

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
 Data File : BF117500.D
 Acq On : 23 Oct 2019 22:57
 Operator : JU
 Sample : K5497-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 170-48-(0-1)

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-BF101819.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	4.934	481	484	494	rBV	21950	31625	2.99%	0.320%
2	5.351	552	555	574	rBV	834790	907468	85.75%	9.181%
3	6.381	726	730	747	rBV	1073866	1058301	100.00%	10.707%
4	6.504	747	751	758	rVB	1186417	1046504	98.89%	10.587%
5	6.734	787	790	800	rBV	296357	288496	27.26%	2.919%
6	6.887	812	816	828	rBV	806958	698583	66.01%	7.067%
7	7.298	882	886	903	rBV	646496	629214	59.46%	6.366%
8	8.010	1004	1007	1028	rBV	397455	382713	36.16%	3.872%
9	9.086	1186	1190	1203	rBV	1064981	902891	85.32%	9.134%
10	9.481	1254	1257	1267	rBV	131092	109020	10.30%	1.103%
11	9.763	1301	1305	1317	rBV	519425	437067	41.30%	4.422%
12	10.551	1436	1439	1450	rBV	581460	608848	57.53%	6.160%
13	11.245	1554	1557	1561	rBV	395808	399196	37.72%	4.039%
14	11.775	1645	1647	1653	rBV2	62662	70409	6.65%	0.712%
15	12.463	1761	1764	1772	rBV	33119	32202	3.04%	0.326%
16	12.557	1778	1780	1785	rBV	16812	21873	2.07%	0.221%
17	12.692	1798	1803	1808	rBV	29165	31691	2.99%	0.321%
18	12.827	1822	1826	1830	rBV	737518	644588	60.91%	6.521%
19	13.733	1976	1980	1992	rBV4	64525	133029	12.57%	1.346%
20	13.892	2003	2007	2011	rBV	265038	283465	26.78%	2.868%
21	14.045	2030	2033	2036	rVB2	15839	13864	1.31%	0.140%
22	14.257	2066	2069	2072	rBV4	14503	17517	1.66%	0.177%
23	14.345	2081	2084	2088	rVB	30341	28544	2.70%	0.289%
24	14.398	2088	2093	2103	rBV	325532	326413	30.84%	3.302%
25	14.645	2131	2135	2139	rVB	39228	42234	3.99%	0.427%
26	14.716	2143	2147	2150	rVB2	15494	17225	1.63%	0.174%
27	14.957	2184	2188	2190	rBV	46713	55601	5.25%	0.563%
28	14.986	2190	2193	2198	rVB2	65457	84581	7.99%	0.856%
29	15.074	2204	2208	2218	rBV	48913	96202	9.09%	0.973%
30	15.151	2218	2221	2225	rVV2	18975	25248	2.39%	0.255%
31	15.204	2228	2230	2235	rVB3	9762	12648	1.20%	0.128%
32	15.315	2245	2249	2258	rVB	248497	325333	30.74%	3.291%
33	15.721	2312	2318	2322	rBV2	32479	45107	4.26%	0.456%
34	15.786	2324	2329	2330	rBV3	10139	13618	1.29%	0.138%

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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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35	16.180	2392	2396	2402	rBV3	18313	33545	3.17%	0.339%
36	16.739	2486	2491	2496	rVB8	10512	18166	1.72%	0.184%
37	16.886	2511	2516	2520	rBV7	5288	11464	1.08%	0.116%

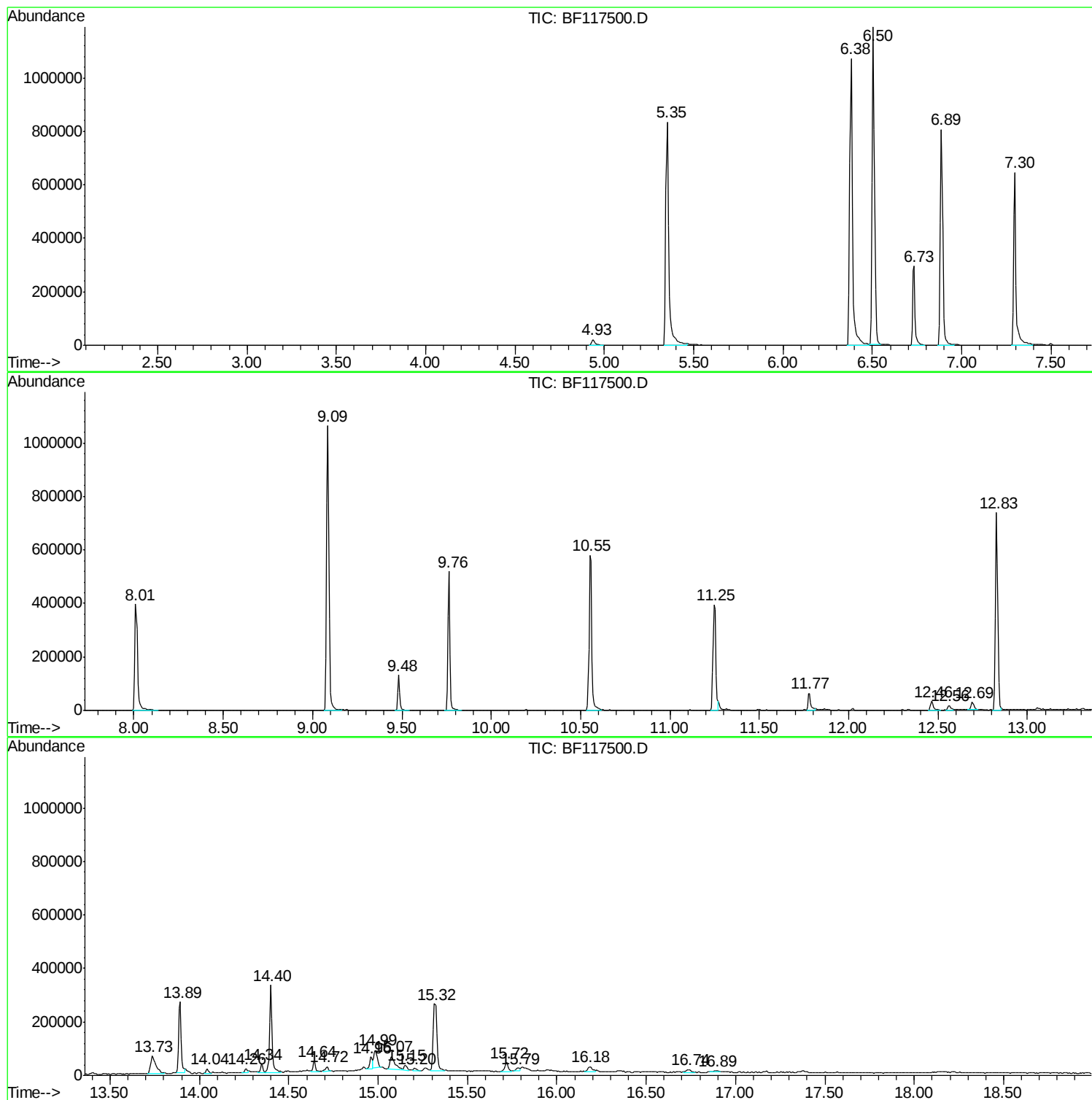
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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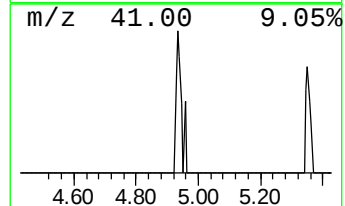
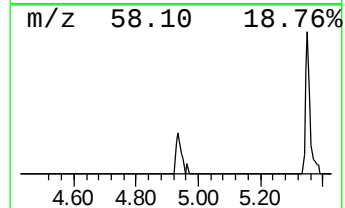
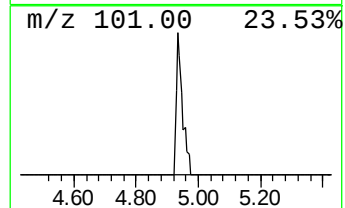
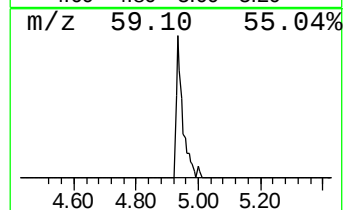
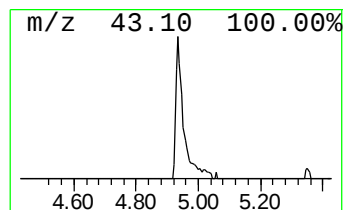
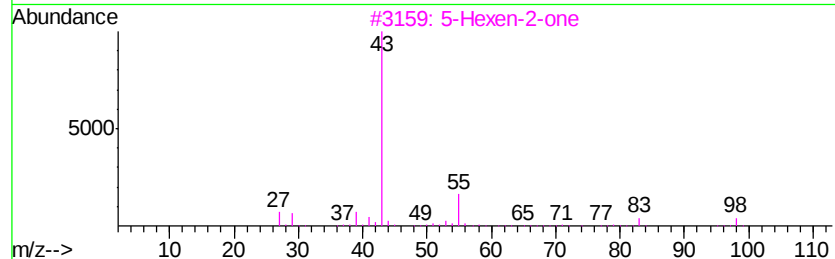
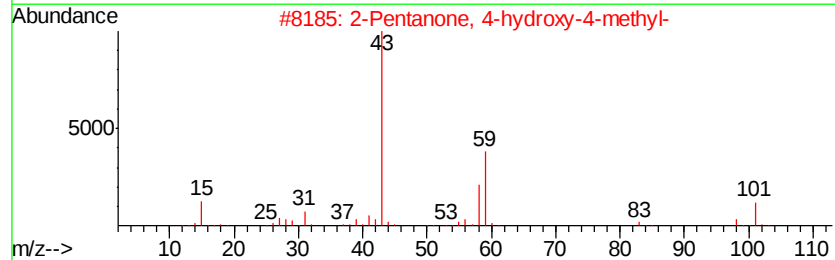
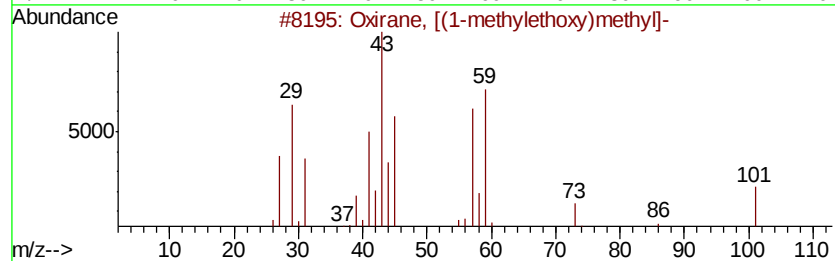
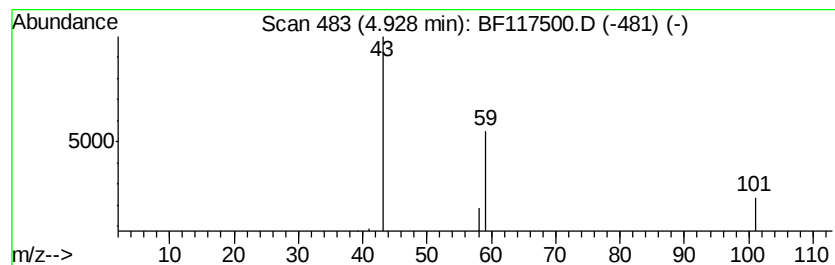
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Oxirane, [(1-methylethoxy)m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.19 ng	31625	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	64
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	7
4		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	7
5		Guanidine	59	CH5N3	000113-00-8	5



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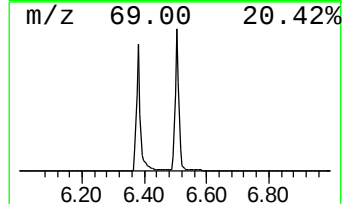
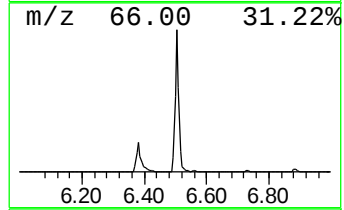
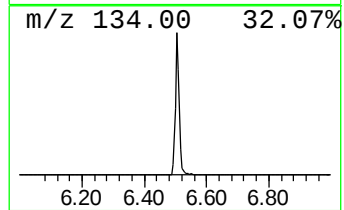
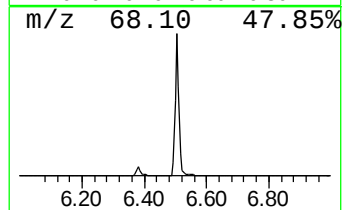
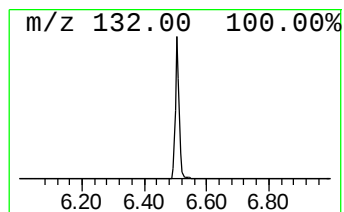
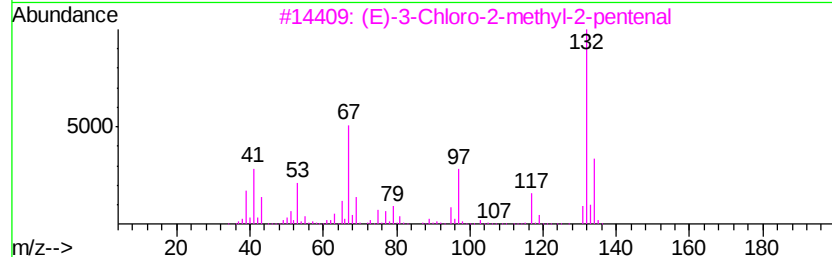
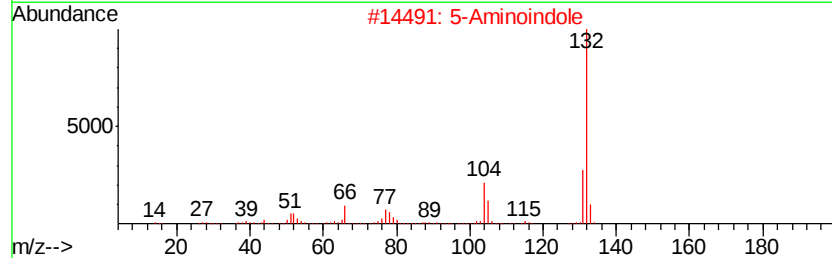
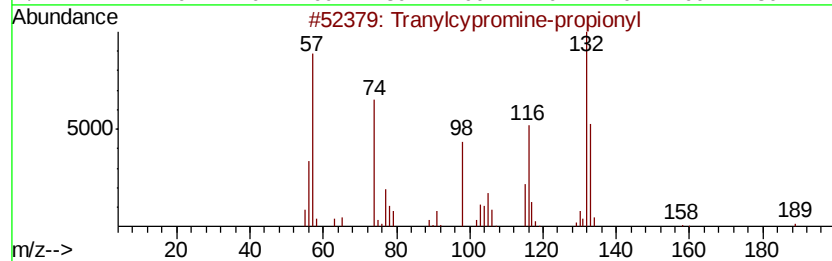
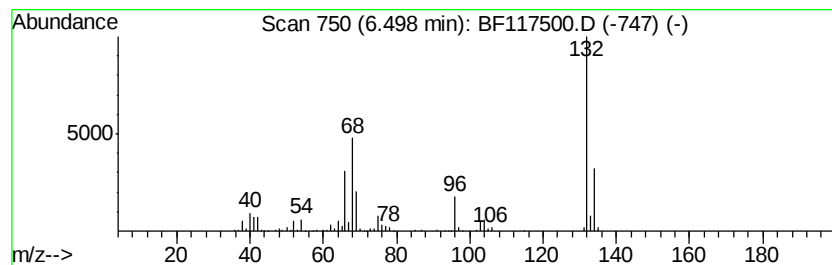
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	72.55 ng	1046500	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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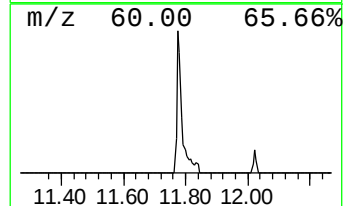
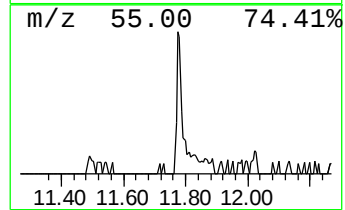
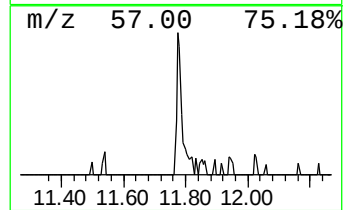
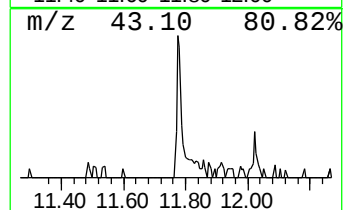
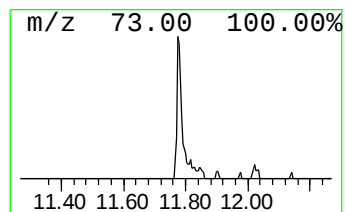
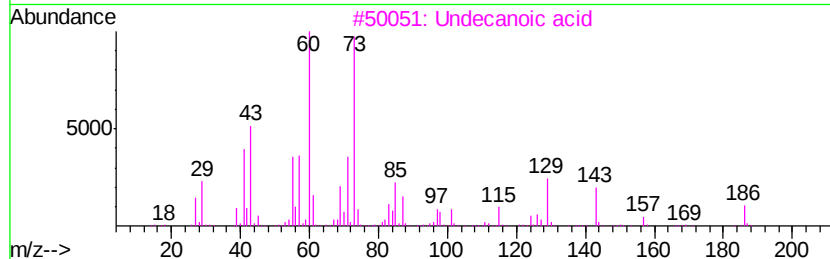
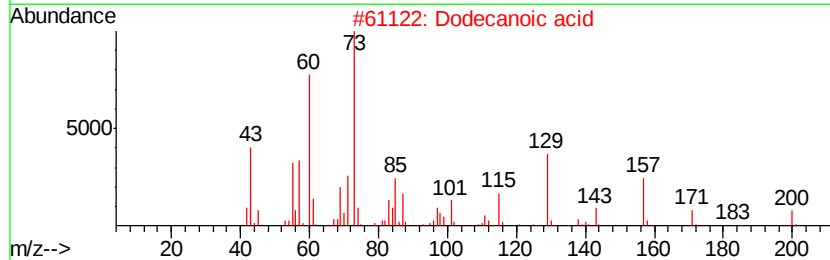
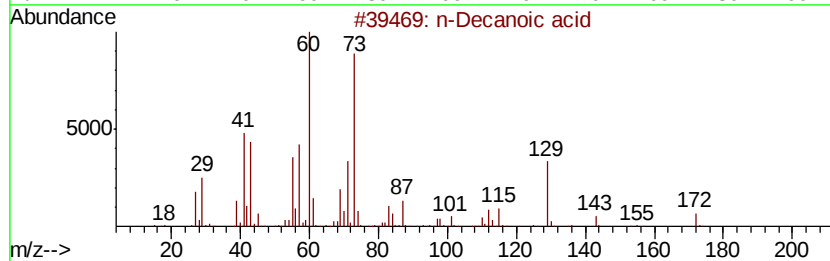
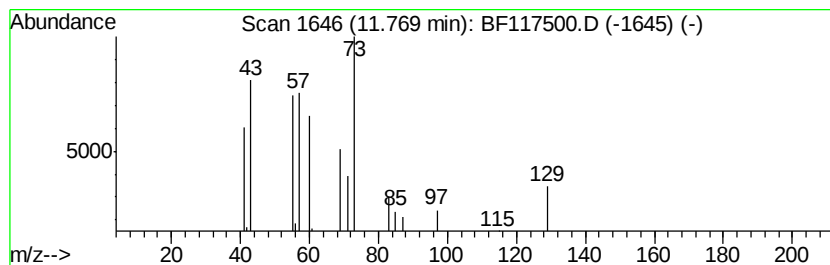
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	3.53 ng	70409	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	59
2	Dodecanoic acid	200	C12H24O2	000143-07-7	50
3	Undecanoic acid	186	C11H22O2	000112-37-8	43
4	Sedoheptulosan	192	C7H12O6	000469-90-9	27
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25



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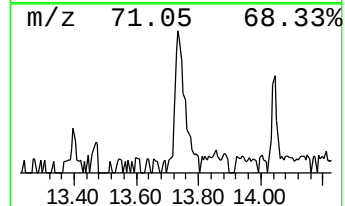
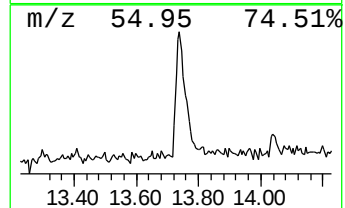
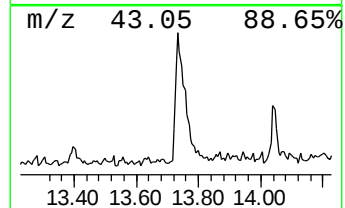
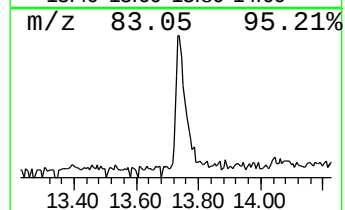
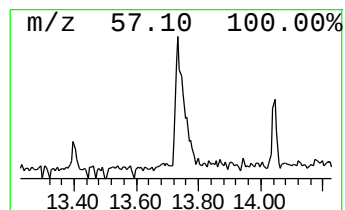
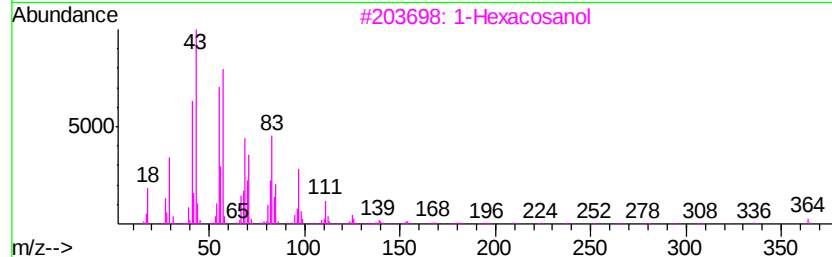
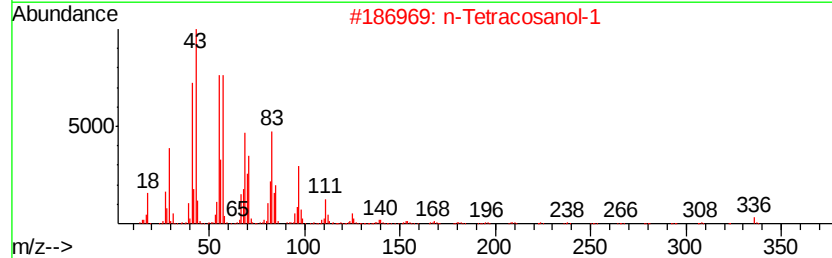
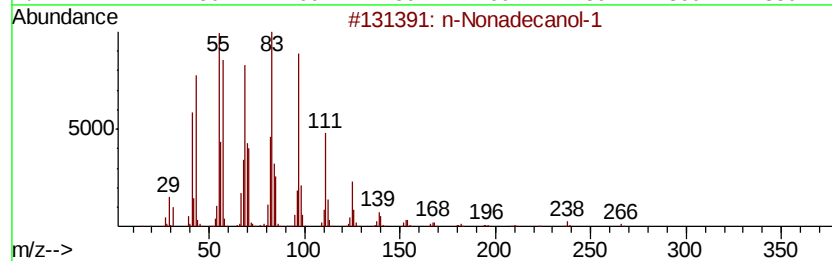
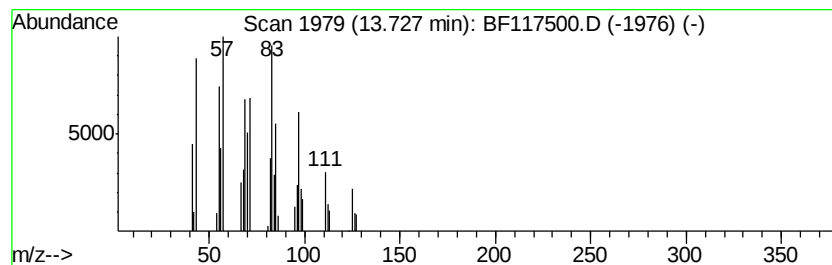
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.73	9.39 ng	133029	Chrysene-d12		13.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Behenic alcohol	326	C22H46O	000661-19-8	90



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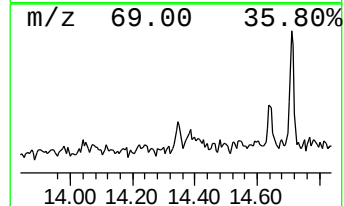
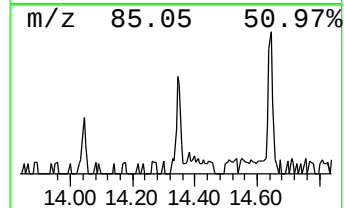
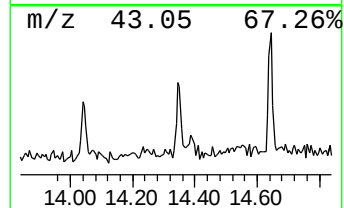
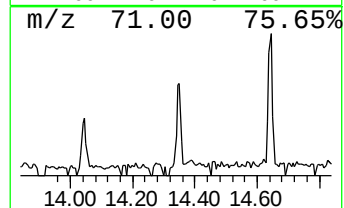
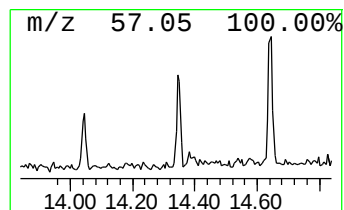
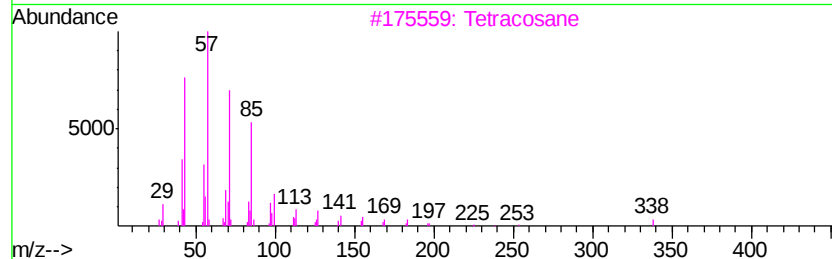
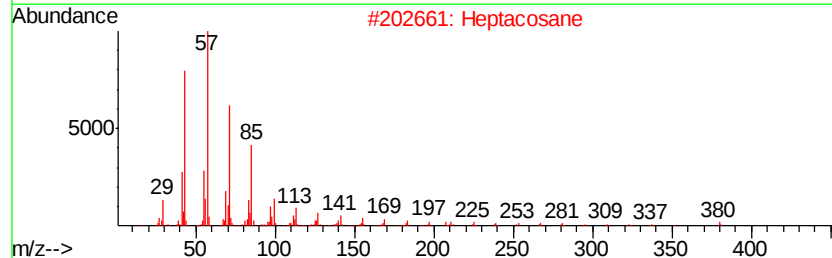
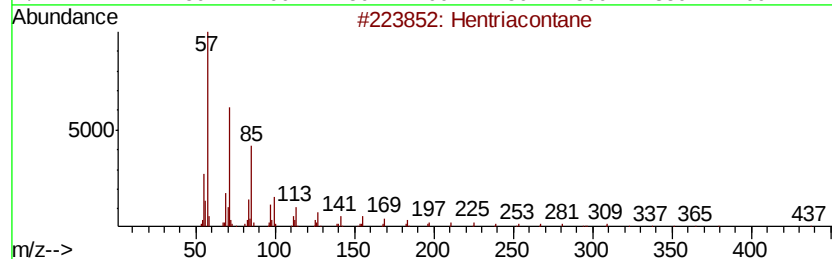
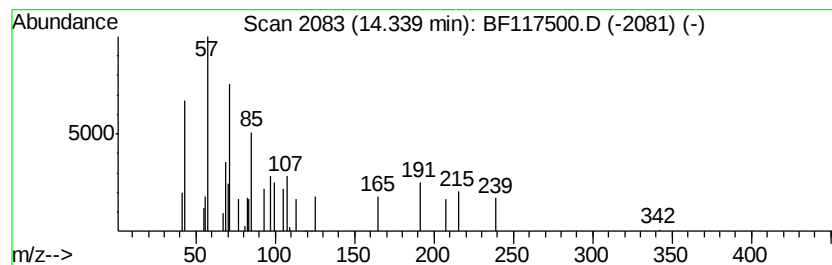
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Hentriacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.01 ng	28544	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	90
2		Heptacosane	380	C27H56	000593-49-7	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		2-methylhexacosane	380	C27H56	1000376-72-7	87
5		Tetratetracontane	619	C44H90	007098-22-8	86



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Acq On : 23 Oct 2019 22:57
Operator : JU
Sample : K5497-01
Misc :
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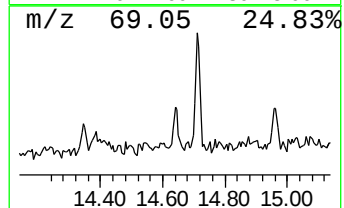
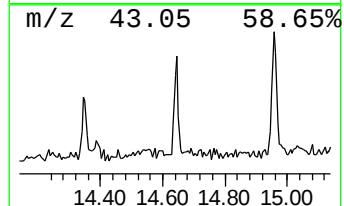
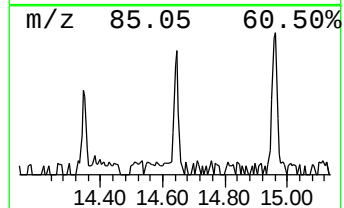
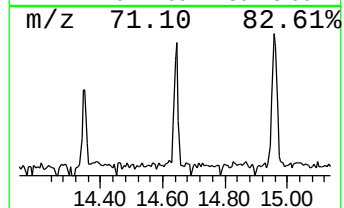
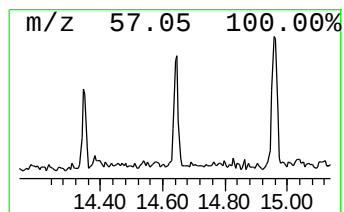
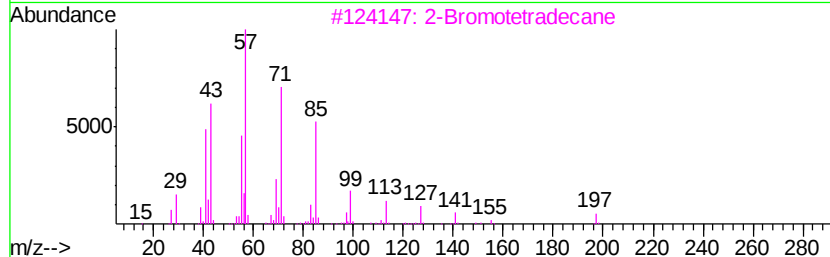
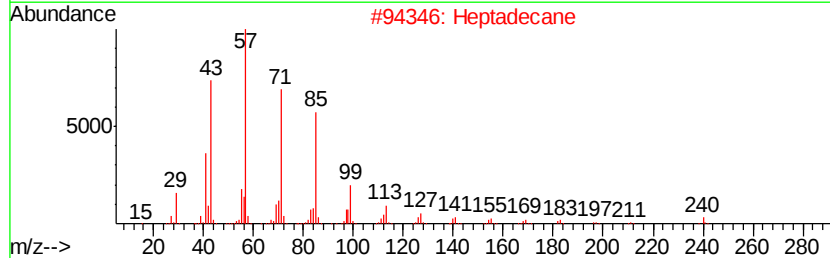
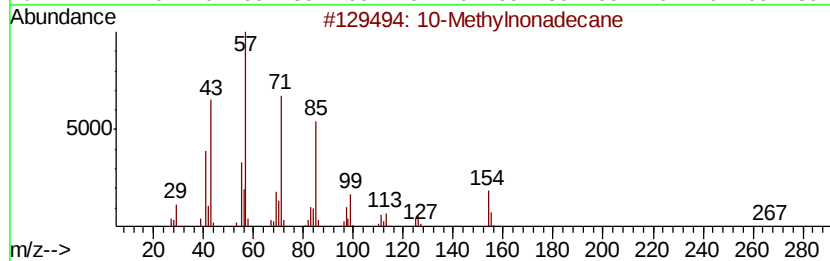
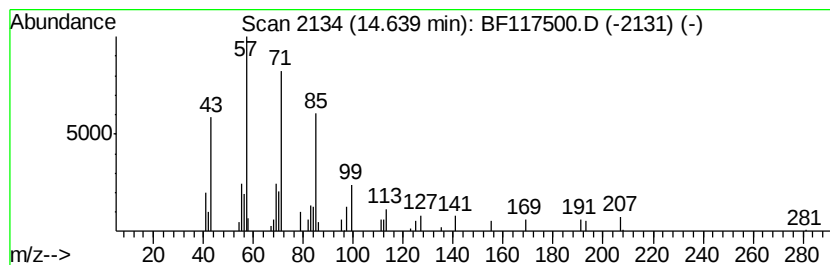
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ClientSampleId :
170-48-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 10-Methylnonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.64	2.60 ng	42234	Perylene-d12		15.32		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Methylnonadecane	282	C20H42	056862-62-5	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			2-Bromotetradecane	276	C14H29Br	074036-95-6	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
Operator : JU
Sample : K5497-01
Misc :
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ClientSampleId :
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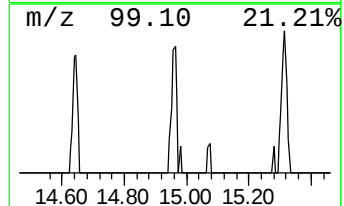
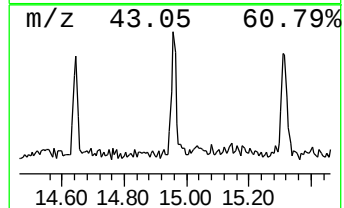
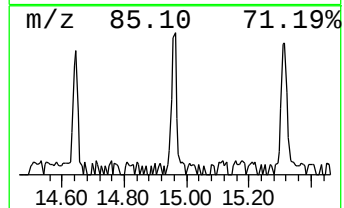
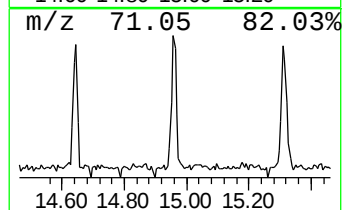
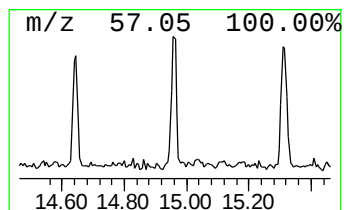
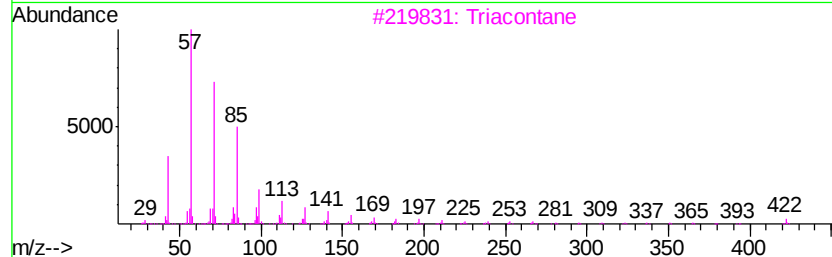
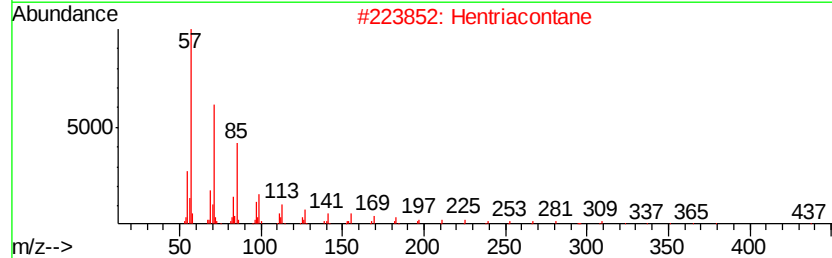
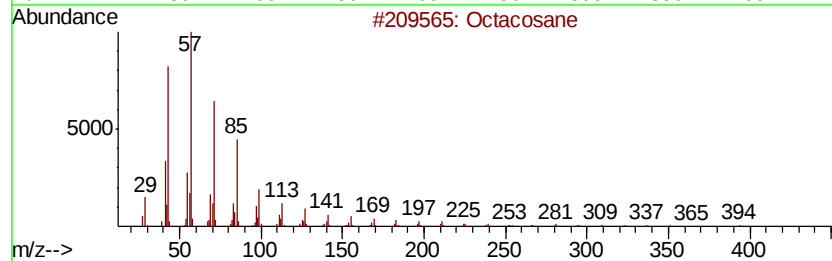
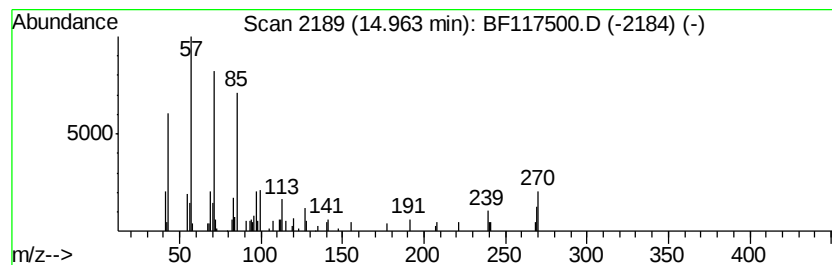
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.42 ng	55601	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Triacontane	422	C30H62	000638-68-6	87
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
Operator : JU
Sample : K5497-01
Misc :
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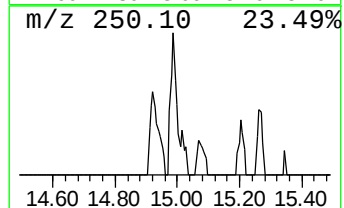
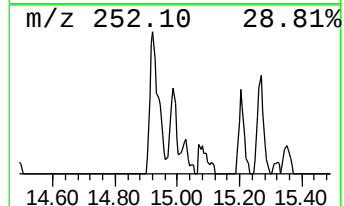
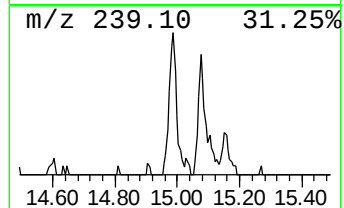
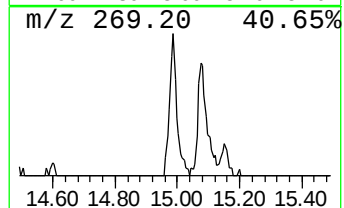
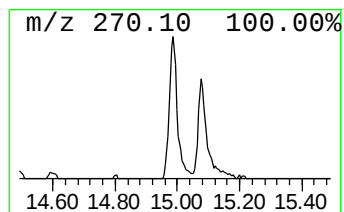
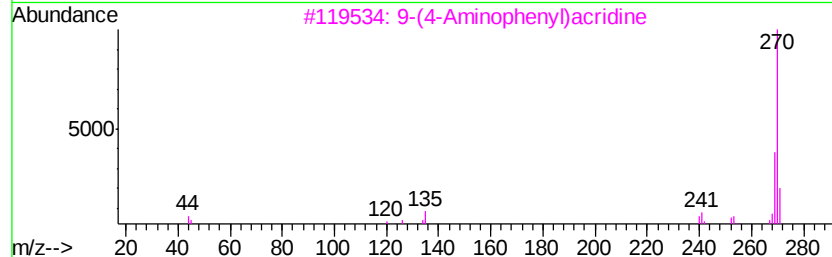
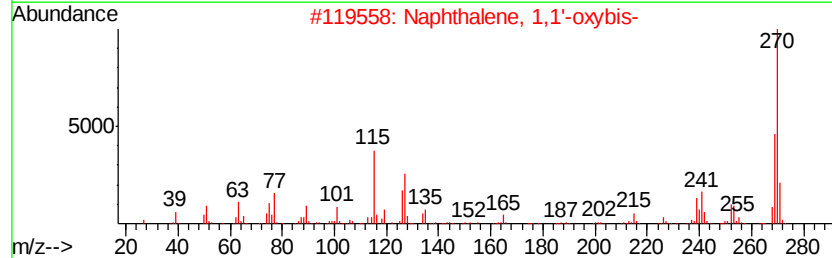
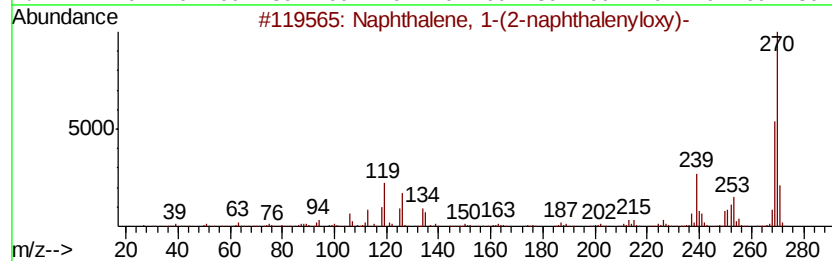
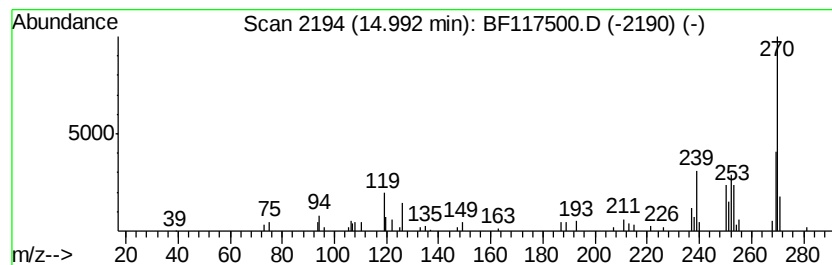
Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1-(2-naphthale... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.99	5.20 ng	84581	Perylene-d12	15.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-(2-naphthalenyloxy)-	270	C20H14O	000611-49-4	91
2	Naphthalene, 1,1'-oxybis-	270	C20H14O	000607-52-3	58
3	9-(4-Aminophenyl)acridine	270	C19H14N2	1000298-83-3	53
4	4-Azafluorenone, 3-methylphenyli...	270	C19H14N2	1000301-74-7	49
5	4-Azafluorenone, 4-methylphenyli...	270	C19H14N2	1000216-54-5	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
Operator : JU
Sample : K5497-01
Misc :
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Instrument :
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ClientSampleId :
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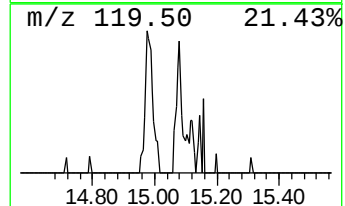
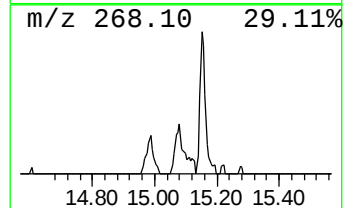
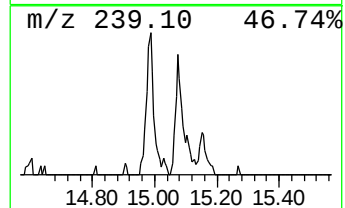
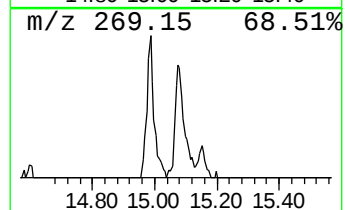
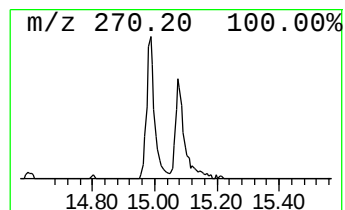
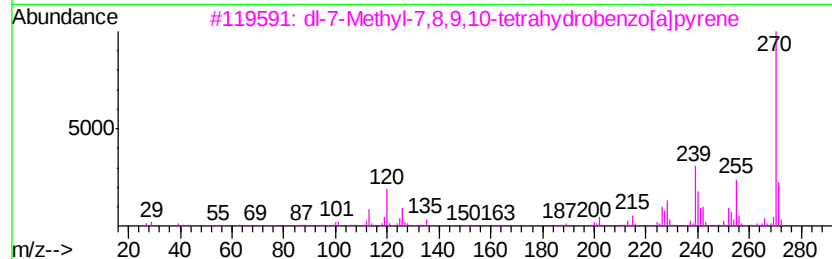
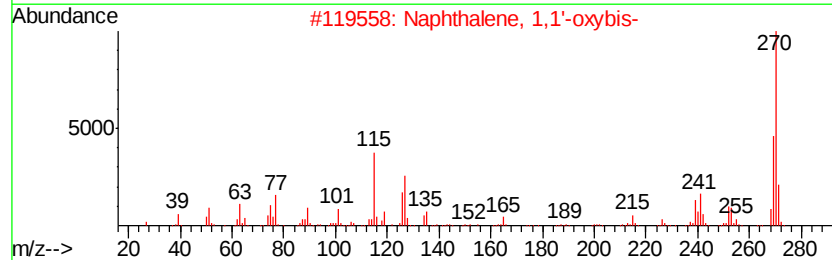
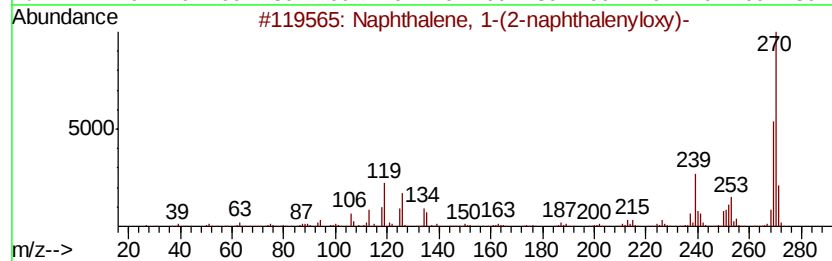
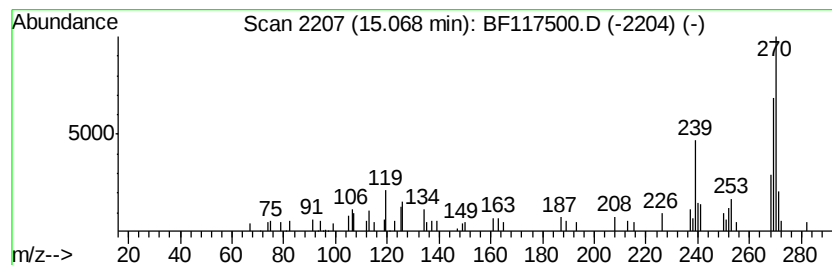
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Naphthalene, 1,1'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	5.91 ng	96202	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-(2-naphthalenyloxy)-	270	C20H14O	000611-49-4	89
2		Naphthalene, 1,1'-oxybis-	270	C20H14O	000607-52-3	68
3		dl-7-Methyl-7,8,9,10-tetrahydrob...	270	C21H18	094849-90-8	55
4		Benz(a)anthracene, 7,9,12-trimet...	270	C21H18	024891-41-6	49
5		Benz(a)anthracene, 7,10,12-trime...	270	C21H18	035187-27-0	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
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Instrument :
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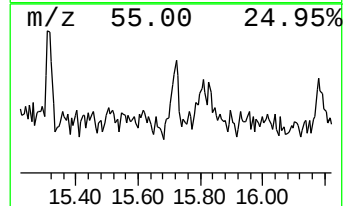
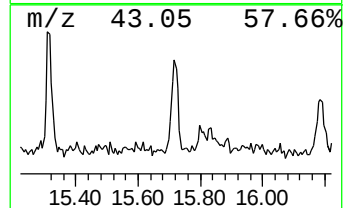
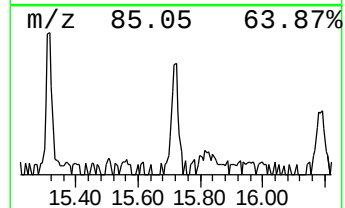
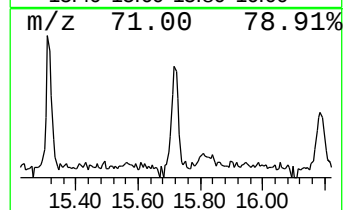
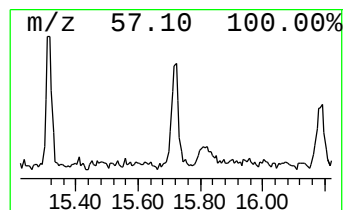
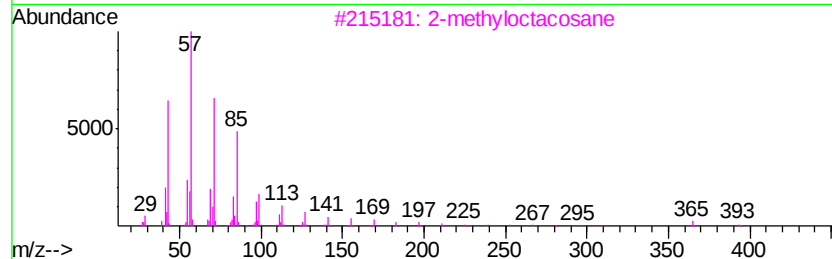
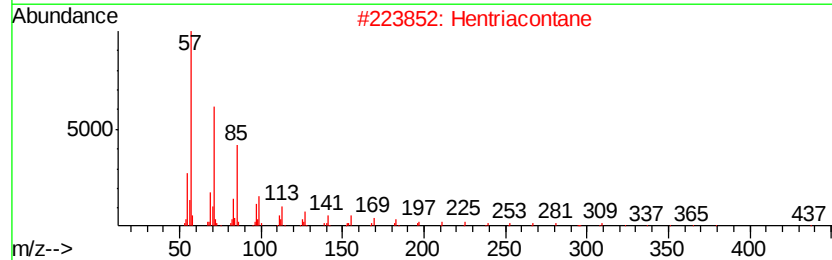
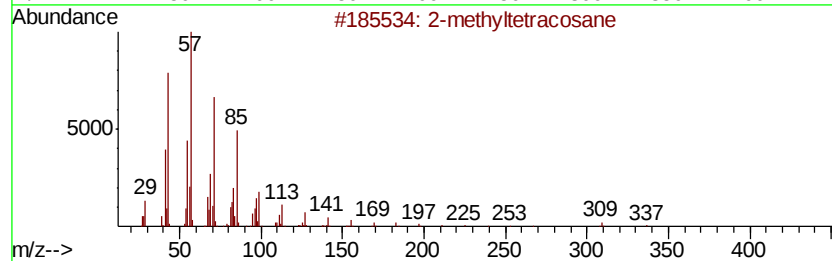
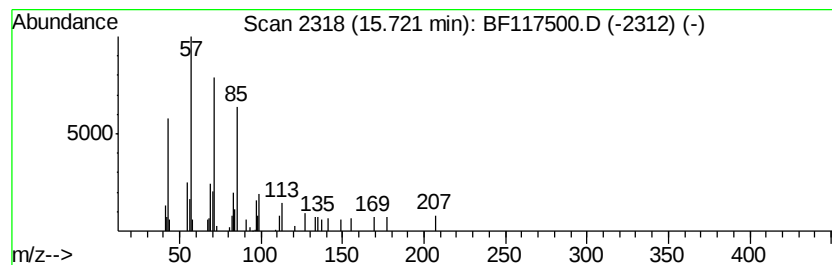
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methyltetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.77 ng	45107	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyltetracosane	352	C25H52	1000376-72-6	90
2			Hentriacontane	437	C31H64	000630-04-6	87
3			2-methyloctacosane	408	C29H60	1000376-72-8	86
4			Octacosane	394	C28H58	000630-02-4	86
5			Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
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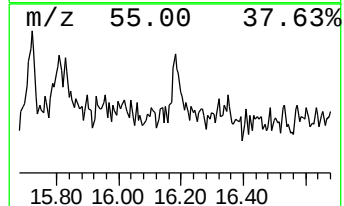
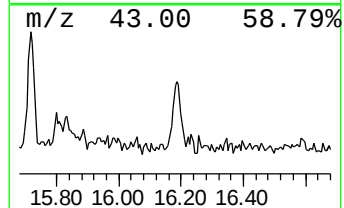
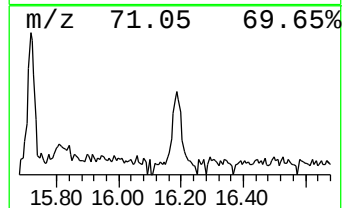
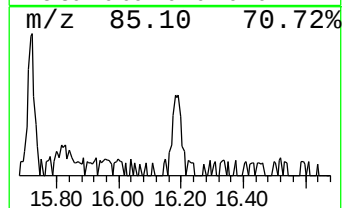
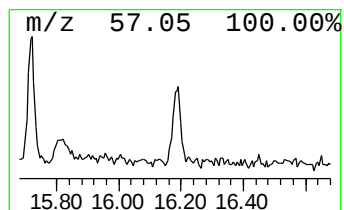
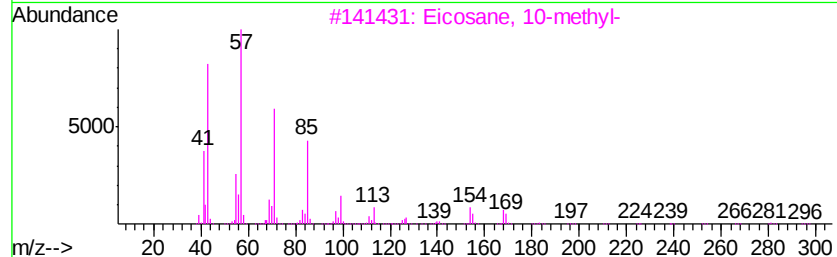
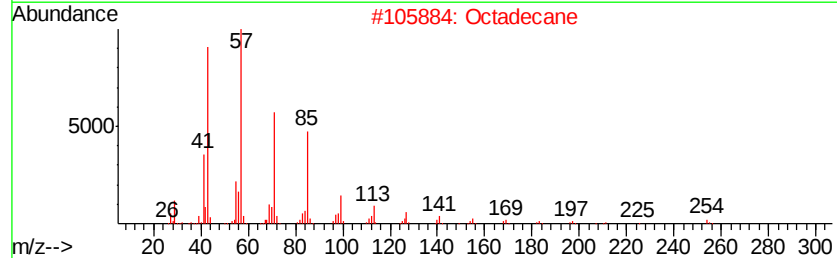
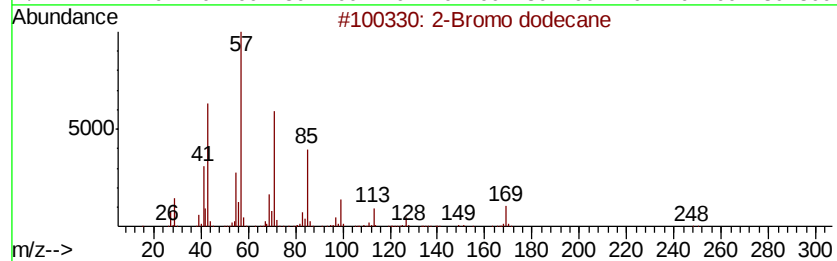
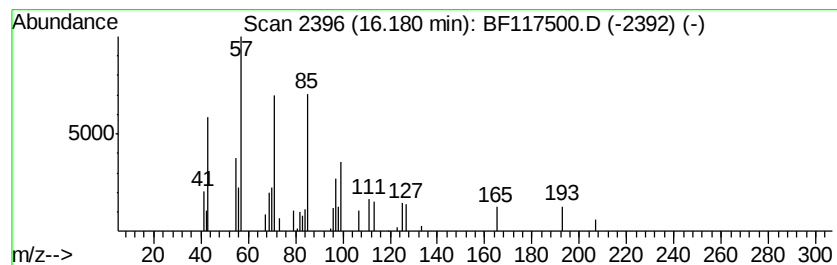
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Bromo dodecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.06 ng	33545	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo dodecane	248	C12H25Br	013187-99-0	53
2			Octadecane	254	C18H38	000593-45-3	53
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	53
4			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	50
5			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102319\
Data File : BF117500.D
Acq On : 23 Oct 2019 22:57
Operator : JU
Sample : K5497-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Oxirane, [(1-meth...	4.93	2.2	ng	31625	1	6.73	288496	20.0
unknown6.50	6.50	72.5	ng	1046500	1	6.73	288496	20.0
n-Decanoic acid	11.77	3.5	ng	70409	4	11.25	399196	20.0
n-Nonadecanol-1	13.73	9.4	ng	133029	5	13.89	283465	20.0
Hentriacontane	14.34	2.0	ng	28544	5	13.89	283465	20.0
10-Methylnonadecane	14.64	2.6	ng	42234	6	15.32	325333	20.0
Octacosane	14.96	3.4	ng	55601	6	15.32	325333	20.0
Naphthalene, 1-(2...	14.99	5.2	ng	84581	6	15.32	325333	20.0
Naphthalene, 1,1'...	15.07	5.9	ng	96202	6	15.32	325333	20.0
2-methyltetracosane	15.72	2.8	ng	45107	6	15.32	325333	20.0
2-Bromo dodecane	16.18	2.1	ng	33545	6	15.32	325333	20.0