

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
 Data File : BF118296.D
 Acq On : 19 Dec 2019 23:07
 Operator : JU
 Sample : K6350-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-1-3

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-BF120619.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	5.063	502	506	519	rVB	266368	331102	13.06%	1.440%
2	5.475	572	576	596	rBV	1871922	1822449	71.91%	7.927%
3	6.134	684	688	692	rBV	136223	108641	4.29%	0.473%
4	6.487	744	748	758	rBV	1918112	1975947	77.96%	8.595%
5	6.557	758	760	766	rVB	33788	29542	1.17%	0.128%
6	6.628	768	772	775	rVV	2569688	2027888	80.01%	8.820%
7	6.857	808	811	820	rVB	706381	552946	21.82%	2.405%
8	7.016	834	838	841	rBV	1780969	1578217	62.27%	6.865%
9	7.422	903	907	924	rBV	1334750	1196116	47.19%	5.203%
10	8.145	1026	1030	1046	rBV	771414	727942	28.72%	3.166%
11	9.222	1209	1213	1226	rBV	2796315	2341496	92.39%	10.185%
12	9.557	1267	1270	1273	rVB	97714	72595	2.86%	0.316%
13	9.616	1277	1280	1290	rVB	183121	190578	7.52%	0.829%
14	9.875	1321	1324	1326	rBV	79337	59813	2.36%	0.260%
15	9.904	1326	1329	1334	rBV	1028597	838207	33.07%	3.646%
16	10.698	1460	1464	1474	rBV	1731137	1663863	65.65%	7.237%
17	11.398	1579	1583	1586	rBV	1031857	921999	36.38%	4.010%
18	11.422	1586	1587	1592	rVB	178011	119279	4.71%	0.519%
19	11.922	1665	1672	1680	rBV2	440807	470003	18.54%	2.044%
20	12.016	1685	1688	1691	rBV	32762	34542	1.36%	0.150%
21	12.616	1787	1790	1801	rBV	279169	330831	13.05%	1.439%
22	12.710	1803	1806	1813	rVV2	84317	97476	3.85%	0.424%
23	12.845	1824	1829	1836	rVB	179032	208654	8.23%	0.908%
24	12.986	1849	1853	1857	rBV	2833884	2534458	100.00%	11.024%
25	13.463	1930	1934	1938	rBV2	27853	31831	1.26%	0.138%
26	13.751	1980	1983	1987	rBV	69703	64080	2.53%	0.279%
27	13.880	2002	2005	2016	rVB2	203144	278457	10.99%	1.211%
28	14.051	2029	2034	2043	rBV	803466	838116	33.07%	3.645%
29	14.204	2057	2060	2066	rBV	36414	46140	1.82%	0.201%
30	14.510	2108	2112	2121	rBV3	57713	91139	3.60%	0.396%
31	14.815	2161	2164	2169	rVB	62540	61318	2.42%	0.267%
32	14.892	2174	2177	2182	rVB	48012	49097	1.94%	0.214%
33	15.104	2210	2213	2217	rBV2	36834	58653	2.31%	0.255%
34	15.163	2219	2223	2228	rVB	83701	97218	3.84%	0.423%

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ClientSampleId :
RO-1-3

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-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.410	2262	2265	2272	rVB	22028	29723	1.17%	0.129%
36	15.480	2274	2277	2282	rVB2	27706	35061	1.38%	0.153%
37	15.539	2282	2287	2302	rBV	570364	840871	33.18%	3.657%
38	15.992	2360	2364	2369	rBV2	65561	98119	3.87%	0.427%
39	16.051	2369	2374	2382	rBV6	41120	98477	3.89%	0.428%
40	16.504	2447	2451	2456	rBV3	22108	37773	1.49%	0.164%

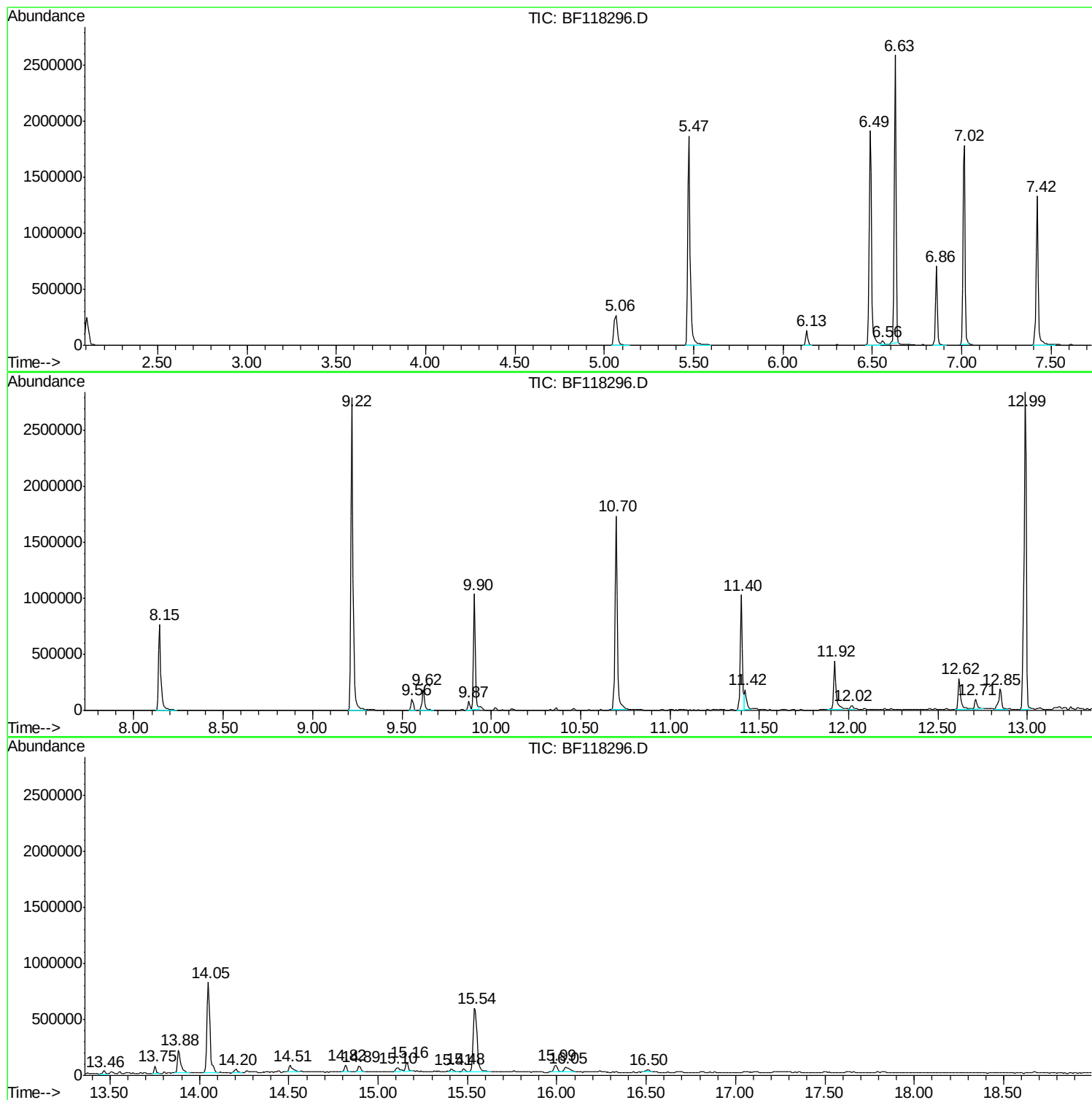
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Instrument :
BNA_F
ClientSampled :
RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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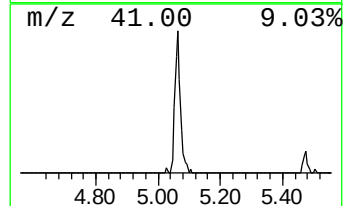
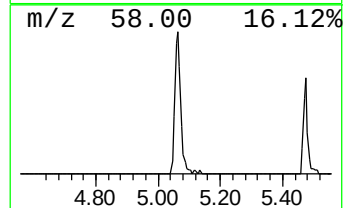
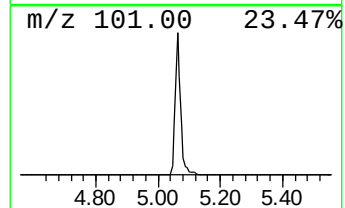
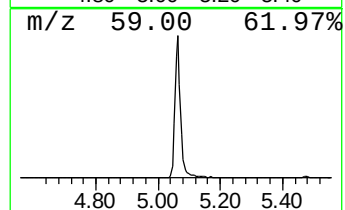
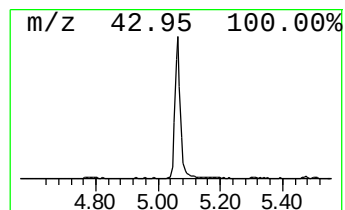
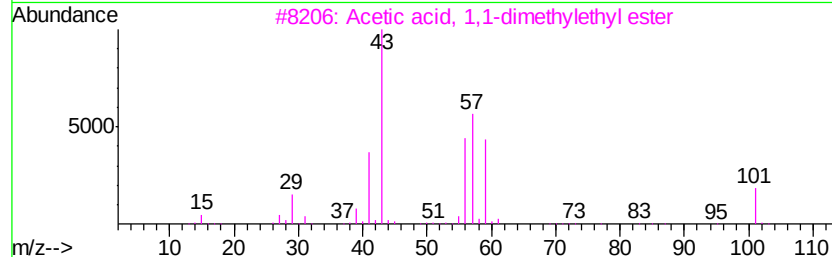
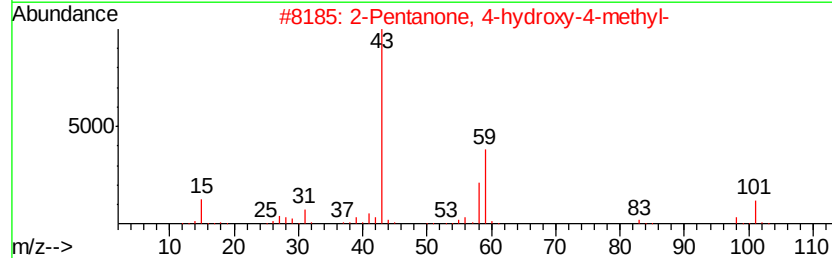
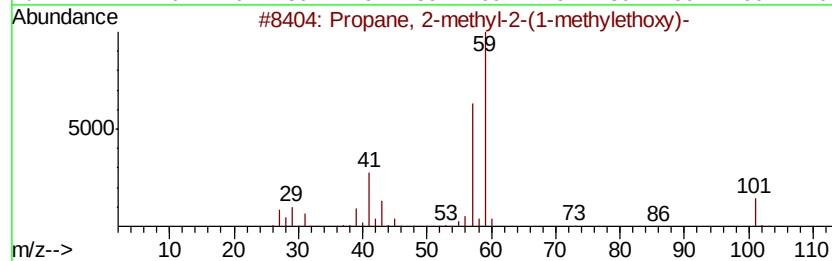
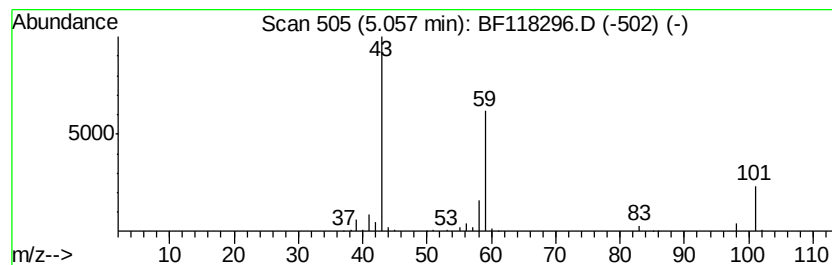
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.06	11.98 ng	331102	1,4-Dichlorobenzene-d4	6.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50	
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17	



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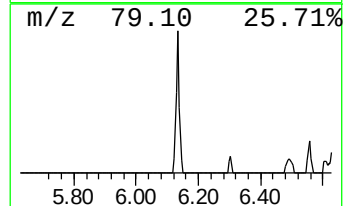
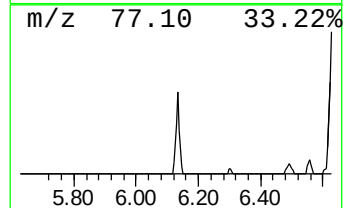
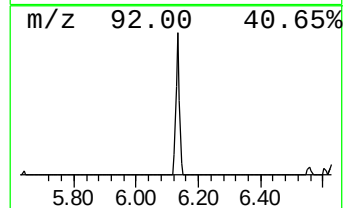
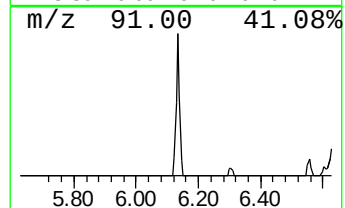
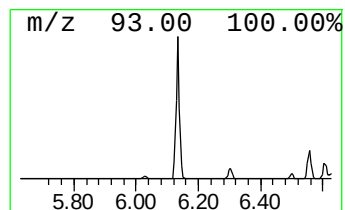
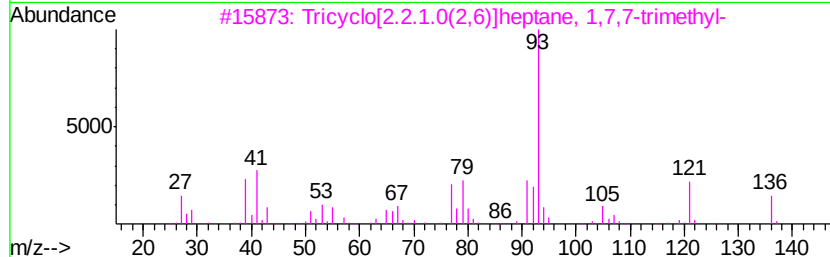
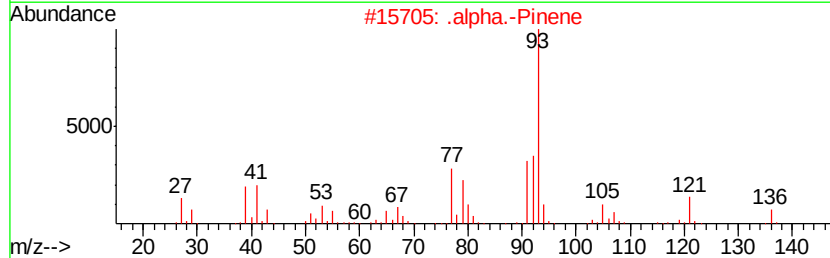
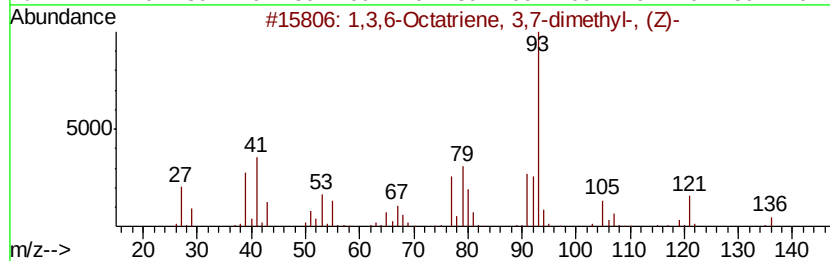
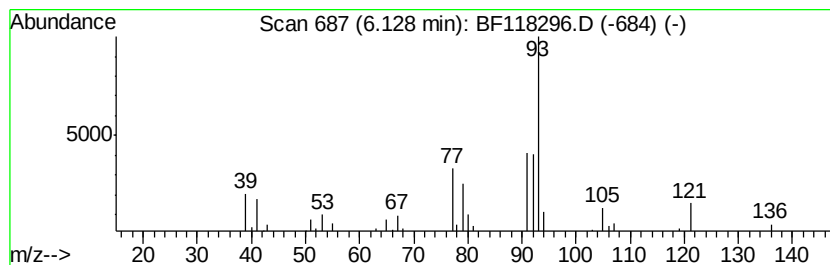
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3,6-Octatriene, 3,7-dimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	3.93 ng	108641	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	91
2		.alpha.-Pinene	136	C10H16	000080-56-8	91
3		Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4		Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	91
5		3,5-Methanocyclopentapyrazole, 3...	164	C10H16N2	087143-58-6	90



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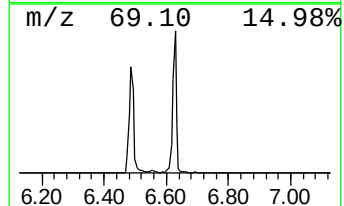
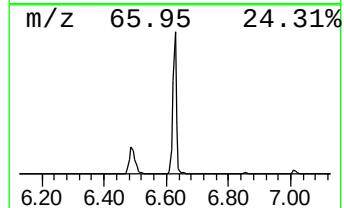
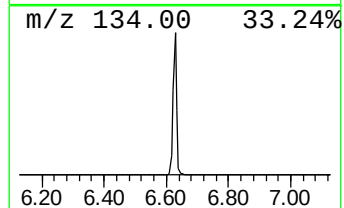
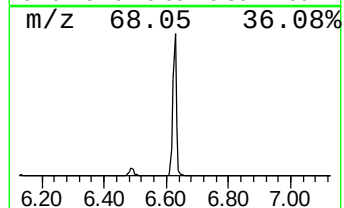
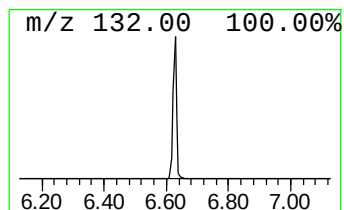
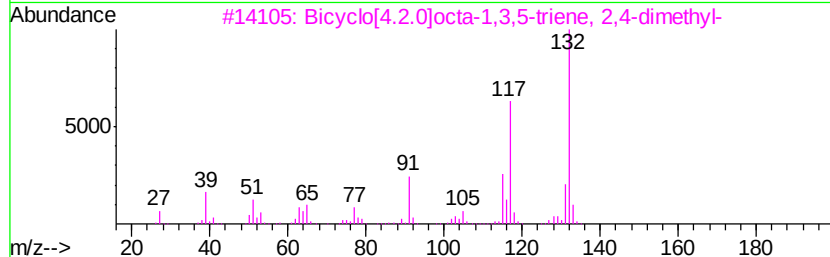
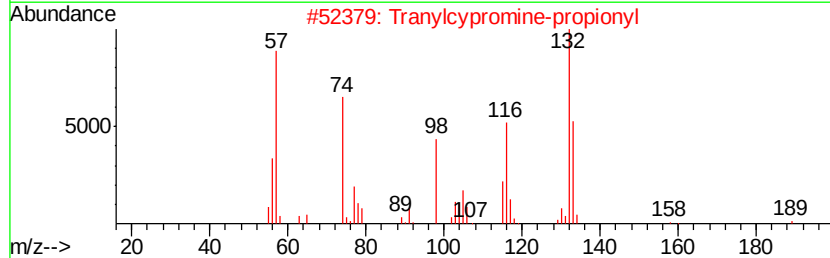
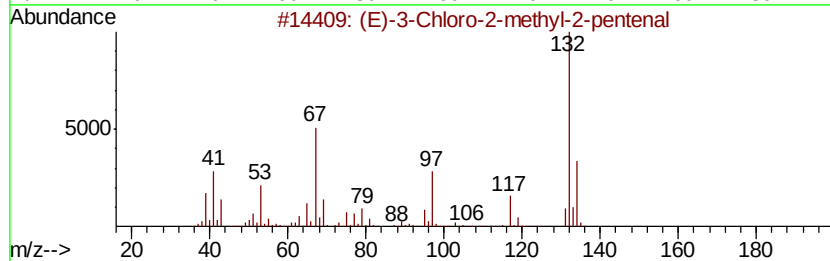
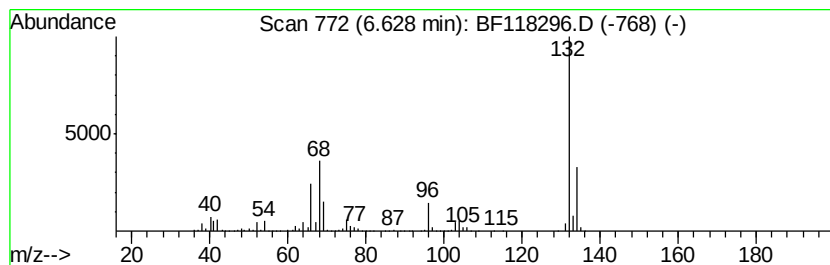
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	73.35 ng	2027890	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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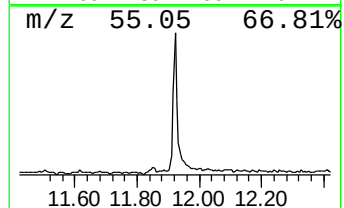
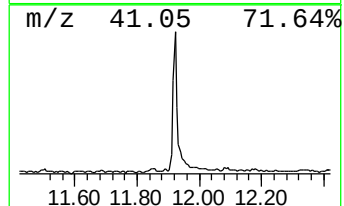
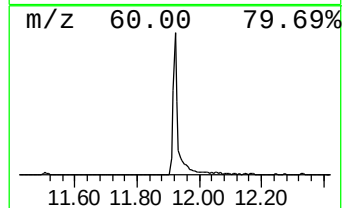
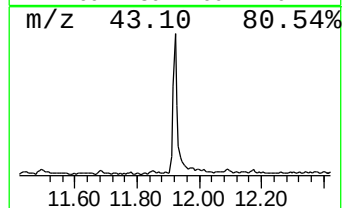
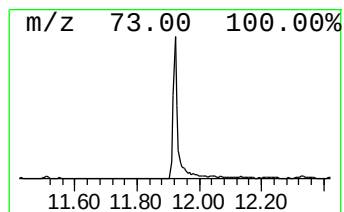
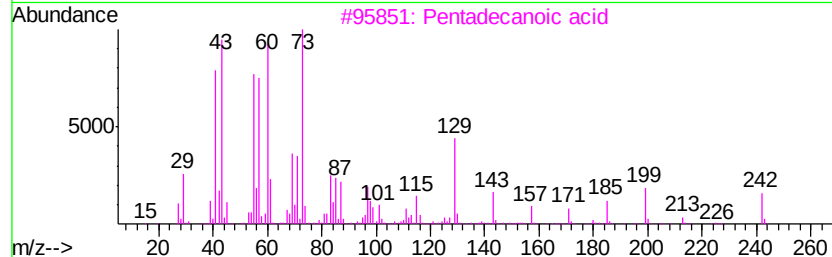
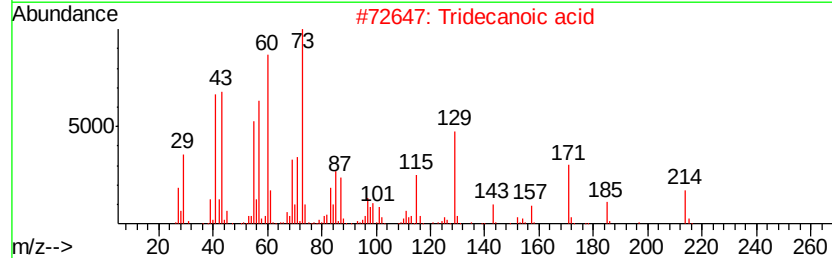
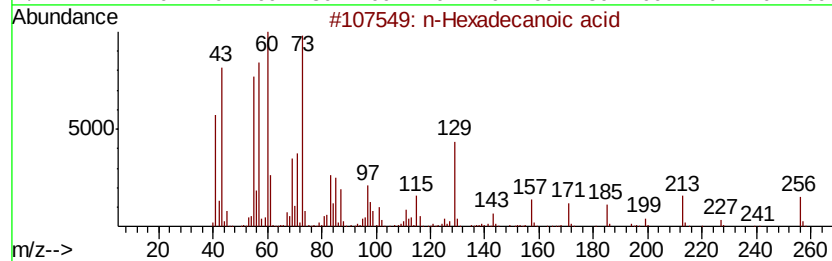
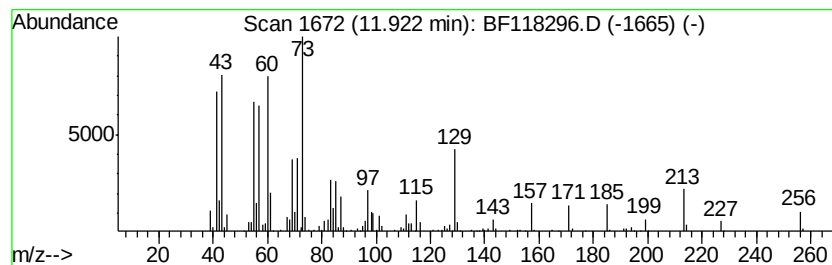
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	10.20 ng	470003	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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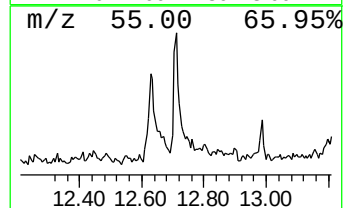
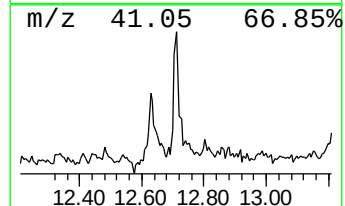
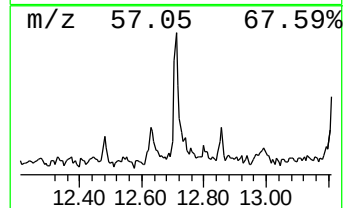
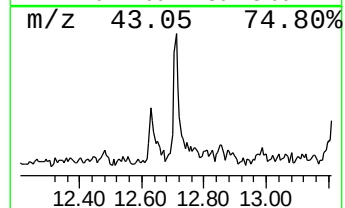
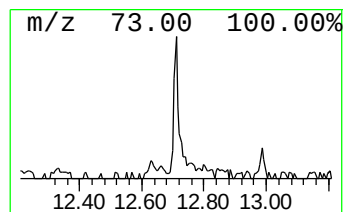
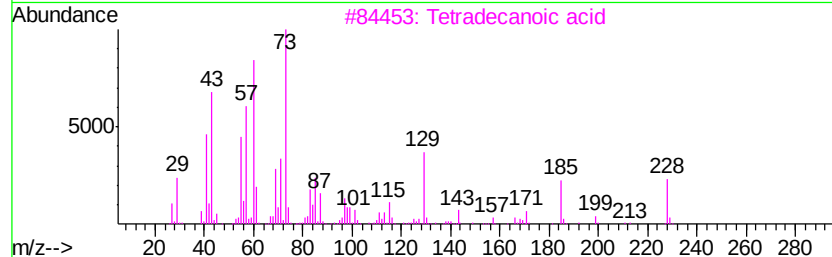
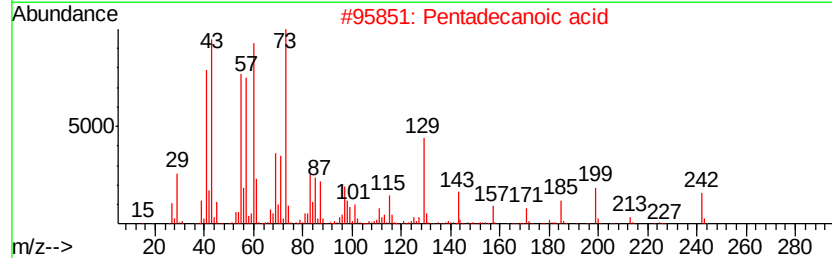
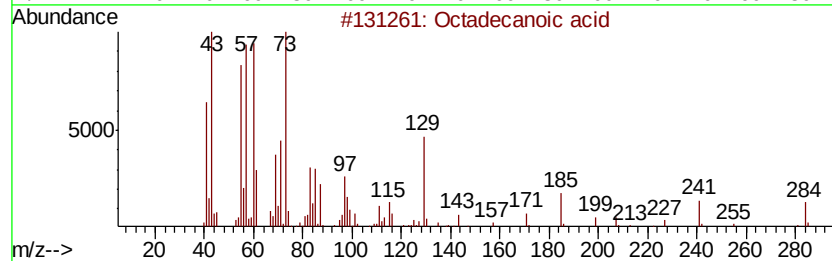
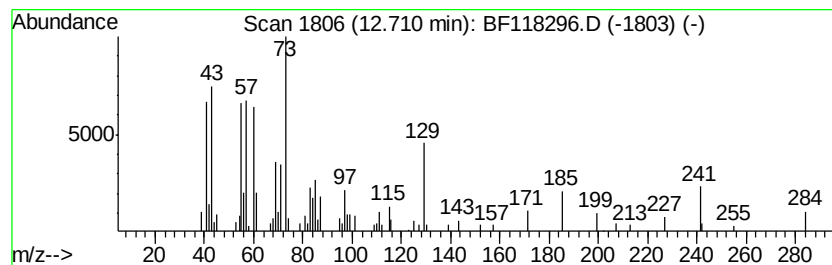
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.71	2.11 ng	97476	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118296.D
Acq On : 19 Dec 2019 23:07
Operator : JU
Sample : K6350-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-1-3

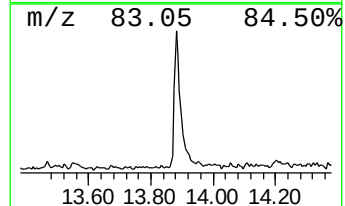
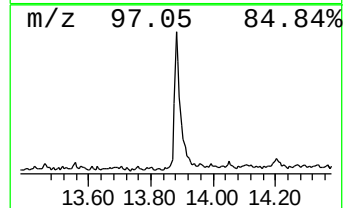
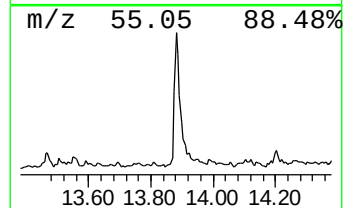
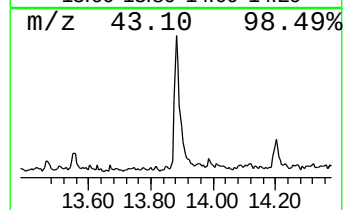
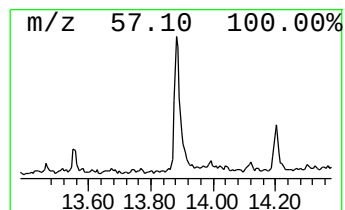
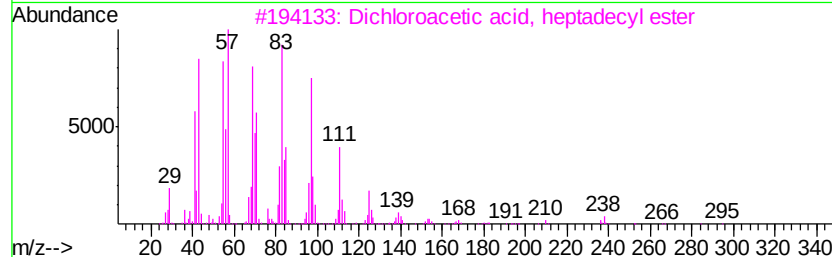
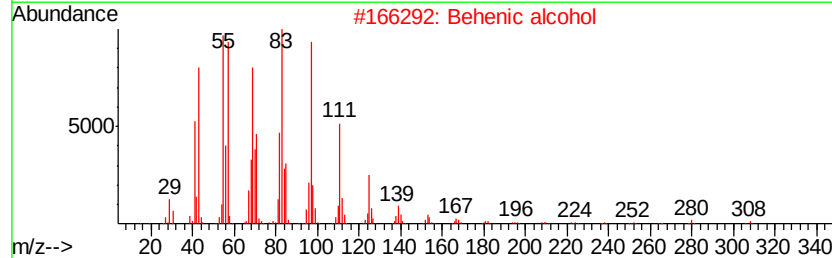
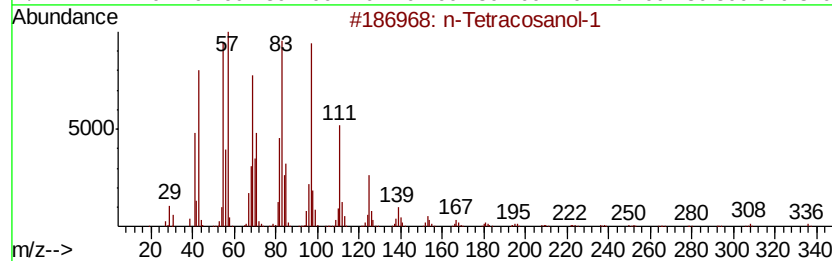
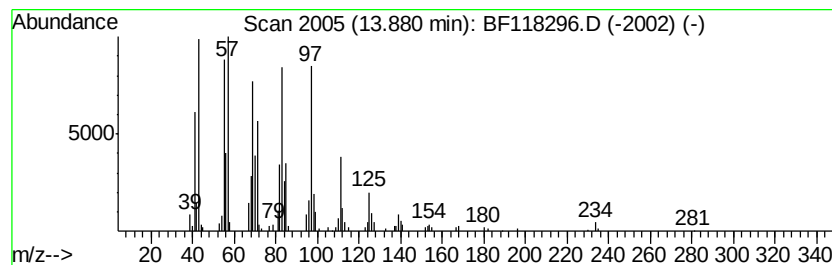
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.64 ng	278457	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118296.D
Acq On : 19 Dec 2019 23:07
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Misc :
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ClientSampleId :
RO-1-3

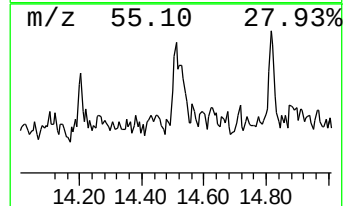
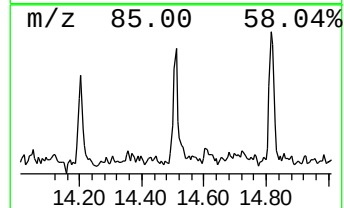
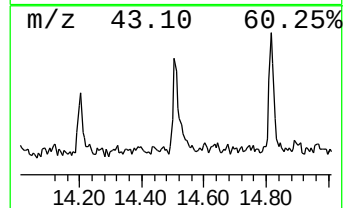
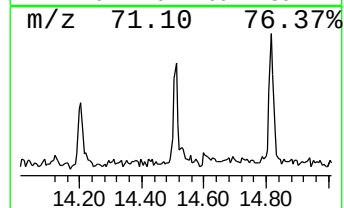
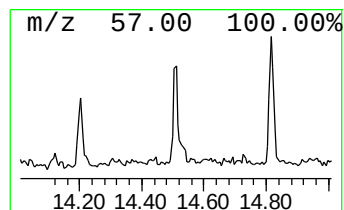
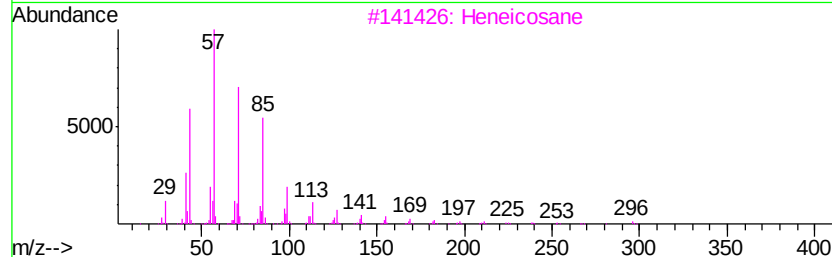
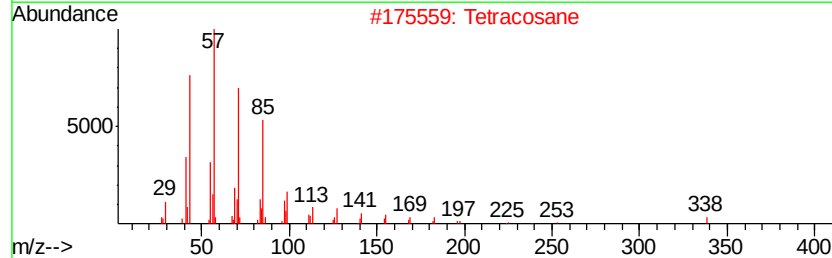
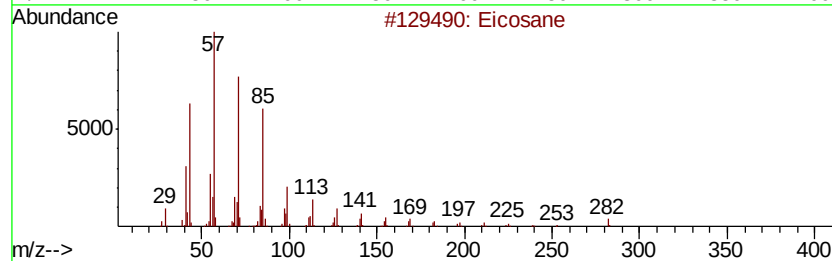
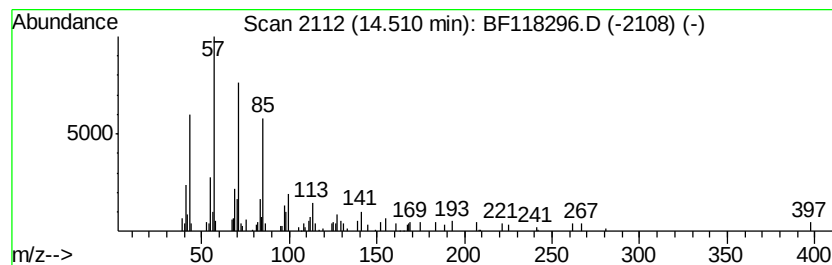
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.17 ng	91139	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118296.D
Acq On : 19 Dec 2019 23:07
Operator : JU
Sample : K6350-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-1-3

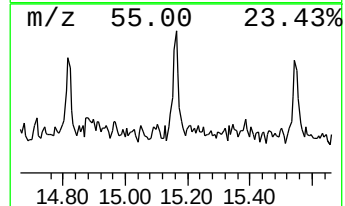
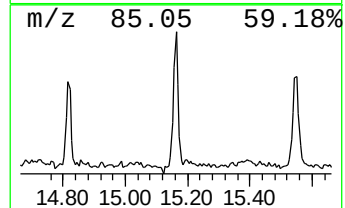
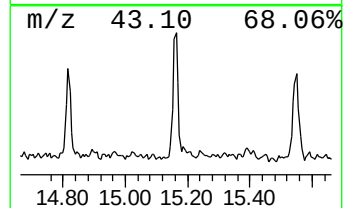
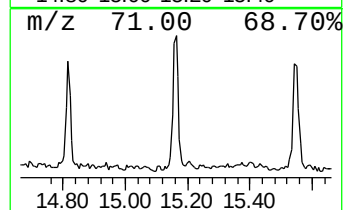
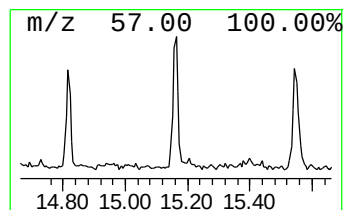
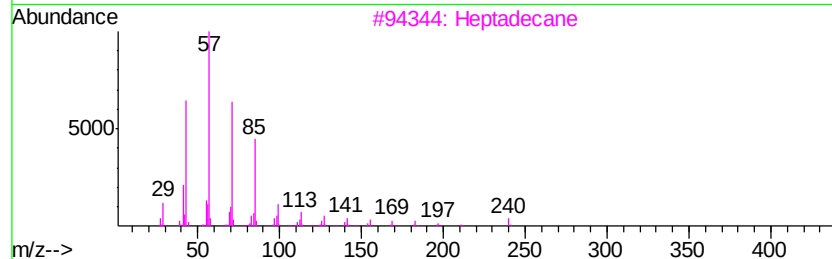
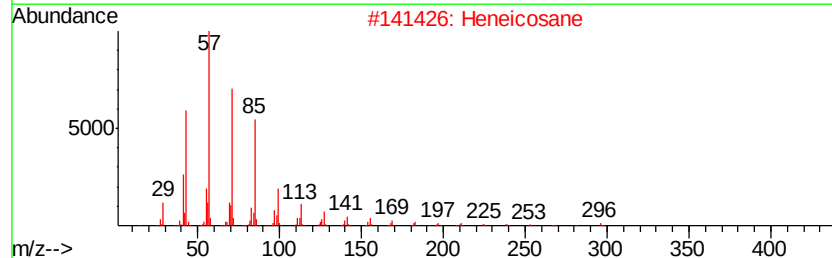
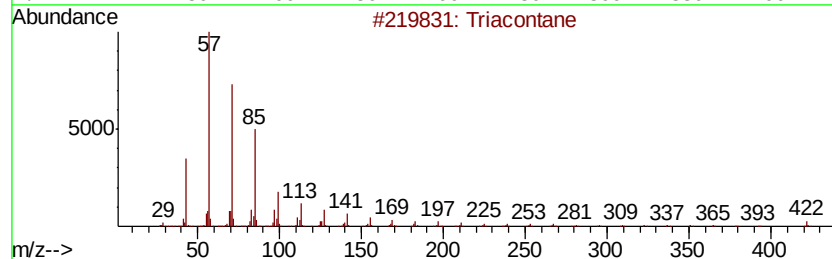
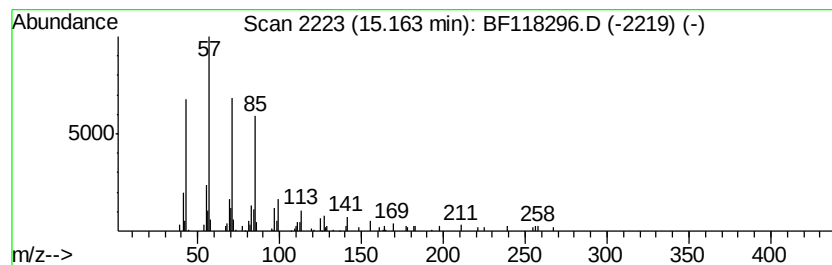
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.31 ng	97218	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane	240	C17H36	000629-78-7	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118296.D
Acq On : 19 Dec 2019 23:07
Operator : JU
Sample : K6350-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

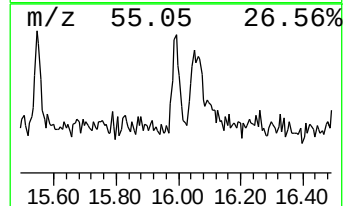
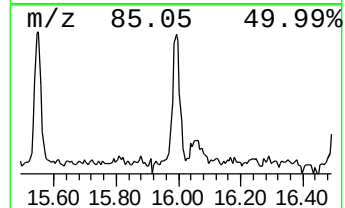
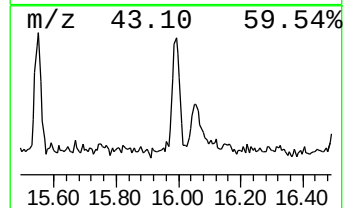
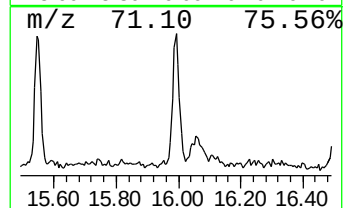
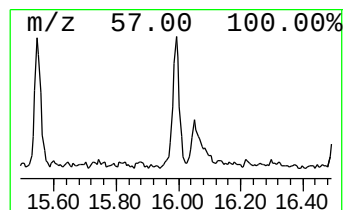
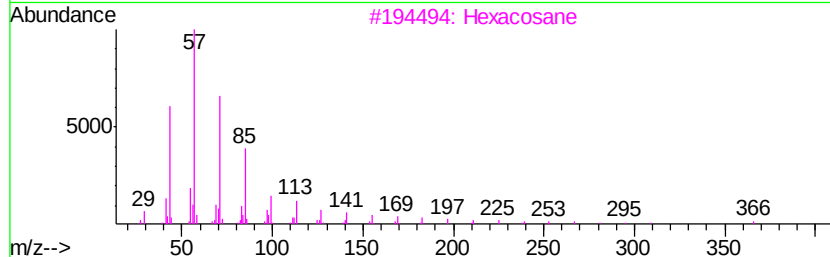
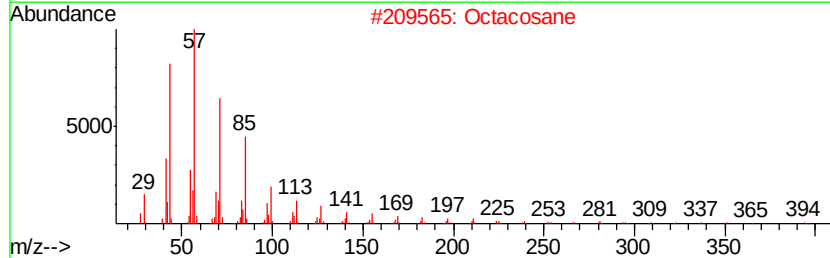
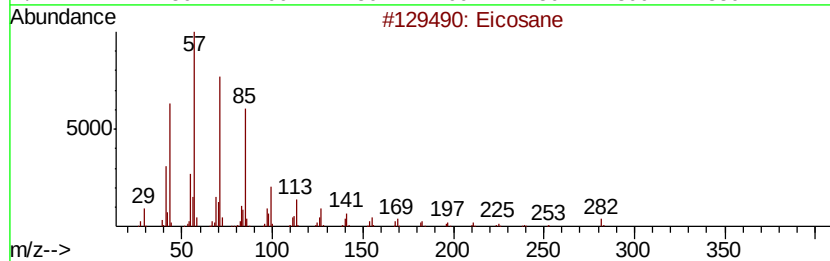
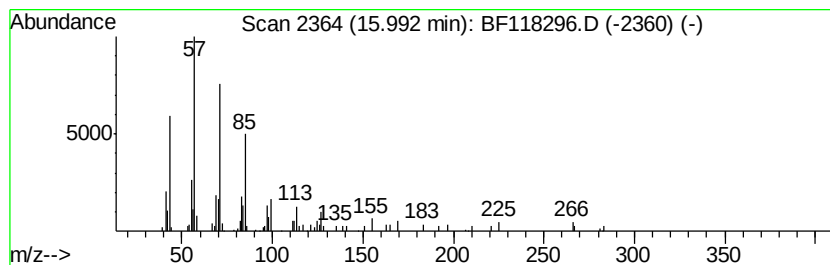
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.33 ng	98119	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Hexacosane	366 C26H54	000630-01-3	91
4	Pentacosane	352 C25H52	000629-99-2	91
5	Heptacosane	380 C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
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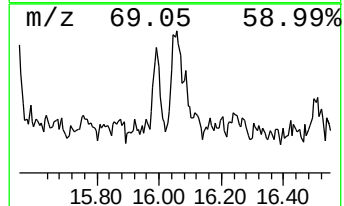
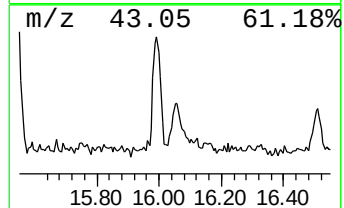
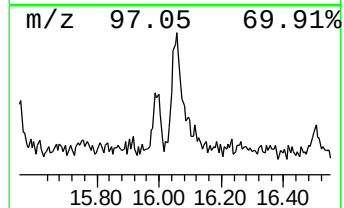
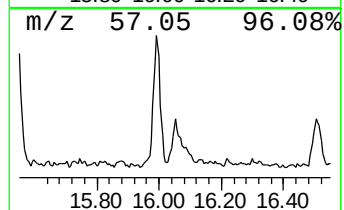
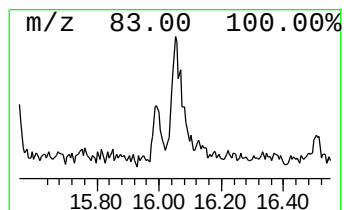
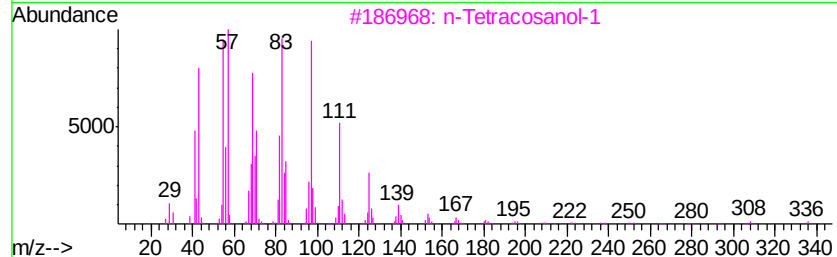
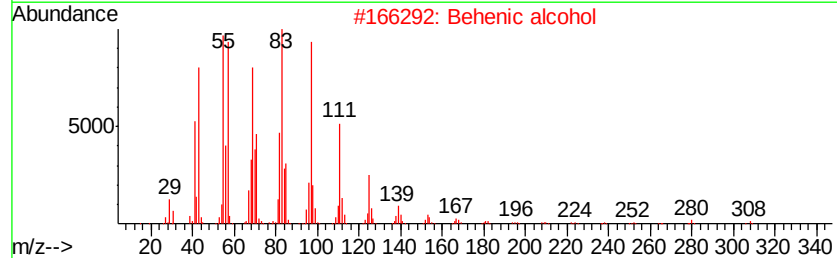
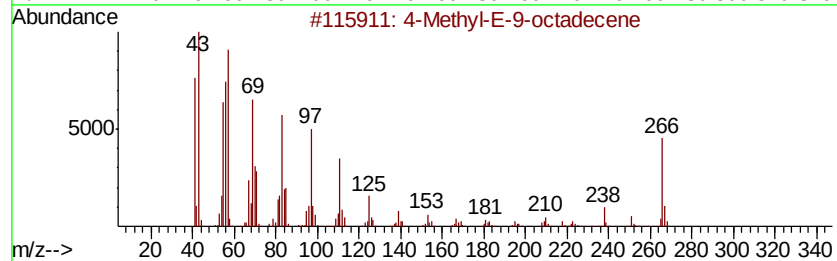
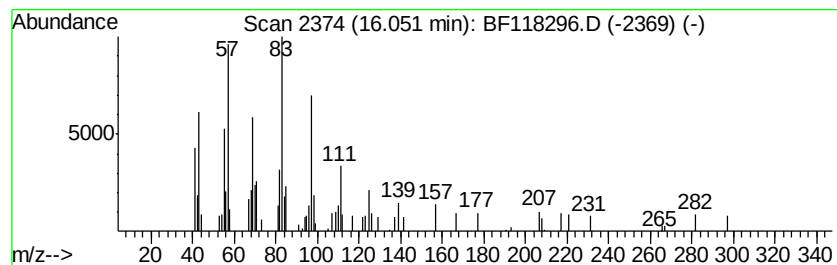
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4-Methyl-E-9-octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.34 ng	98477	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	4-Methyl-E-9-octadecene	266 C19H38	1000130-87-1	64
2	Behenic alcohol	326 C22H46O	000661-19-8	60
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	60
4	1-Heneicosanol	312 C21H44O	015594-90-8	49
5	Cycloheptanol, 2-methylene	126 C8H14O	016240-38-3	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121919\
Data File : BF118296.D
Acq On : 19 Dec 2019 23:07
Operator : JU
Sample : K6350-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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
Propane, 2-methyl...	5.06	12.0	ng	331102	1	6.86	552946	20.0
1,3,6-Octatriene,...	6.13	3.9	ng	108641	1	6.86	552946	20.0
unknown6.63	6.63	73.3	ng	2027890	1	6.86	552946	20.0
n-Hexadecanoic acid	11.92	10.2	ng	470003	4	11.40	921999	20.0
Octadecanoic acid	12.71	2.1	ng	97476	4	11.40	921999	20.0
n-Tetracosanol-1	13.88	6.6	ng	278457	5	14.05	838116	20.0
Eicosane	14.51	2.2	ng	91139	5	14.05	838116	20.0
Triacontane	15.16	2.3	ng	97218	6	15.54	840871	20.0
Octacosane	15.99	2.3	ng	98119	6	15.54	840871	20.0
4-Methyl-E-9-octa...	16.05	2.3	ng	98477	6	15.54	840871	20.0