

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030920\
 Data File : BF119301.D
 Acq On : 9 Mar 2020 23:55
 Operator : CG/JU
 Sample : L1837-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-065

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-BF022020.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	4.922	478	482	491	rBV	88198	125436	5.68%	0.682%
2	5.351	552	555	581	rBV	1225892	1586405	71.89%	8.623%
3	6.375	726	729	746	rBV	1355096	1559185	70.66%	8.475%
4	6.722	785	788	799	rVB	632774	554457	25.13%	3.014%
5	6.881	811	815	825	rBV	1512809	1451664	65.79%	7.891%
6	7.286	881	884	902	rBV	1018887	1067558	48.38%	5.803%
7	8.004	1003	1006	1027	rVB	791935	718527	32.56%	3.906%
8	9.080	1185	1189	1205	rBV	2321548	2206623	100.00%	11.995%
9	9.475	1253	1256	1267	rVB	147724	149444	6.77%	0.812%
10	9.757	1300	1304	1317	rVB	967301	882254	39.98%	4.796%
11	10.545	1435	1438	1454	rBV	1282078	1415584	64.15%	7.695%
12	11.239	1553	1556	1564	rBV	920254	891382	40.40%	4.845%
13	11.769	1643	1646	1654	rBV3	66586	100317	4.55%	0.545%
14	12.457	1760	1763	1767	rBV	37936	38575	1.75%	0.210%
15	12.557	1777	1780	1785	rBV2	21718	31972	1.45%	0.174%
16	12.692	1797	1803	1806	rBV	30385	36191	1.64%	0.197%
17	12.821	1821	1825	1828	rBV	2360010	2027351	91.88%	11.020%
18	13.733	1975	1980	1992	rBV5	63280	203546	9.22%	1.106%
19	13.880	2002	2005	2018	rVB	633618	663468	30.07%	3.606%
20	14.033	2028	2031	2034	rVB2	31030	26041	1.18%	0.142%
21	14.339	2079	2083	2085	rBV	106810	102528	4.65%	0.557%
22	14.374	2085	2089	2101	rVB5	37008	85662	3.88%	0.466%
23	14.633	2129	2133	2136	rVB	46867	47046	2.13%	0.256%
24	14.704	2142	2145	2152	rVB2	47198	58624	2.66%	0.319%
25	14.768	2154	2156	2163	rVB5	35463	36724	1.66%	0.200%
26	14.915	2177	2181	2182	rBV	20922	26607	1.21%	0.145%
27	14.945	2182	2186	2191	rVB	322385	370618	16.80%	2.015%
28	15.204	2226	2230	2233	rBV4	18809	27291	1.24%	0.148%
29	15.309	2243	2248	2261	rVB	529369	735638	33.34%	3.999%
30	15.486	2274	2278	2283	rBV3	42449	58053	2.63%	0.316%
31	15.621	2296	2301	2304	rBV6	14213	23850	1.08%	0.130%
32	15.704	2310	2315	2321	rVB	141634	209813	9.51%	1.140%
33	16.168	2390	2394	2398	rVB7	20189	28460	1.29%	0.155%
34	16.439	2435	2440	2446	rVB2	36059	66048	2.99%	0.359%

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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-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.715	2482	2487	2498	rVB9	25184	67536	3.06%	0.367%
36	17.015	2535	2538	2550	rVB9	27482	66819	3.03%	0.363%
37	17.233	2568	2575	2588	rVB10	73935	241005	10.92%	1.310%
38	17.386	2598	2601	2608	rVB4	47117	91244	4.14%	0.496%
39	17.703	2651	2655	2657	rBV4	28224	47631	2.16%	0.259%
40	18.015	2694	2708	2713	rBV4	59540	230570	10.45%	1.253%
41	18.415	2772	2776	2782	rBV9	17155	39127	1.77%	0.213%

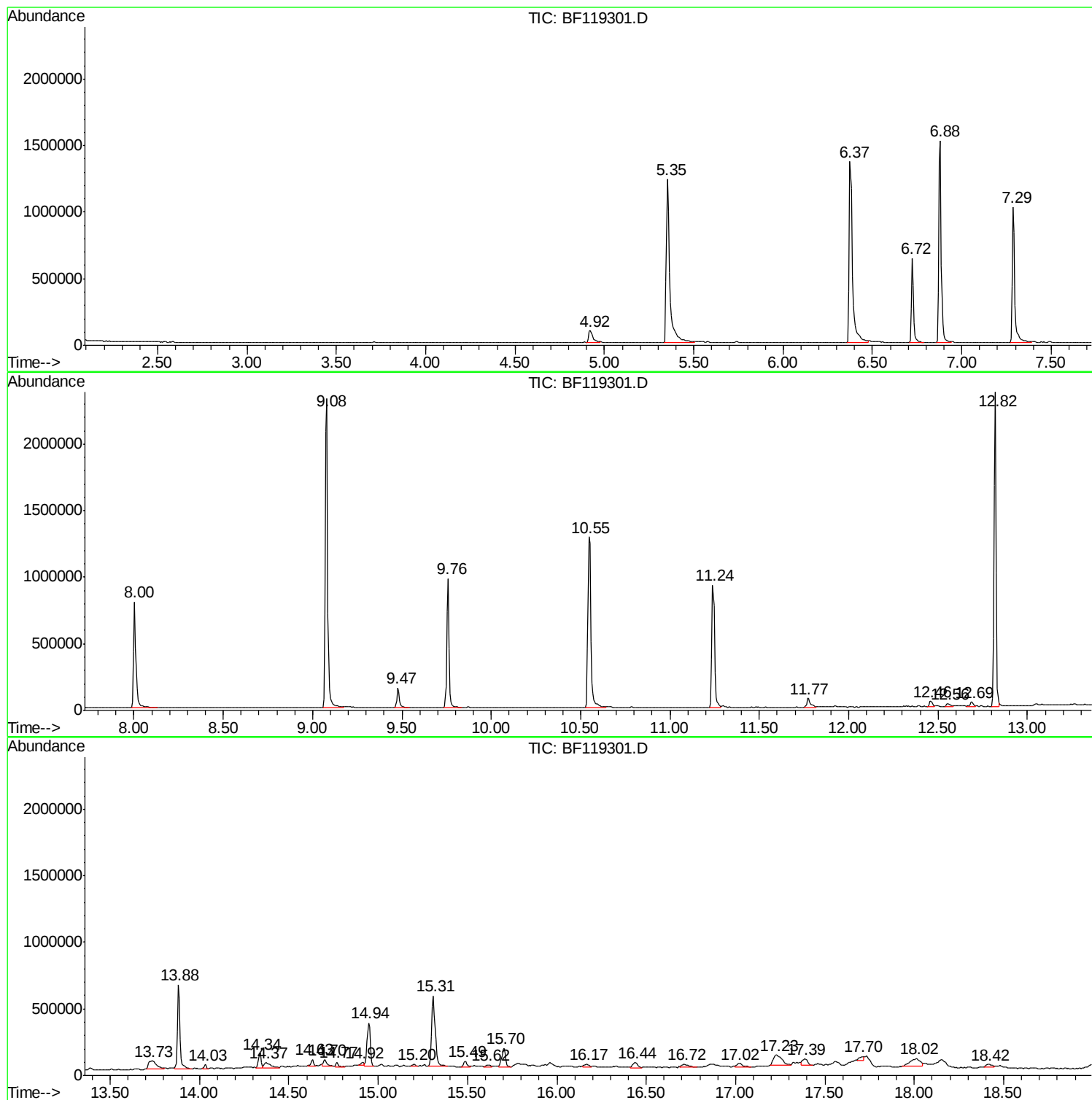
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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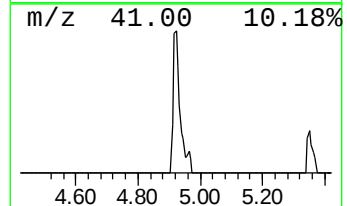
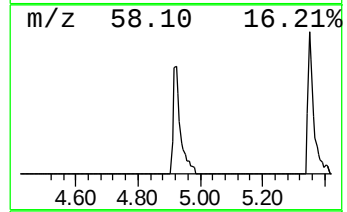
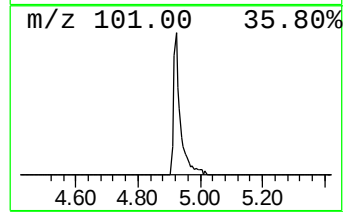
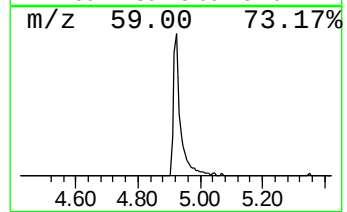
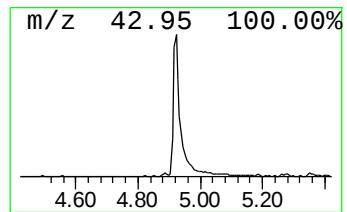
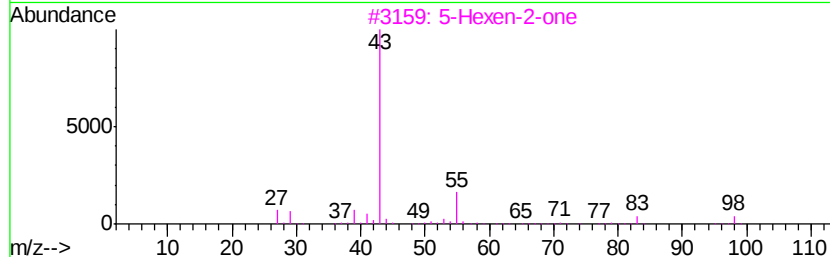
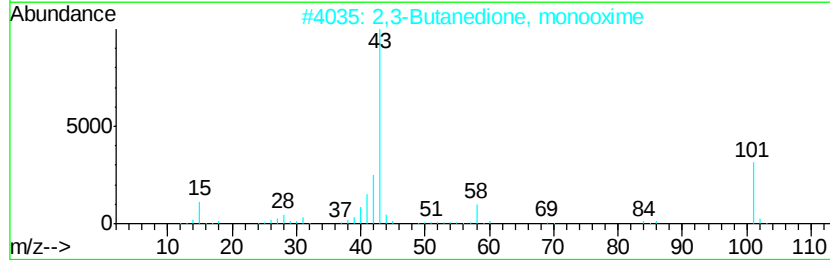
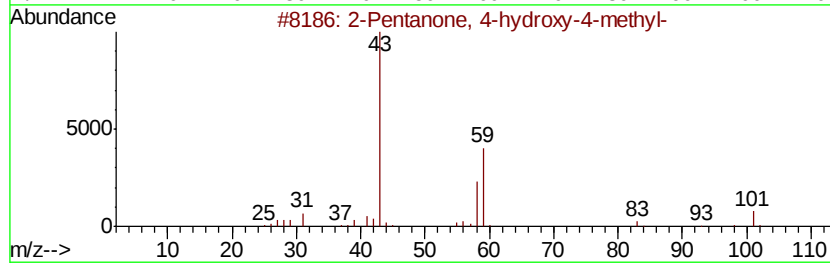
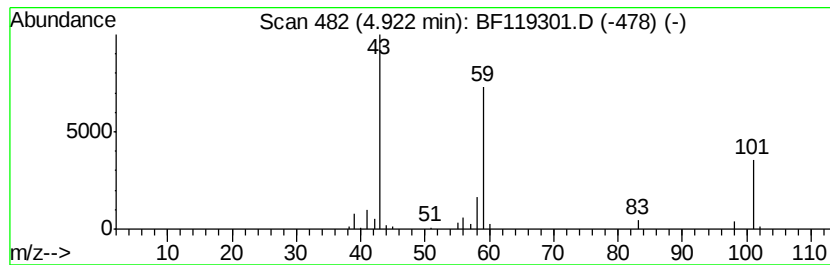
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
4.92	4.52 ng	125436	1,4-Dichlorobenzene-d4		6.72
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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Instrument :
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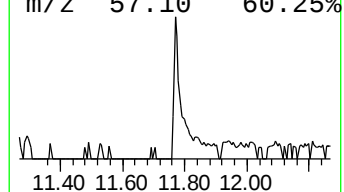
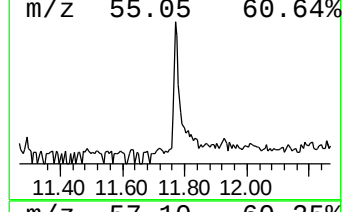
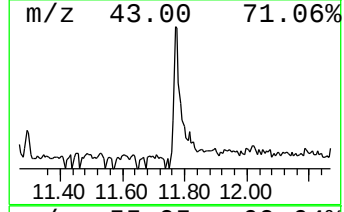
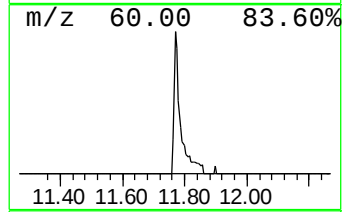
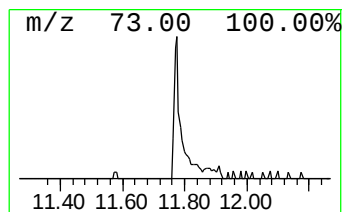
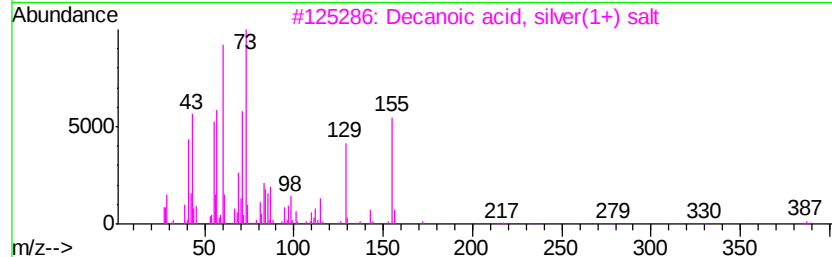
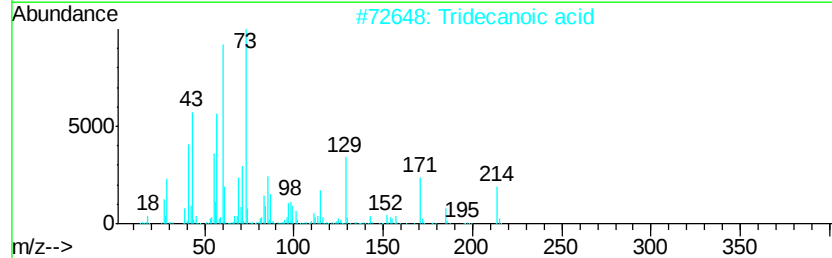
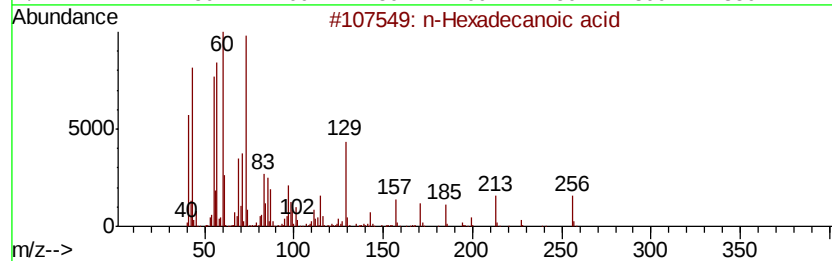
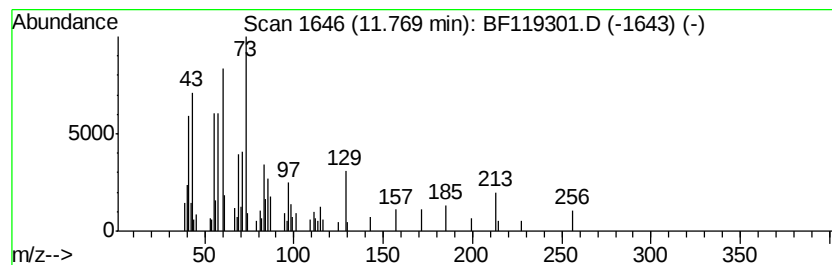
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.25 ng	100317	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	74
3		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		Undecanoic acid	186	C11H22O2	000112-37-8	35



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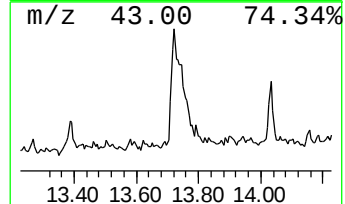
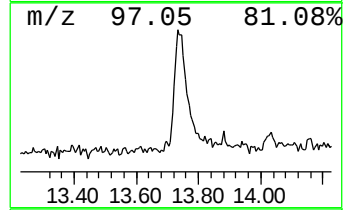
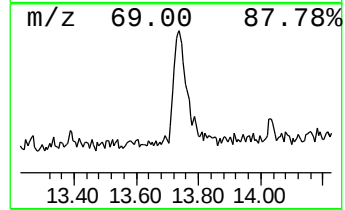
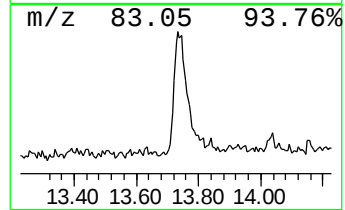
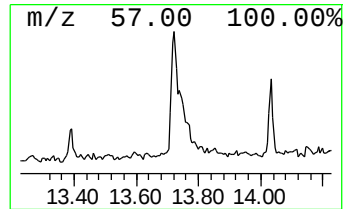
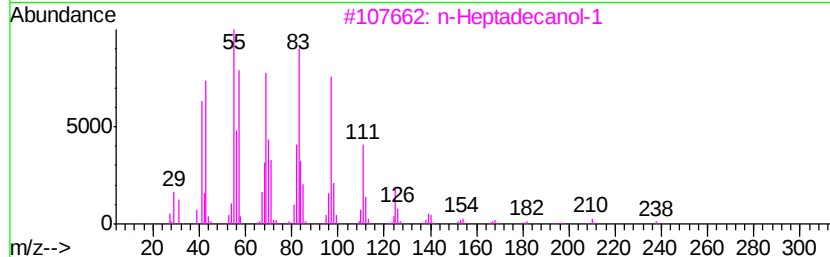
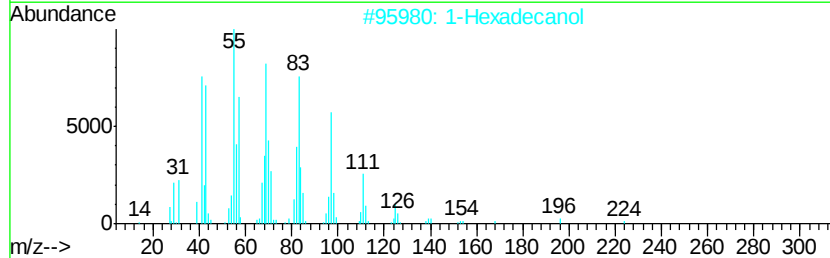
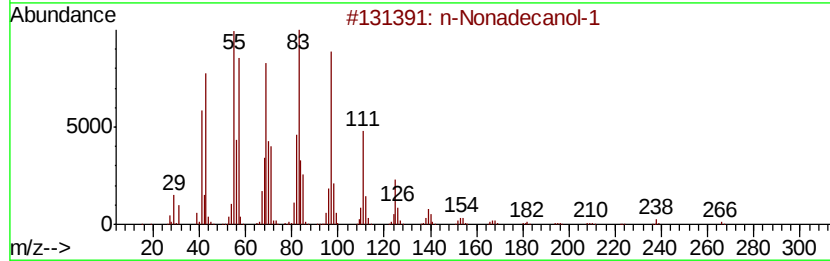
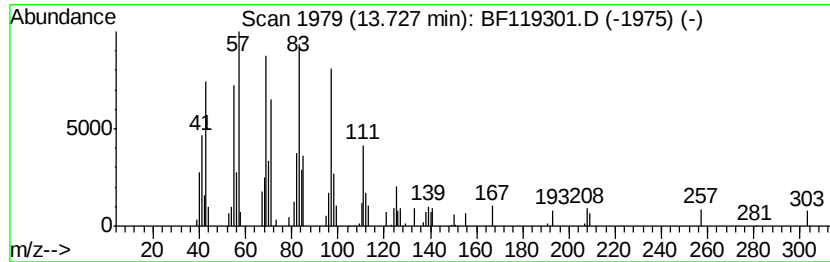
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.14 ng	203546	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4		5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	90
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90



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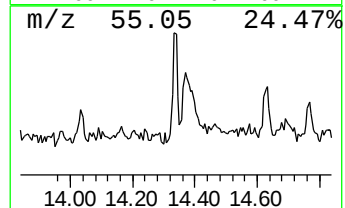
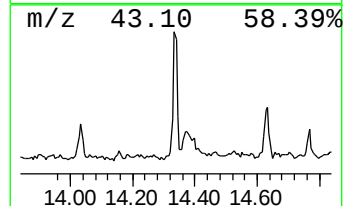
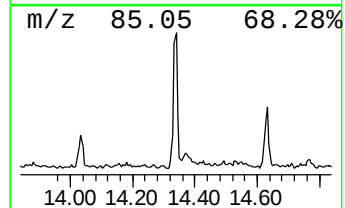
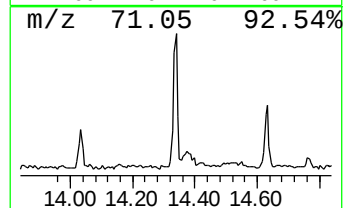
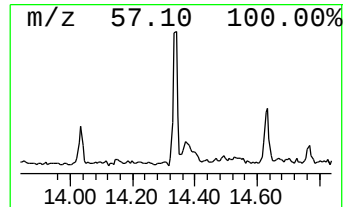
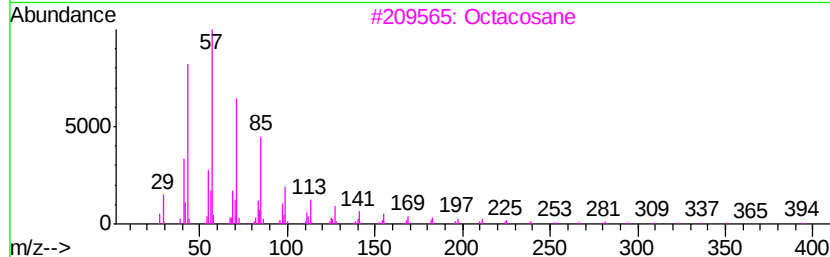
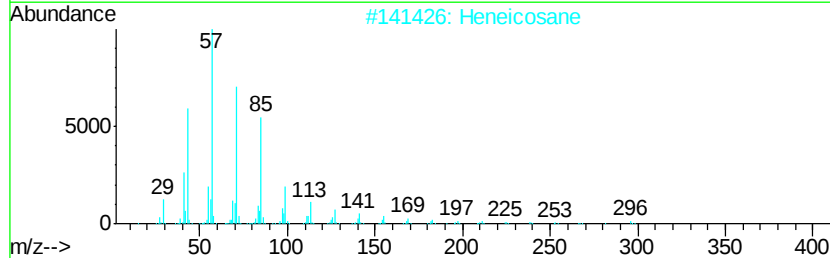
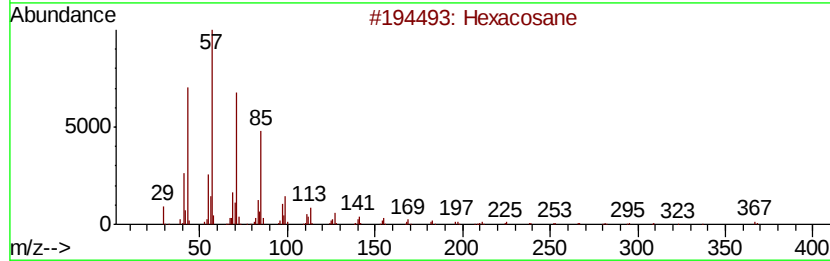
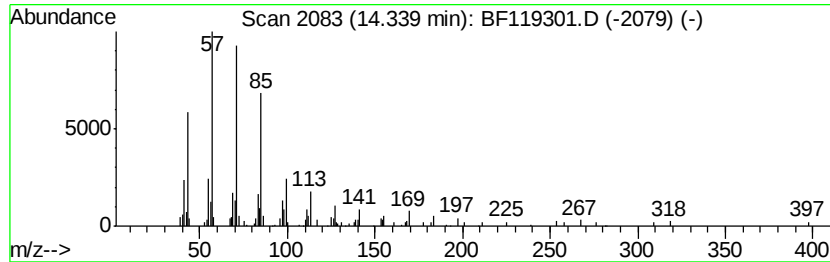
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.09 ng	102528	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Docosane		310	C22H46	000629-97-0	91



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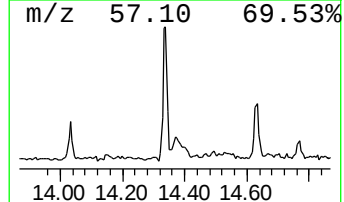
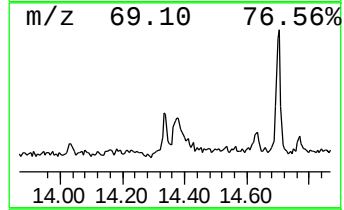
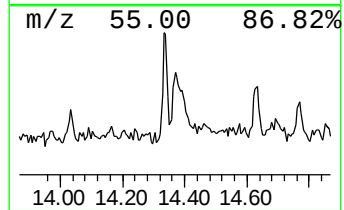
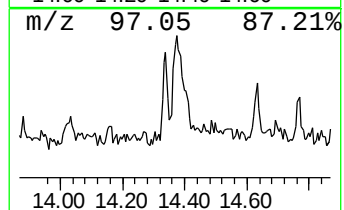
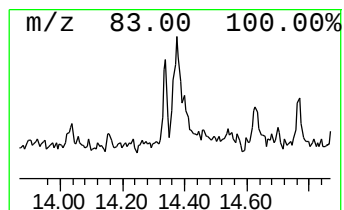
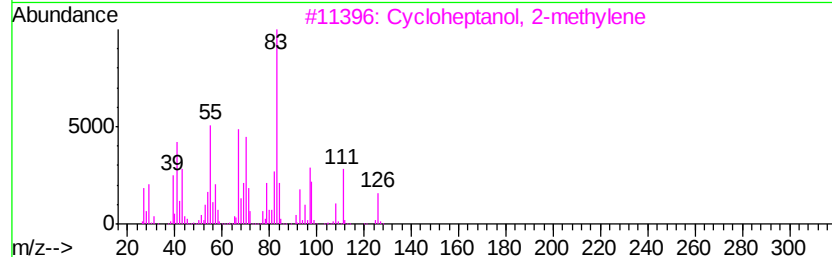
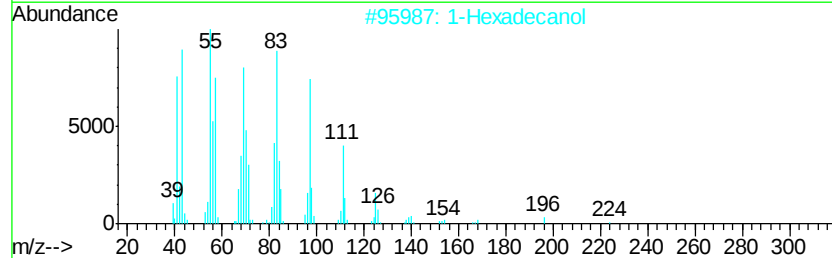
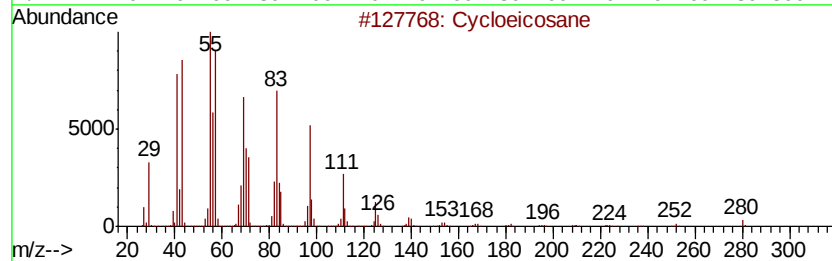
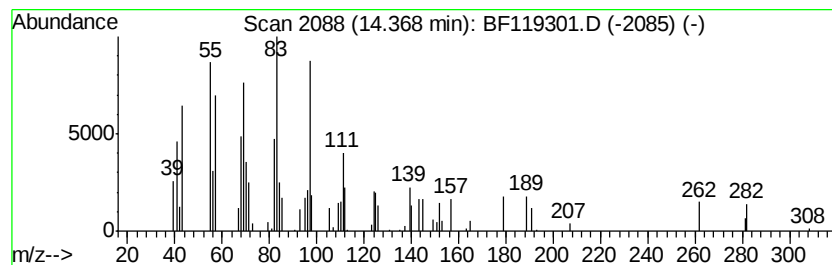
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloeicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.58 ng	85662	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloeicosane	280	C20H40	000296-56-0	58
2		1-Hexadecanol	242	C16H34O	036653-82-4	49
3		Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	49
4		1-Octadecanol	270	C18H38O	000112-92-5	49
5		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	46



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Data File : BF119301.D
Acq On : 9 Mar 2020 23:55
Operator : CG/JU
Sample : L1837-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-065

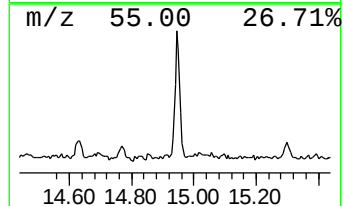
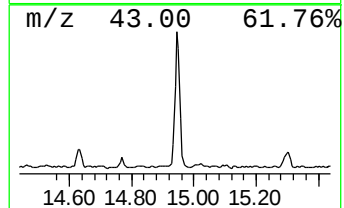
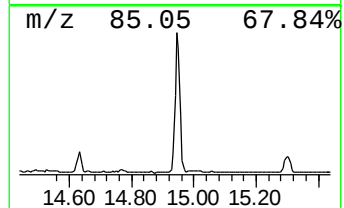
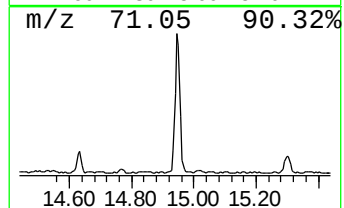
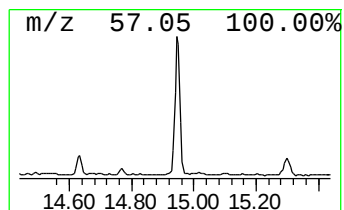
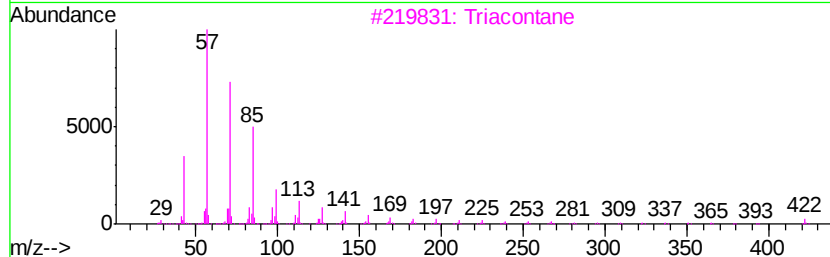
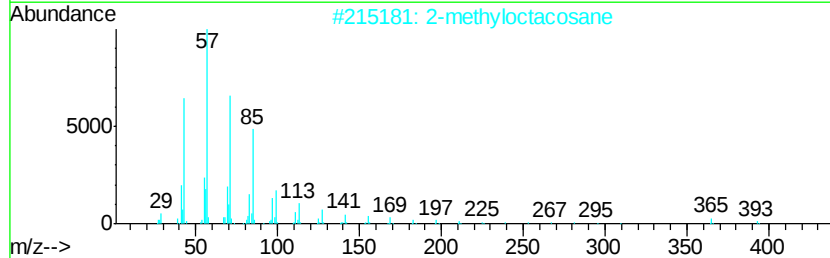
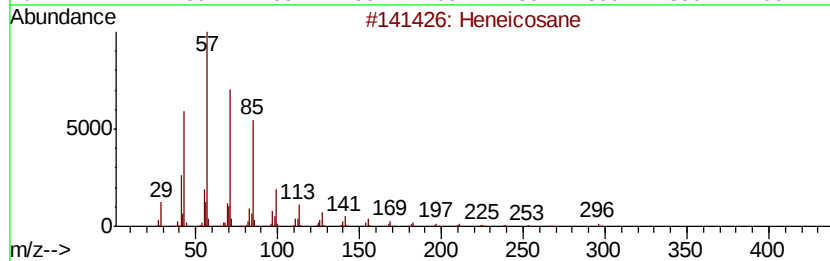
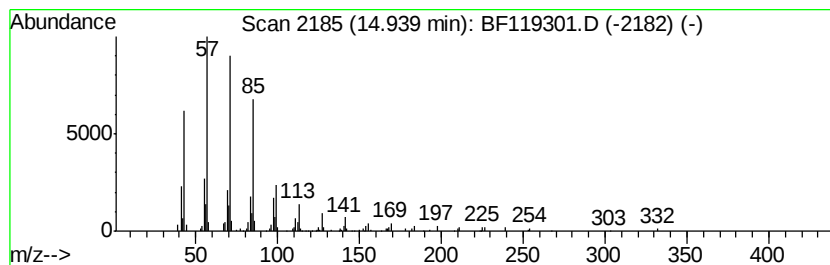
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	10.08 ng	370618	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	triacontane		422	C30H62	000638-68-6	91
4	2-methylhexacosane		380	C27H56	1000376-72-7	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030920\
Data File : BF119301.D
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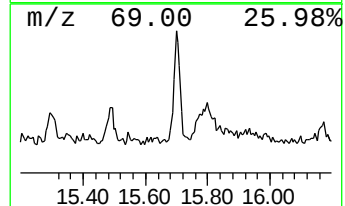
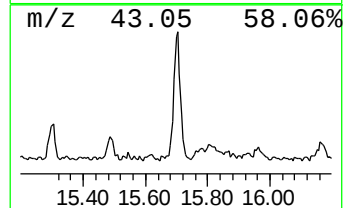
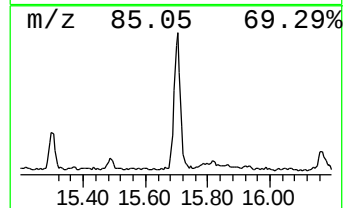
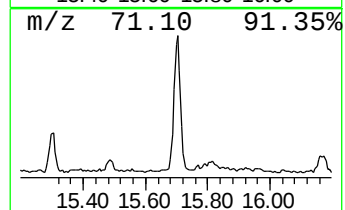
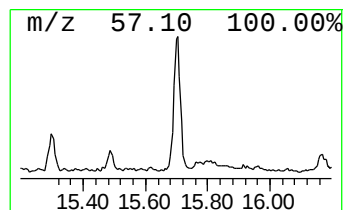
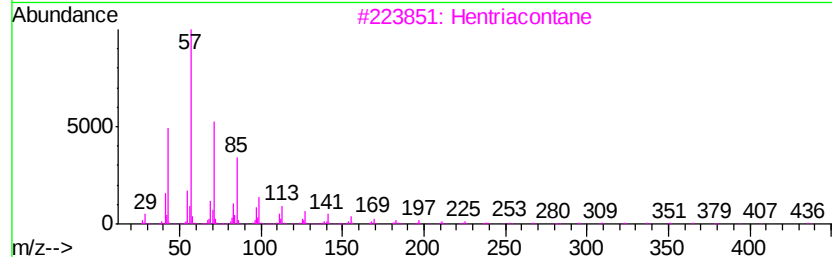
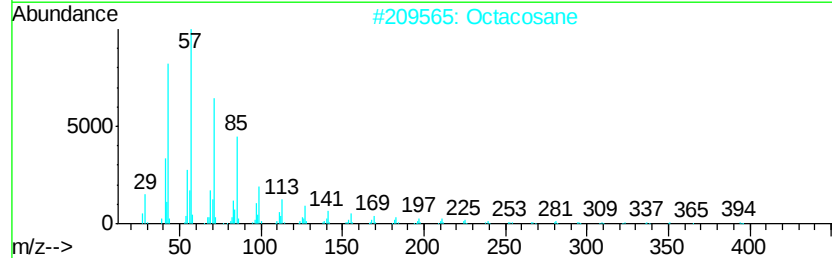
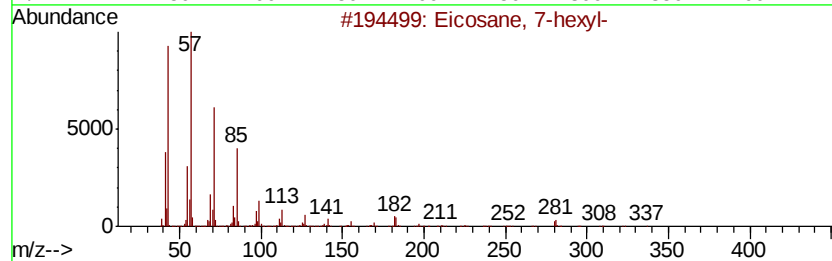
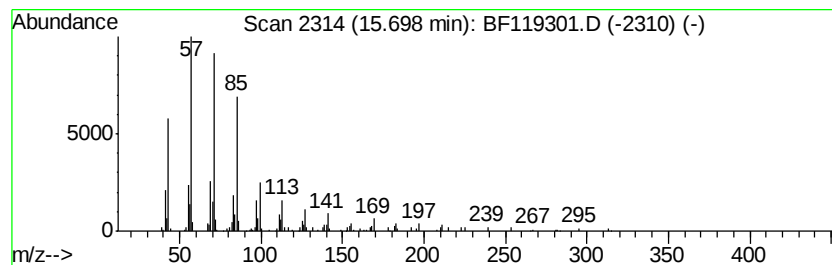
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	5.70 ng	209813	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91	
2	Octacosane	394	C28H58	000630-02-4	90	
3	Hentriacontane	437	C31H64	000630-04-6	90	
4	Hexacosane	366	C26H54	000630-01-3	90	
5	2-methyloctacosane	408	C29H60	1000376-72-8	87	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030920\
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Acq On : 9 Mar 2020 23:55
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Sample : L1837-01
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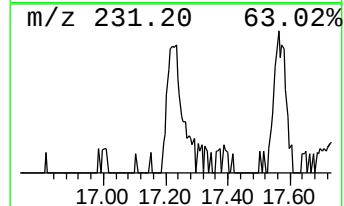
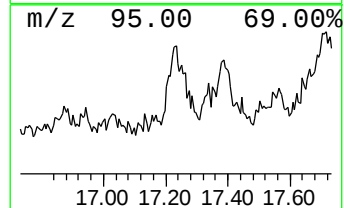
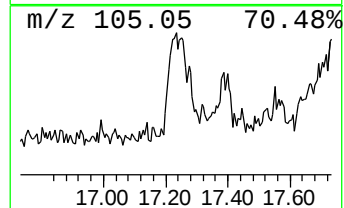
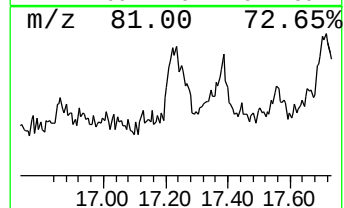
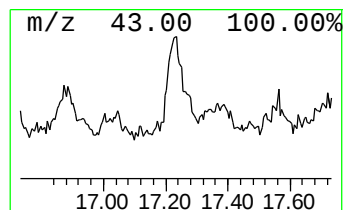
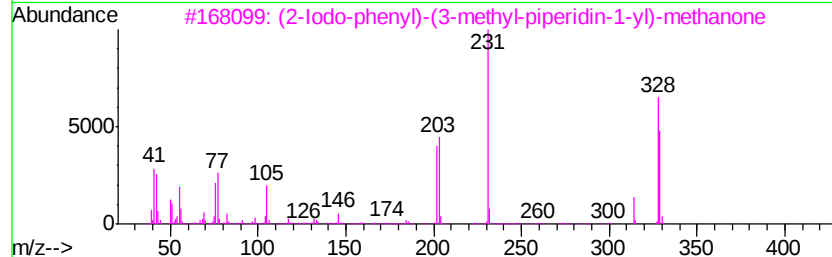
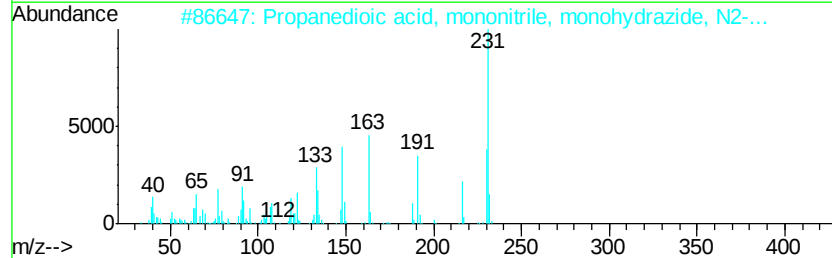
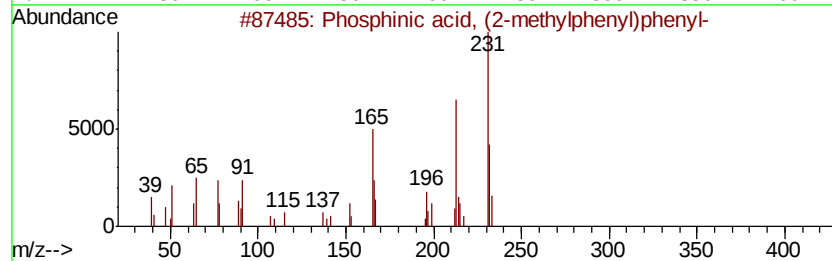
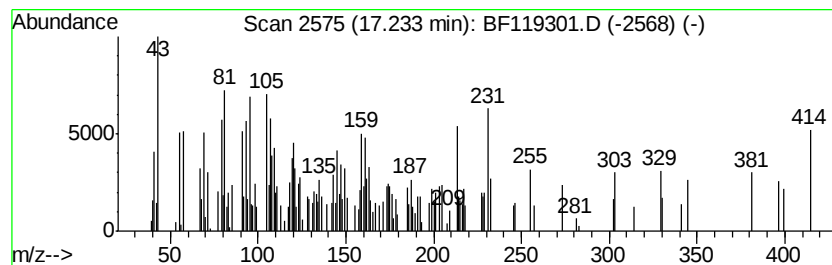
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.23	6.55 ng	241005	Perylene-d12	15.31		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phosphinic acid, (2-methylphenyl)...	232	C13H13O2P	018593-18-5	11
2		Propanedioic acid, mononitrile, ...	231	C12H13N3O2	004980-37-4	11
3		(2-Iodo-phenyl)-(3-methyl-piperi...	329	C13H16INO	333349-53-4	11
4		4-Methoxycarbonylamino-benzenesu...	273	C11H15NO5S	304882-97-1	11
5		4,8-Propanoborepino[1,2-b][1,2,5...	260	C16H30B2O	139688-22-5	10



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Operator : CG/JU
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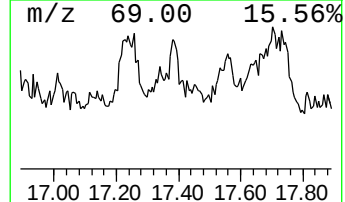
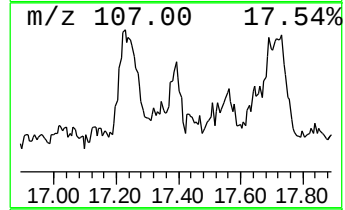
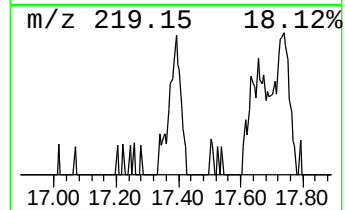
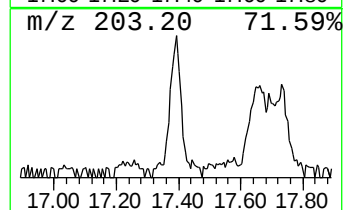
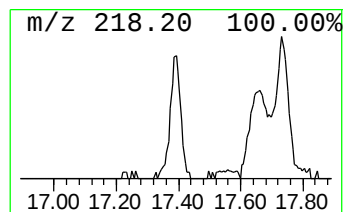
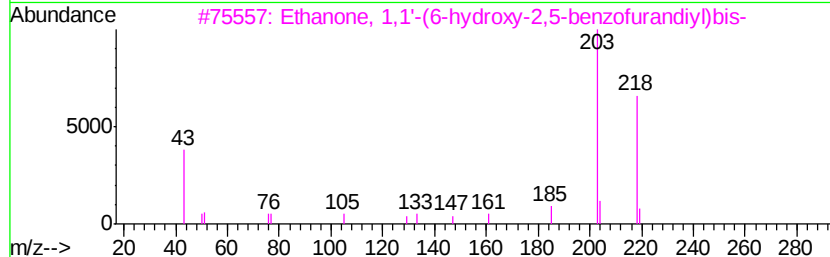
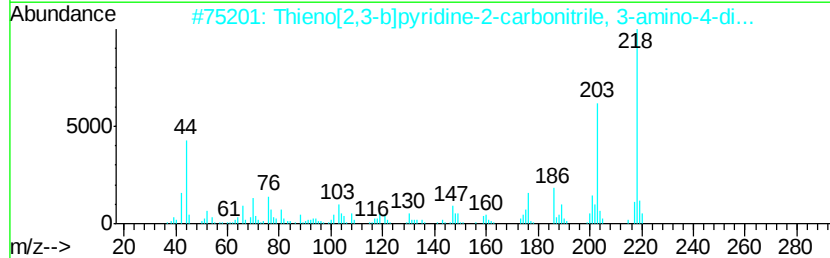
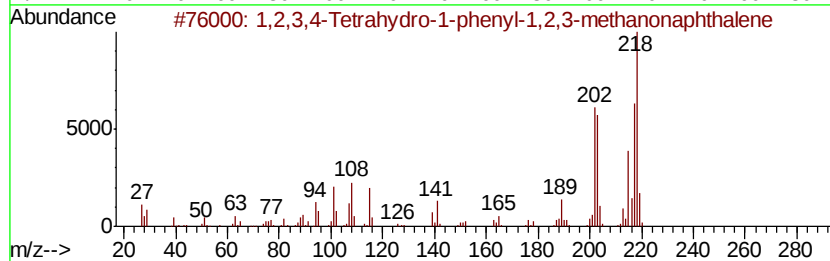
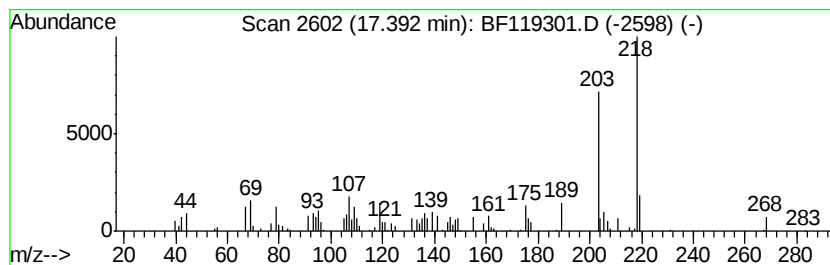
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2,3,4-Tetrahydro-1-phenyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	2.48 ng	91244	Perylene-d12	15.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	64
2			Thieno[2,3-b]pyridine-2-carbonit...	218	C10H10N4S	147992-88-9	64
3			Ethanone, 1,1'-(6-hydroxy-2,5-be...	218	C12H10O4	053947-86-7	58
4			9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	53
5			6-Benzyl-2-thiouracil	218	C11H10N2OS	006336-50-1	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030920\
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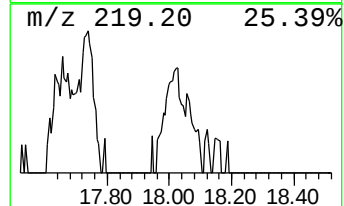
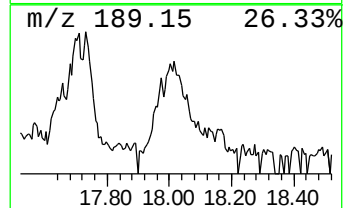
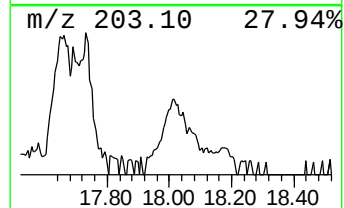
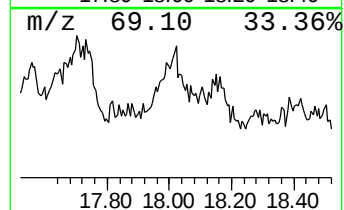
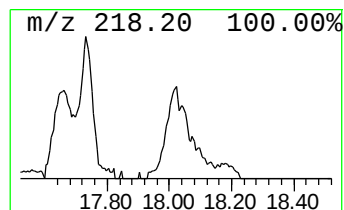
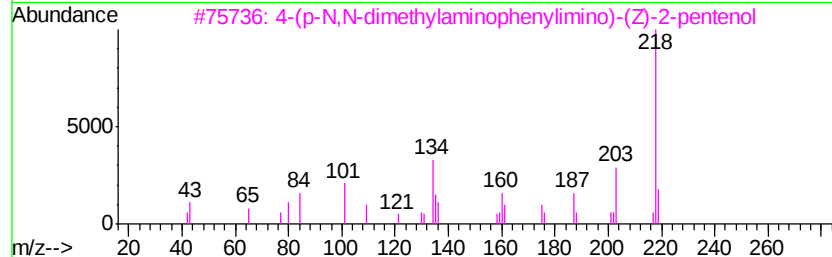
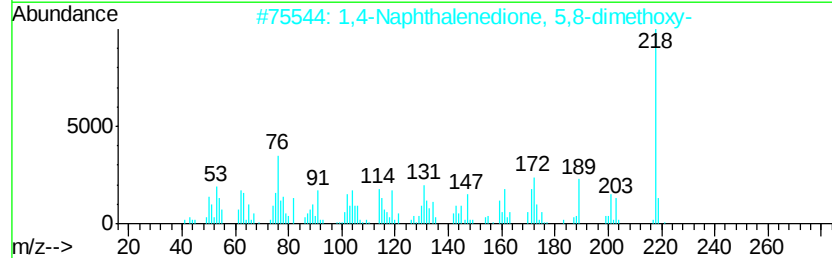
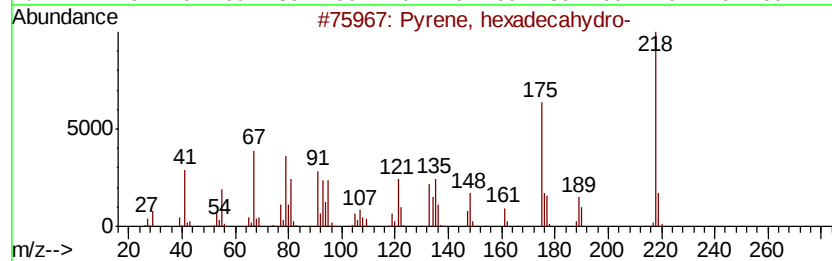
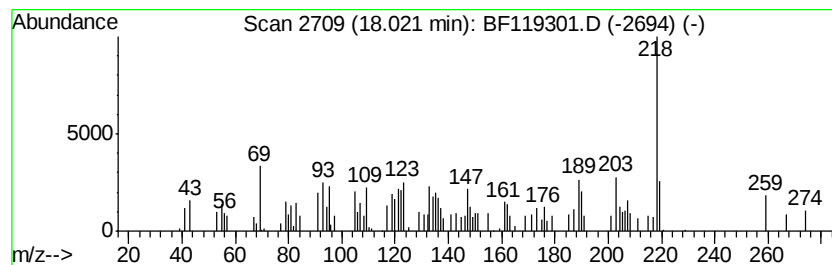
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	6.27 ng	230570	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	46
2		1,4-Naphthalenedione, 5,8-dimeth...	218	C12H10O4	015013-16-8	43
3		4-(p-N,N-dimethylaminophenylimin...	218	C13H18N2O	1000100-07-8	41
4		Indeno[2,1-b]chromene,	218	C16H10O	000243-24-3	38
5		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	4.5	ng	125436	1	6.72	554457	20.0
n-Hexadecanoic acid	11.77	2.3	ng	100317	4	11.24	891382	20.0
n-Nonadecanol-1	13.73	6.1	ng	203546	5	13.88	663468	20.0
Hexacosane	14.34	3.1	ng	102528	5	13.88	663468	20.0
Cycloeicosane	14.37	2.6	ng	85662	5	13.88	663468	20.0
Heneicosane	14.94	10.1	ng	370618	6	15.31	735638	20.0
Eicosane, 7-hexyl-	15.70	5.7	ng	209813	6	15.31	735638	20.0
(DEL) Alkane: Str...	17.23	6.5	ng	241005	6	15.31	735638	20.0
1,2,3,4-Tetrahydr...	17.39	2.5	ng	91244	6	15.31	735638	20.0
unknown18.02	18.02	6.3	ng	230570	6	15.31	735638	20.0