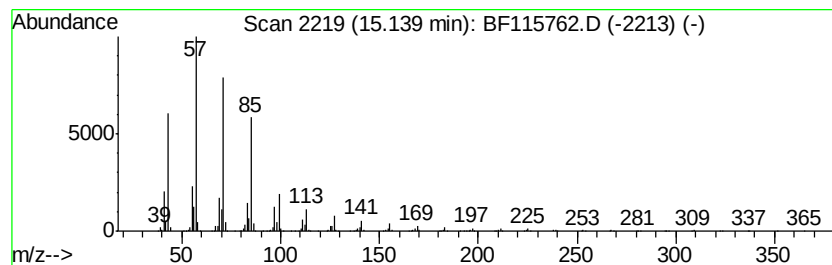
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane, 10-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	14.10 ng	2988190	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072519\
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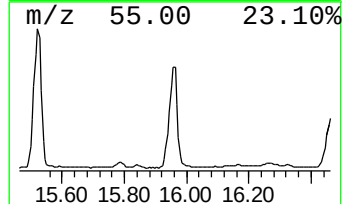
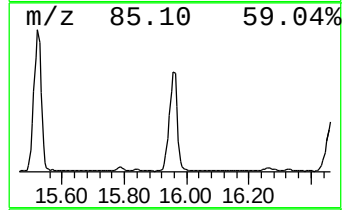
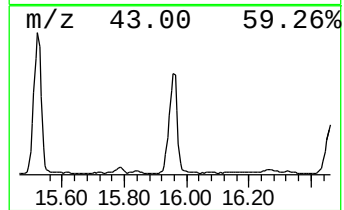
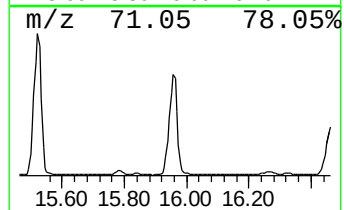
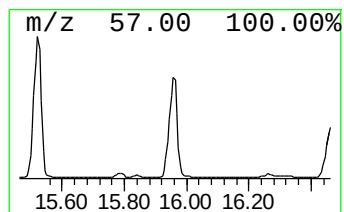
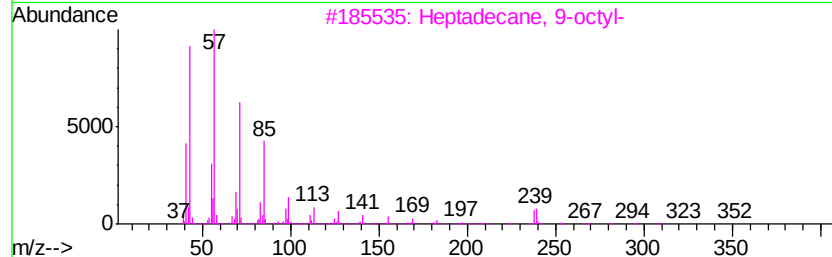
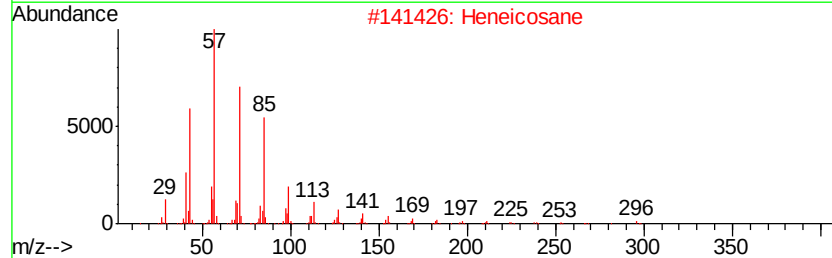
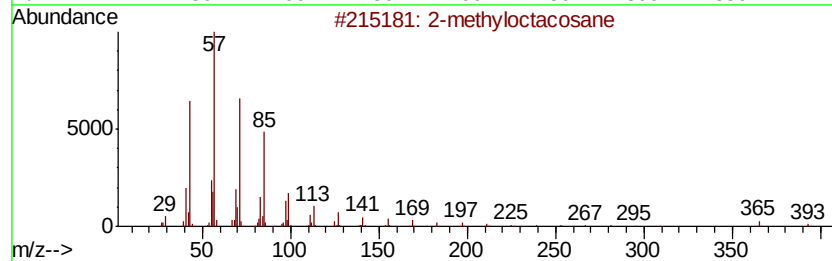
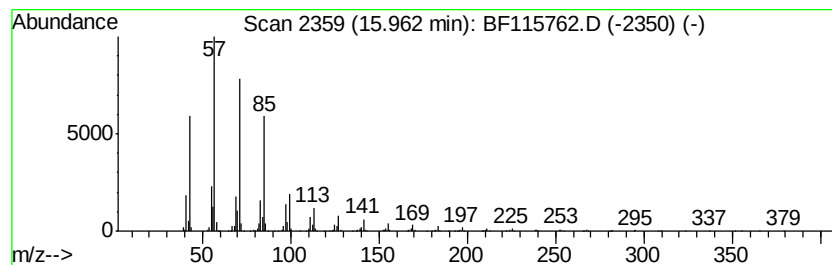
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 15 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	11.20 ng	2373350	Perylene-d12	15.50

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		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072519\
Data File : BF115762.D
Acq On : 25 Jul 2019 16:53
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Sample : K3990-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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...	2.15	14.8	ng	571423	1	6.87	773596	20.0
unknown6.64	6.64	76.0	ng	2941490	1	6.87	773596	20.0
n-Hexadecanoic acid	11.92	10.5	ng	729167	4	11.39	1393360	20.0
Octadecanoic acid	12.70	5.0	ng	348724	4	11.39	1393360	20.0
Trifluoroacetic a...	13.93	7.2	ng	483802	5	14.03	1351670	20.0
Heptadecane	14.16	4.1	ng	275555	5	14.03	1351670	20.0
Hexacosane	14.19	5.9	ng	401271	5	14.03	1351670	20.0
Eicosane	14.47	10.1	ng	684718	5	14.03	1351670	20.0
Heneicosane	14.80	11.8	ng	2495470	6	15.50	4237900	20.0
Eicosane, 10-methyl-	15.14	14.1	ng	2988190	6	15.50	4237900	20.0
2-methyloctacosane	15.96	11.2	ng	2373350	6	15.50	4237900	20.0