

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
 Data File : BF135368.D
 Acq On : 20 Sep 2023 20:50
 Operator : CG\JU
 Sample : 04304-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	491	496	506	rVB	73731	102334	3.26%	0.414%
2	5.398	559	563	582	rBV	3187318	3135537	100.00%	12.683%
3	6.404	729	734	737	rBV	3061620	3068827	97.87%	12.413%
4	6.757	791	794	800	rBV	928443	739459	23.58%	2.991%
5	7.322	885	890	893	rBV	2111364	1984253	63.28%	8.026%
6	8.033	1007	1011	1015	rBV	997801	896935	28.61%	3.628%
7	9.027	1176	1180	1182	rBV4	22603	34193	1.09%	0.138%
8	9.057	1182	1185	1188	rBV	60309	56253	1.79%	0.228%
9	9.116	1188	1195	1198	rBV	3184150	2791289	89.02%	11.291%
10	9.145	1198	1200	1203	rVB3	37691	40197	1.28%	0.163%
11	9.198	1203	1209	1211	rBV5	66280	103966	3.32%	0.421%
12	9.339	1230	1233	1234	rBV2	43566	45519	1.45%	0.184%
13	9.363	1234	1237	1239	rVV3	47049	58509	1.87%	0.237%
14	9.422	1244	1247	1250	rBV4	113330	139969	4.46%	0.566%
15	9.516	1260	1263	1266	rBV	240016	195766	6.24%	0.792%
16	9.545	1266	1268	1270	rVV2	63331	50119	1.60%	0.203%
17	9.604	1276	1278	1279	rBV2	57353	40684	1.30%	0.165%
18	9.657	1284	1287	1291	rBV3	128706	254429	8.11%	1.029%
19	9.698	1291	1294	1297	rVB2	197598	198878	6.34%	0.804%
20	9.739	1299	1301	1303	rBV3	89248	80418	2.56%	0.325%
21	9.792	1307	1310	1313	rVB	960141	860070	27.43%	3.479%
22	10.051	1352	1354	1357	rBV2	214951	209550	6.68%	0.848%
23	10.198	1377	1379	1382	rBV2	184251	181492	5.79%	0.734%
24	10.451	1419	1422	1428	rVB	583517	652186	20.80%	2.638%
25	10.592	1443	1446	1448	rBV	923223	833324	26.58%	3.371%
26	10.722	1465	1468	1474	rVB	1205796	1227717	39.15%	4.966%
27	11.192	1544	1548	1552	rVB	1281199	1383480	44.12%	5.596%
28	11.292	1562	1565	1573	rBV3	742037	997315	31.81%	4.034%
29	11.539	1605	1607	1610	rVB	419164	342923	10.94%	1.387%
30	12.274	1730	1732	1737	rVB	279404	293750	9.37%	1.188%
31	12.739	1809	1811	1813	rVB	208338	147094	4.69%	0.595%
32	12.886	1832	1836	1839	rBV	1909075	1826121	58.24%	7.387%
33	13.945	2011	2016	2019	rBV2	731629	760044	24.24%	3.074%
34	14.986	2189	2193	2196	rBV	130816	187000	5.96%	0.756%
35	15.280	2241	2243	2248	rVB	72132	97441	3.11%	0.394%
36	15.345	2251	2254	2259	rVB	100310	131117	4.18%	0.530%

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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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.409	2261	2265	2269	rBV	473105	573773	18.30%	2.321%
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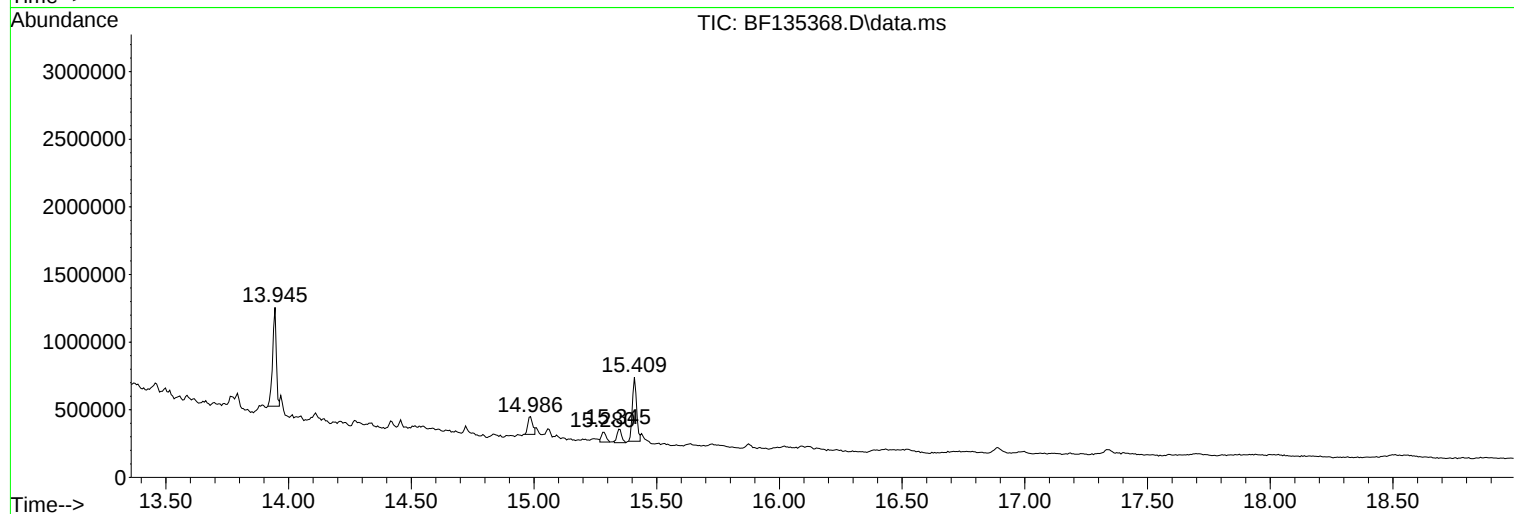
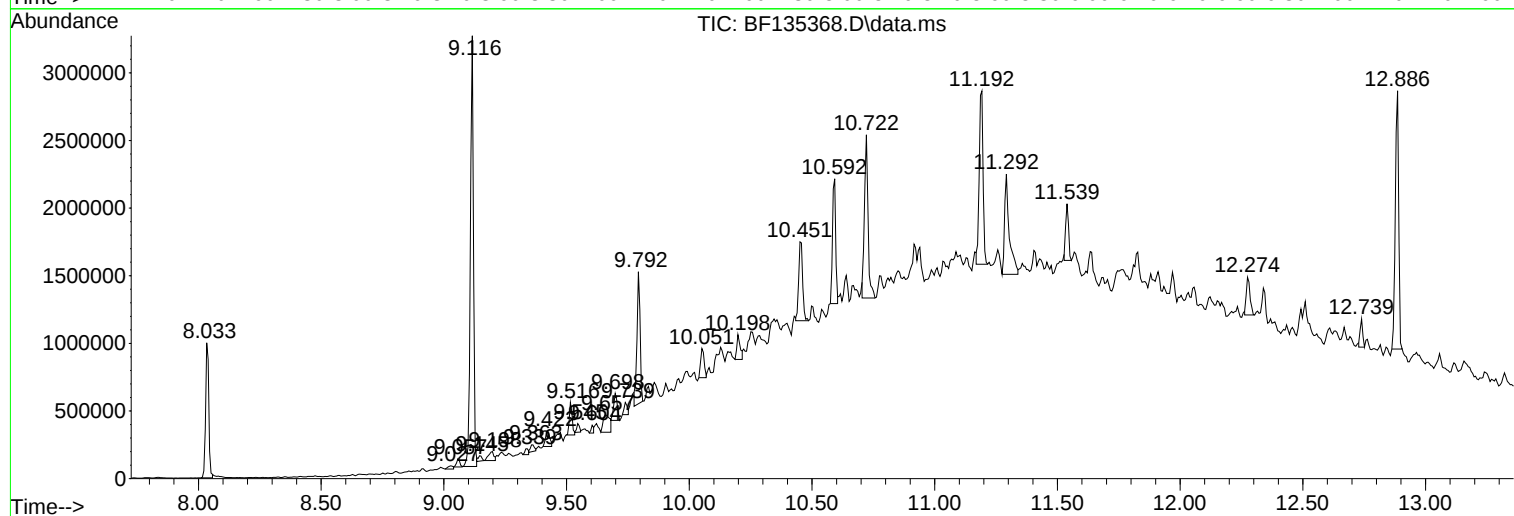
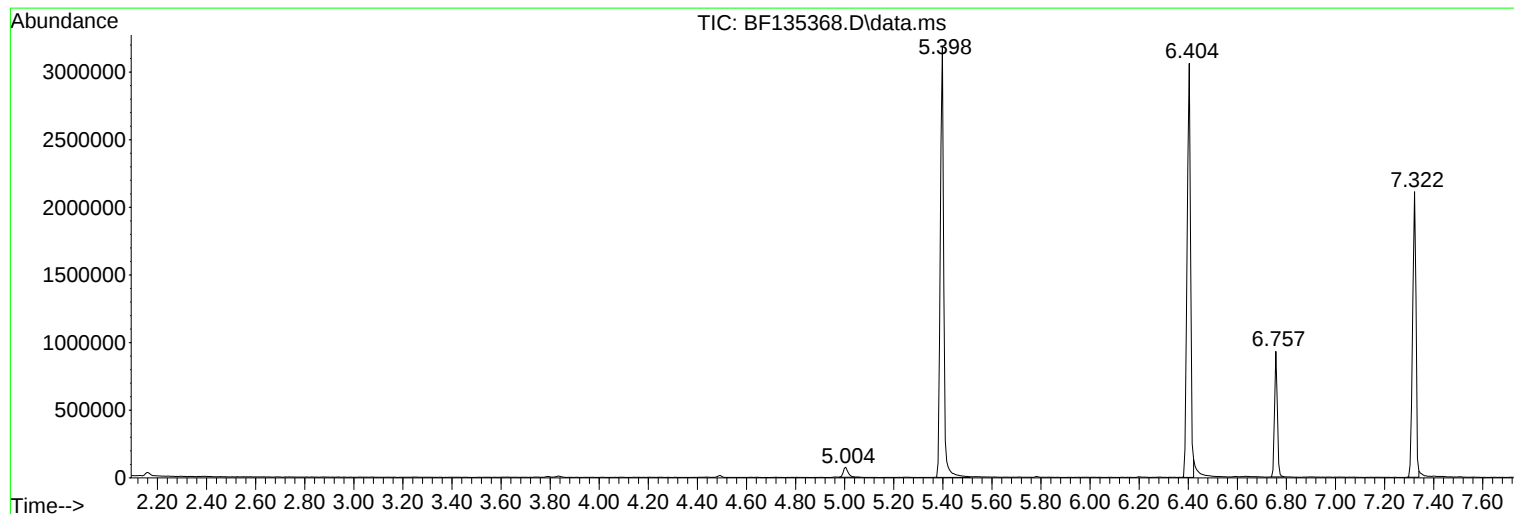
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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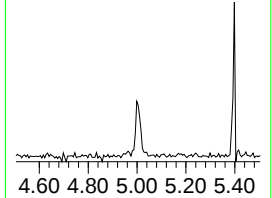
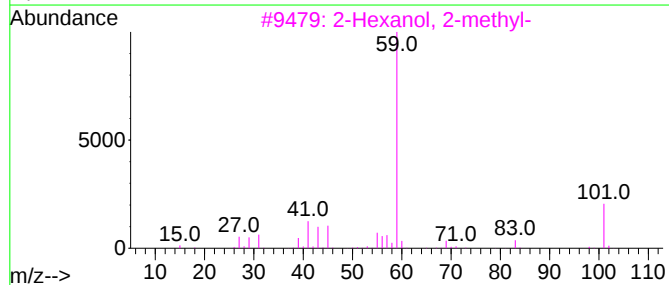
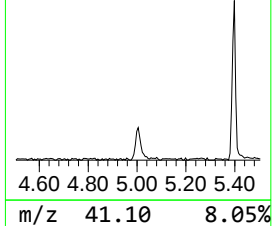
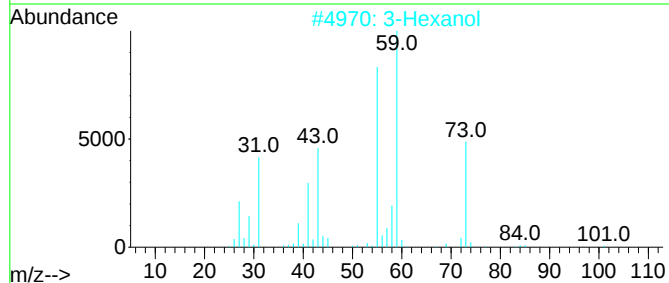
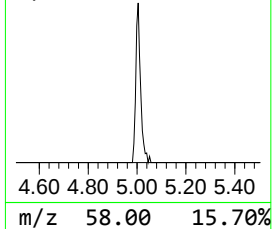
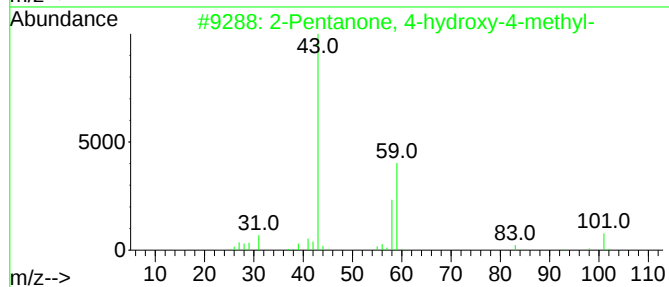
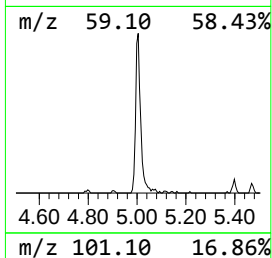
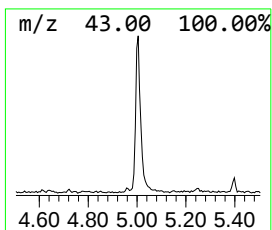
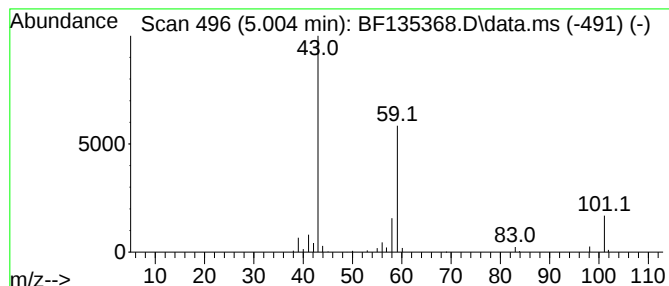
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.77 ng	102334	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Guanidine	59	CH5N3	000113-00-8	9		



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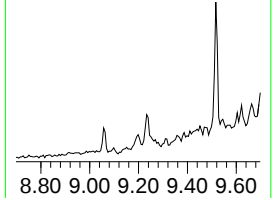
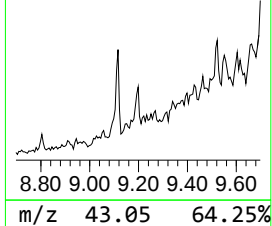
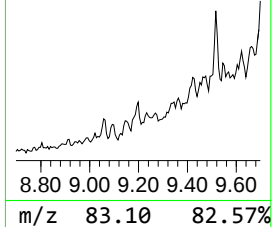
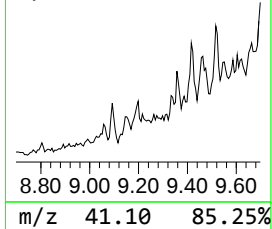
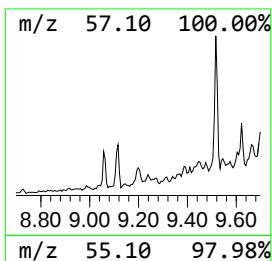
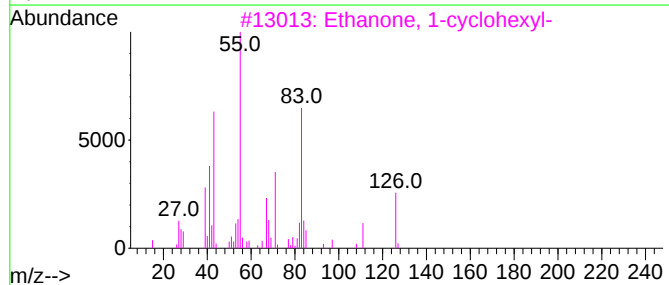
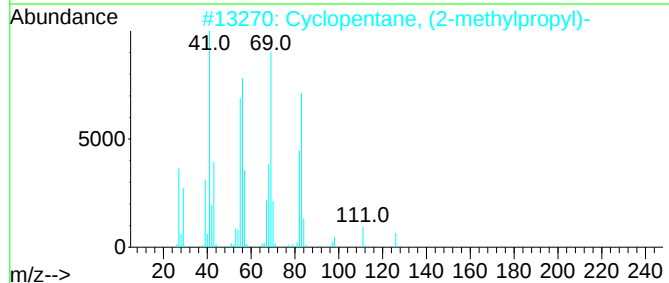
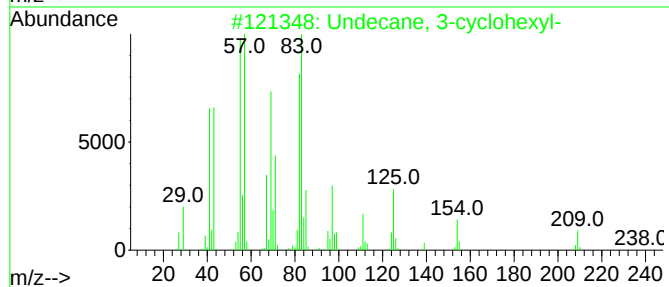
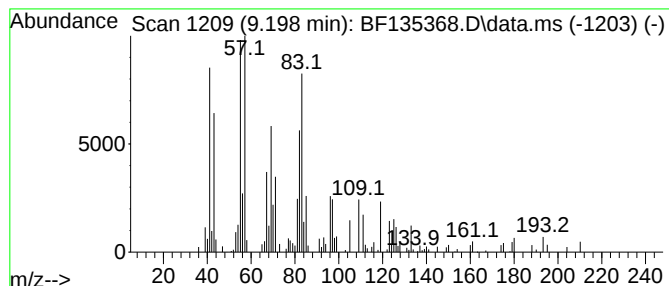
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Undecane, 3-cyclohexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.198	2.42 ng	103966	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3-cyclohexyl-	238	C17H34	013151-78-5	50
2			Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	43
3			Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	41
4			Acetic acid, mercapto-, cyclohex...	174	C8H14O2S	016849-98-2	38
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38



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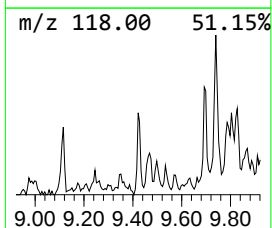
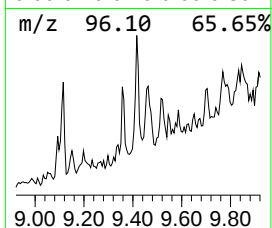
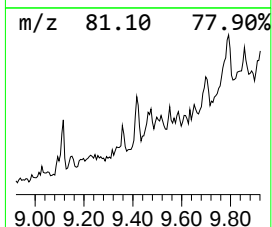
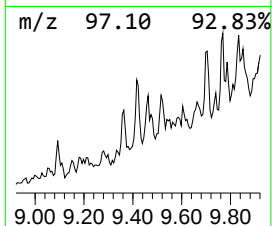
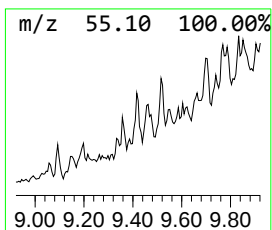
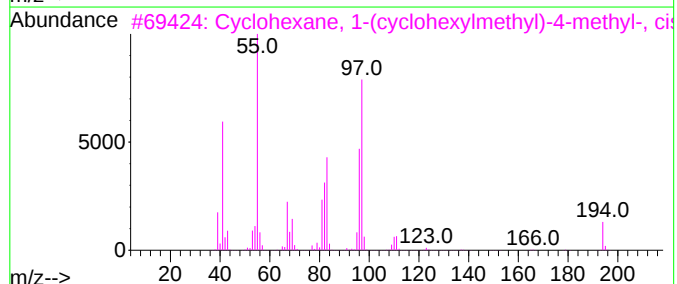
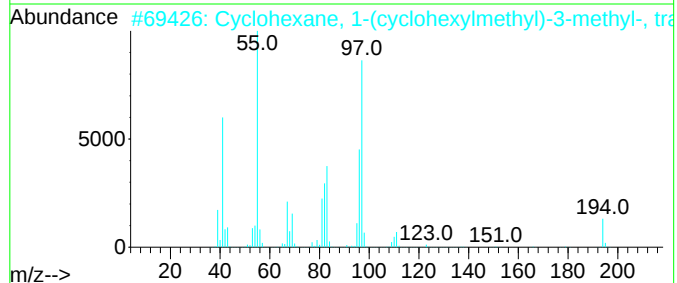
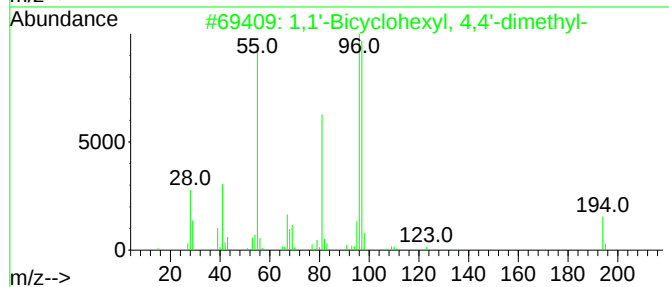
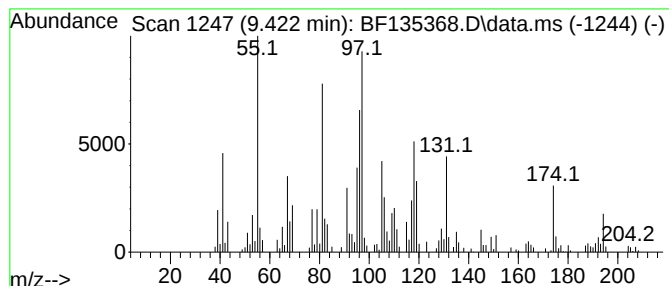
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.422 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.422	3.25 ng	139969	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl, 4,4'-dimethyl-	194	C14H26	054823-99-3	38		
2	Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-95-9	30		
3	Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-97-1	30		
4	2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	25		
5	Isomycorene	136	C10H16	006876-07-9	25		



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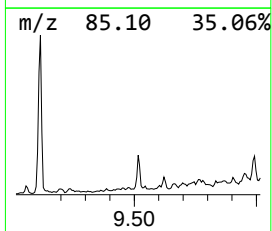
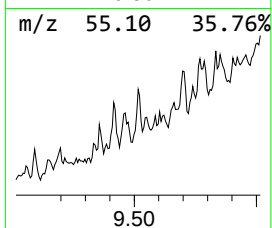
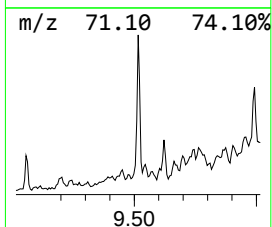
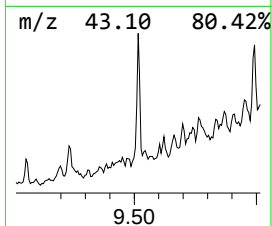
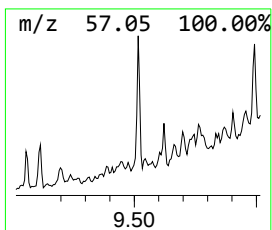
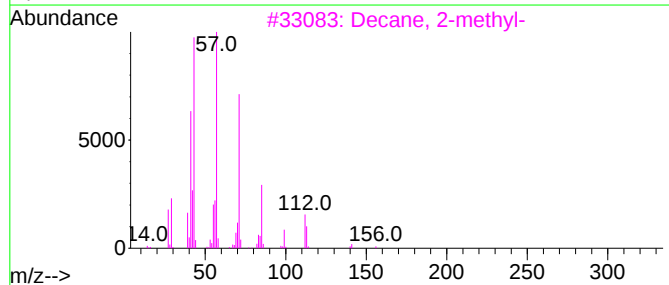
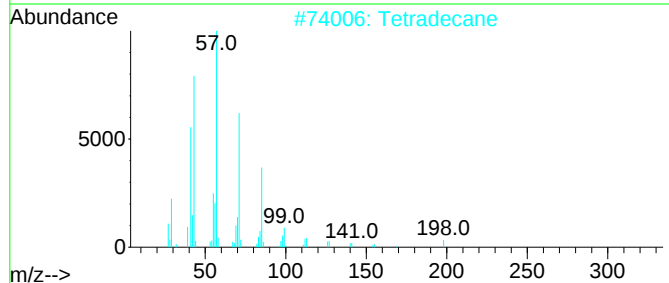
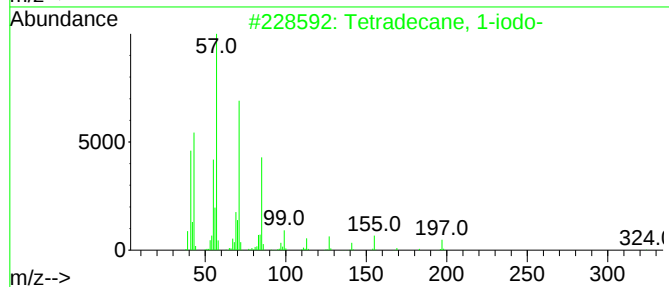
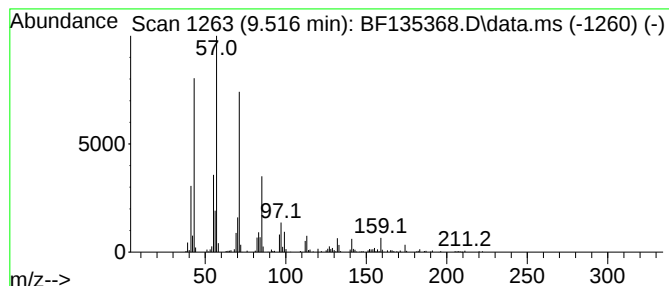
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.516	4.55 ng	195766	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
2			Tetradecane	198	C14H30	000629-59-4	72
3			Decane, 2-methyl-	156	C11H24	006975-98-0	72
4			Hexadecane	226	C16H34	000544-76-3	72
5			Bacchotricuneatin c	342	C20H22O5	066563-30-2	64



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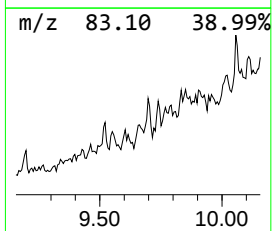
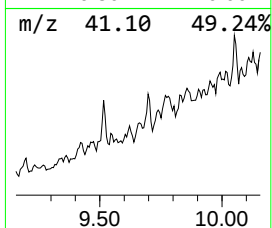
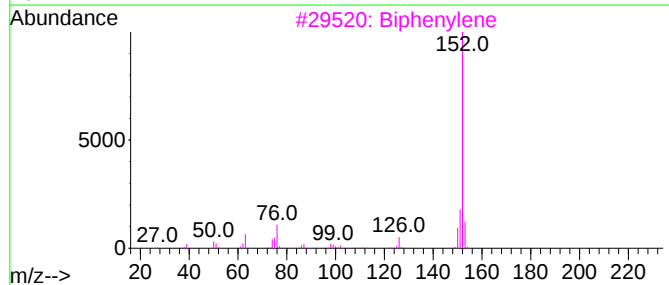
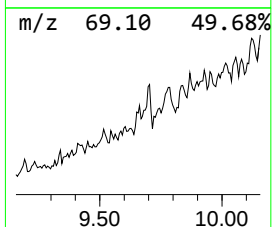
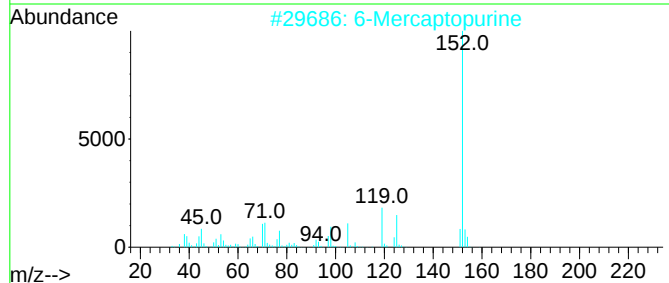
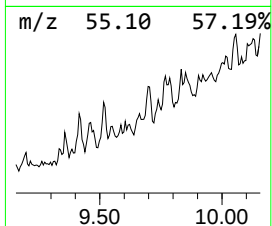
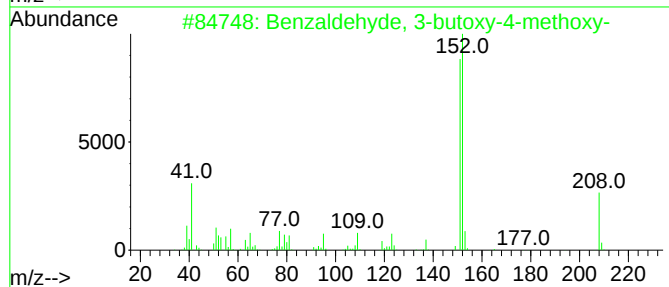
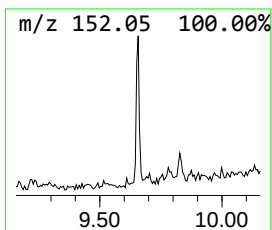
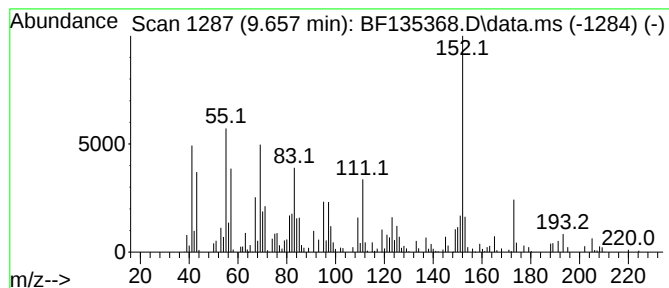
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.657 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	5.92 ng	254429	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3-butoxy-4-methoxy-	208	C12H16O3	034127-96-3	41
2			6-Mercaptopurine	152	C5H4N4S	000050-44-2	41
3			Biphenylene	152	C12H8	000259-79-0	41
4			Acenaphthylene	152	C12H8	000208-96-8	41
5			Piperidine, 1-(cyanoacetyl)-	152	C8H12N2O	015029-30-8	38



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Data File : BF135368.D
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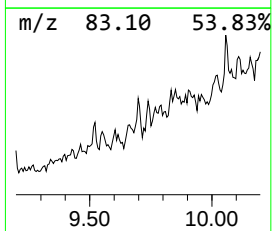
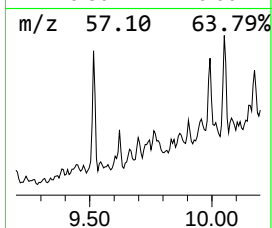
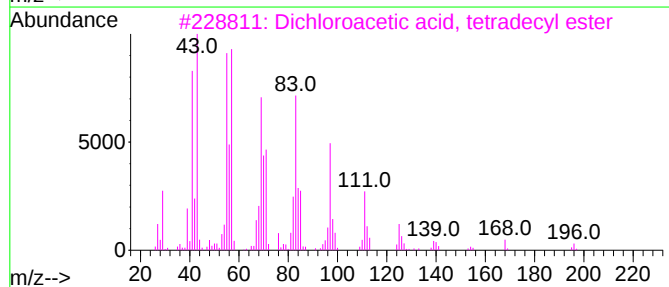
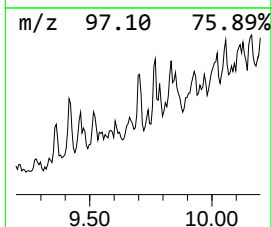
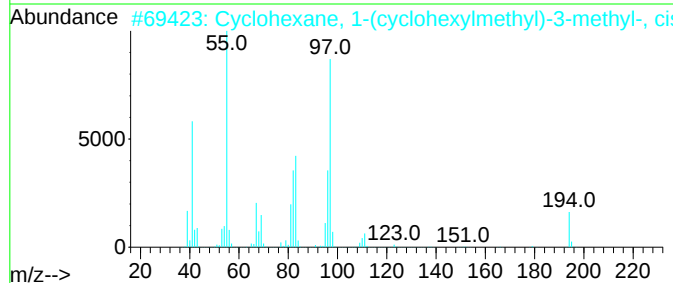
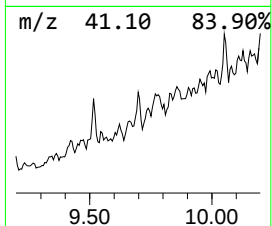
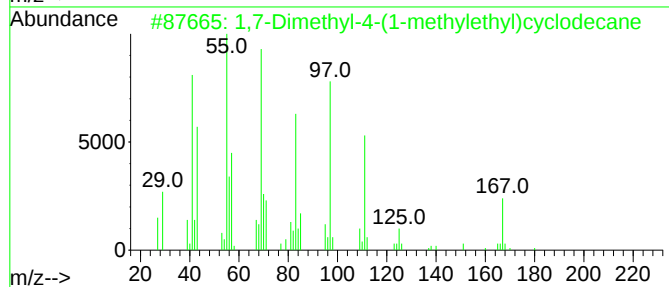
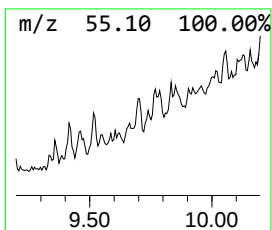
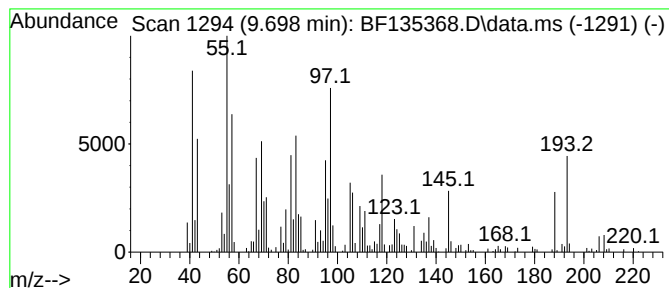
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.698 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.698	4.62 ng	198878	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	27
2			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-96-0	27
3			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	25
4			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	25
5			Cycloheptane, methyl-	112	C8H16	004126-78-7	25



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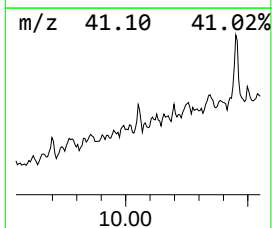
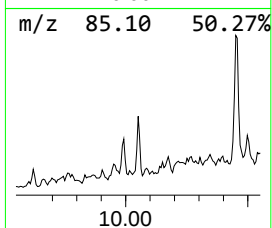
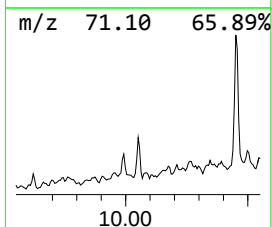
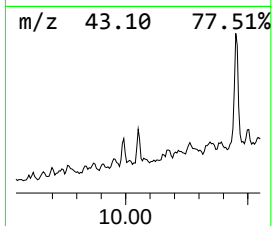
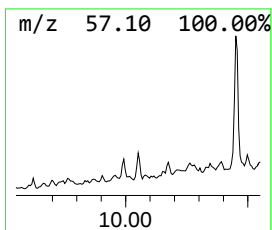
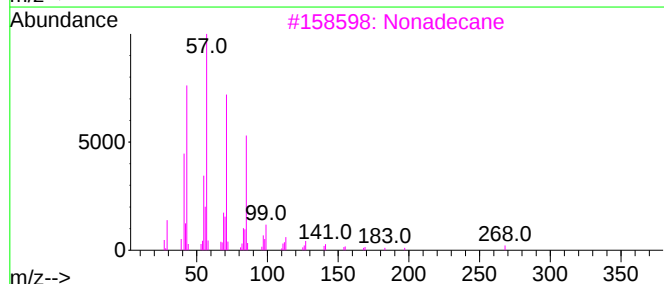
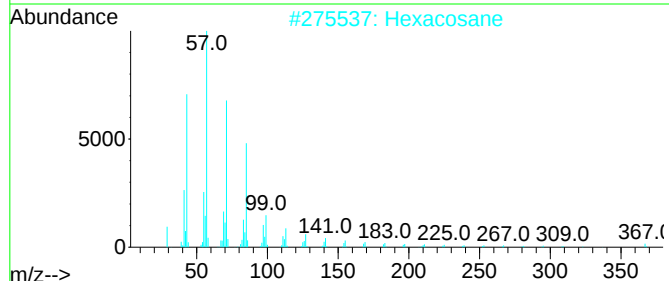
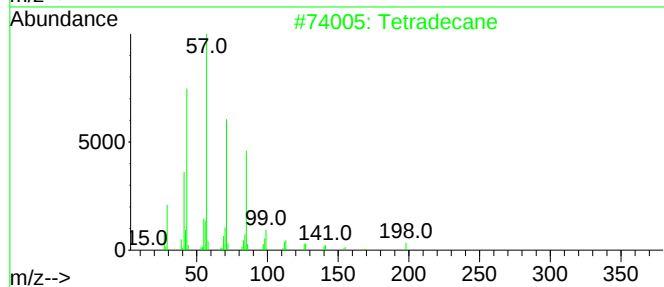
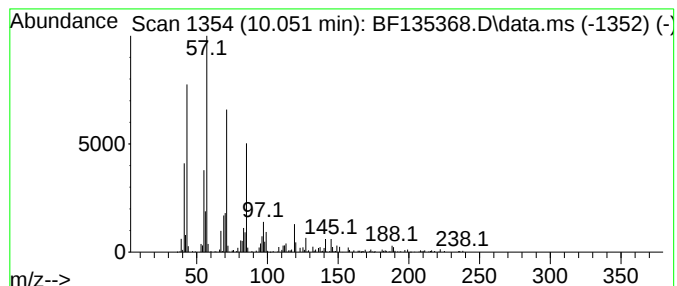
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.051	4.87 ng	209550	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	72
2			Hexacosane	366	C26H54	000630-01-3	64
3			Nonadecane	268	C19H40	000629-92-5	64
4			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	59
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	52



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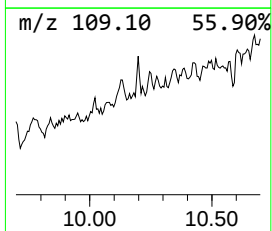
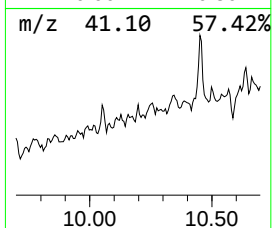
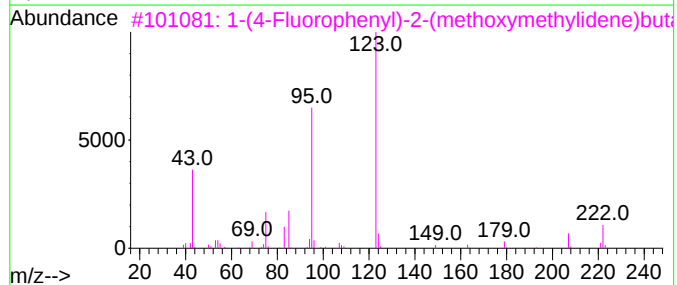
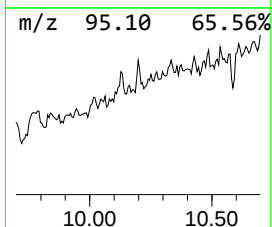
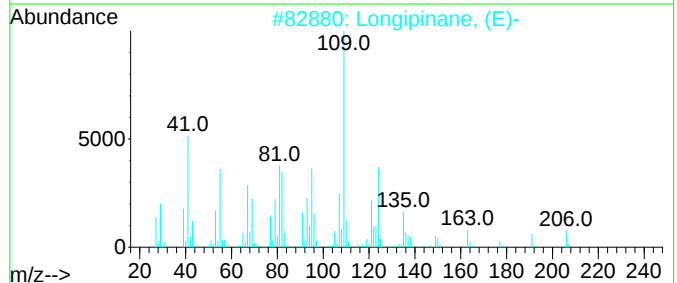
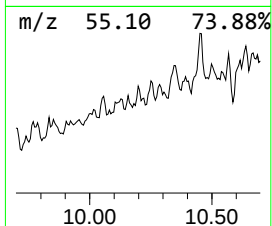
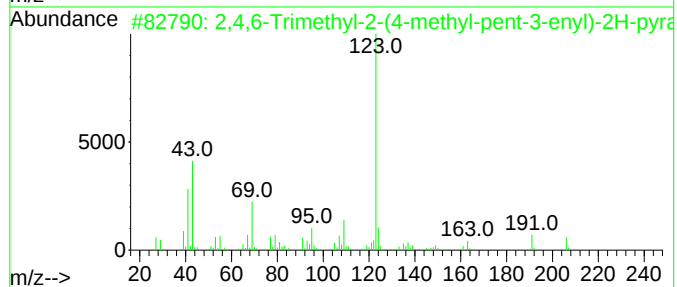
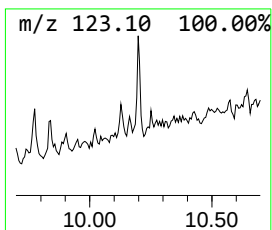
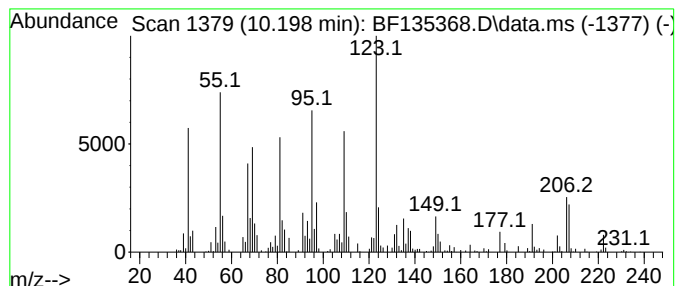
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2,4,6-Trimethyl-2-(4-methyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	4.22 ng	181492	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trimethyl-2-(4-methyl-pent...	206	C14H22O	1000193-58-6	52		
2	Longipinane, (E)-	206	C15H26	1000156-14-5	50		
3	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	38		
4	1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	38		
5	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	25		



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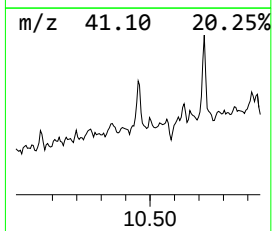
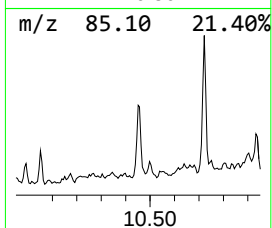
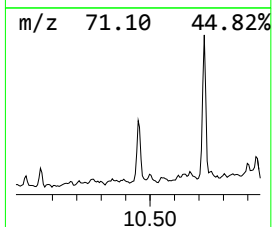
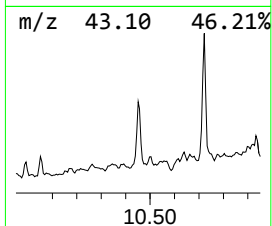
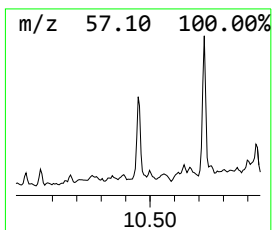
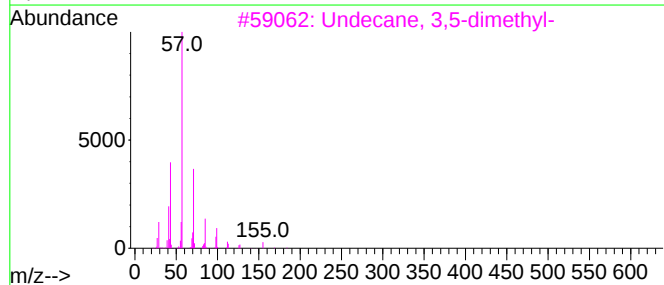
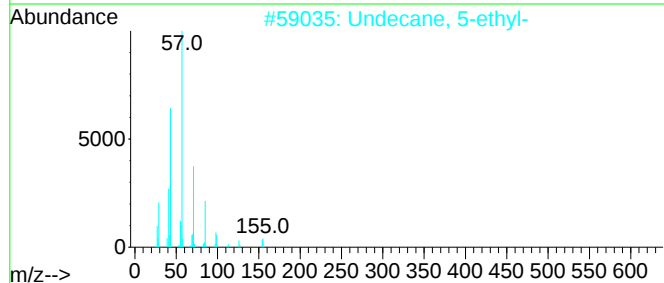
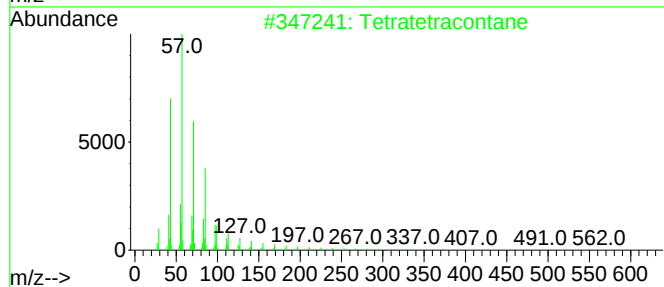
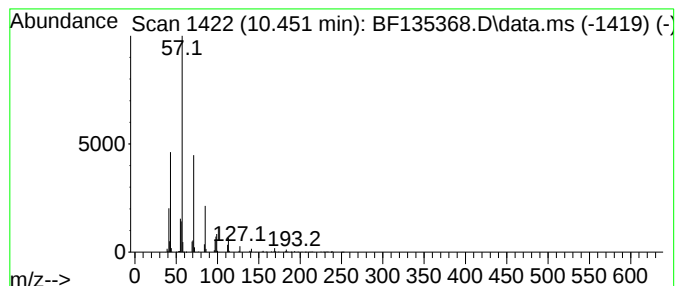
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	15.17 ng	652186	Acenaphthene-d10	9.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	78
2			Undecane, 5-ethyl-	184	C13H28	017453-94-0	78
3			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	72
4			Heptacosane	380	C27H56	000593-49-7	64
5			Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
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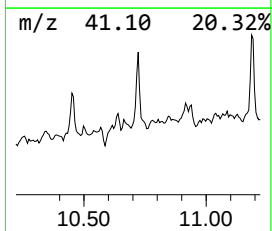
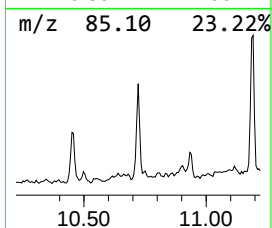
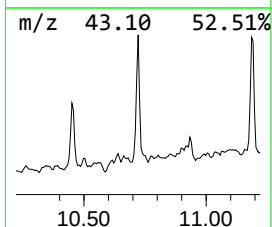
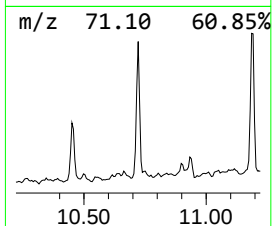
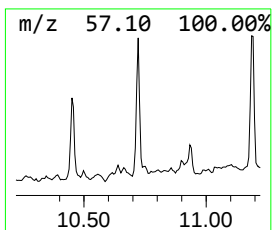
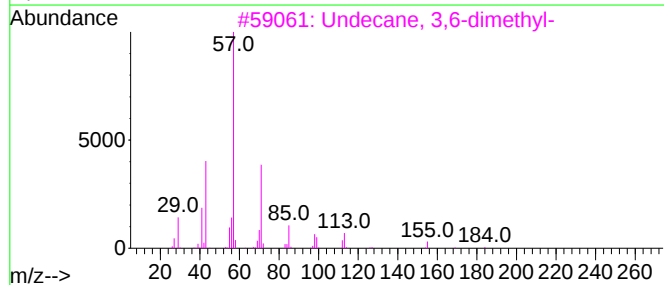
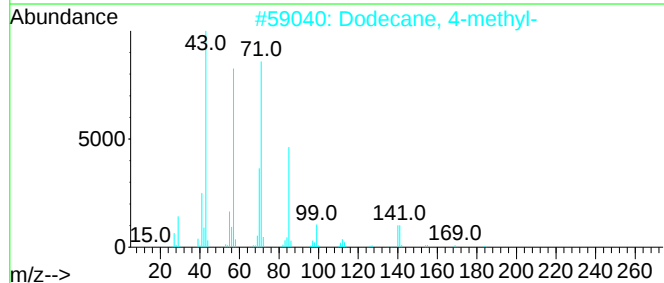
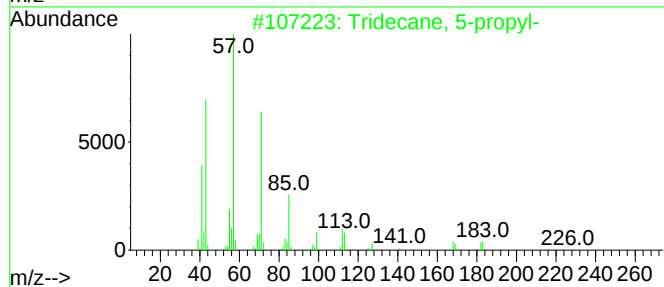
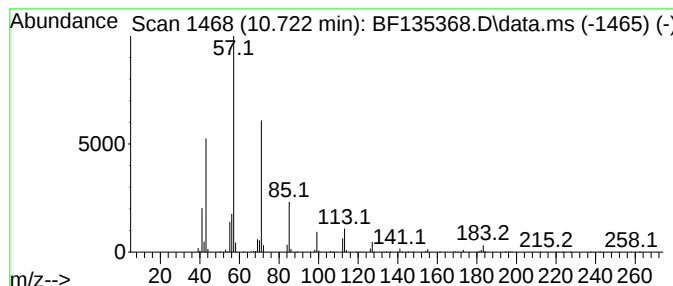
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tridecane, 5-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	24.62 ng	1227720	Phenanthrene-d10	11.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
2		Dodecane, 4-methyl-	184	C13H28	006117-97-1	68
3		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	58
4		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	53
5		Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	52



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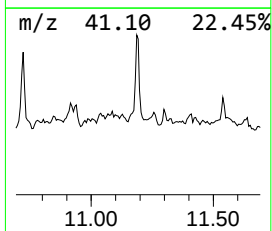
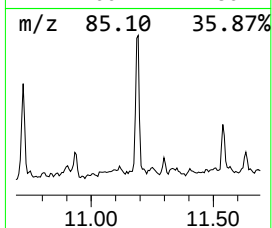
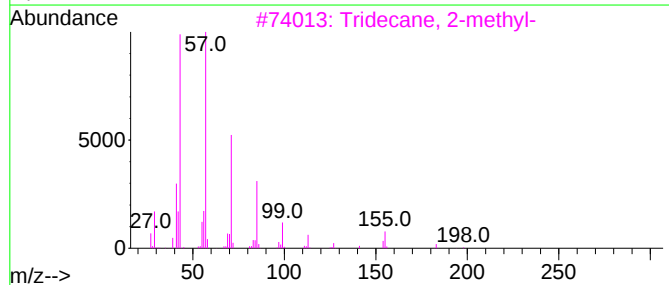
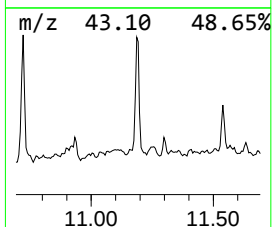
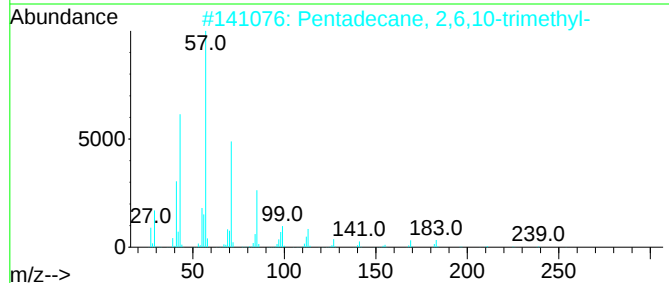
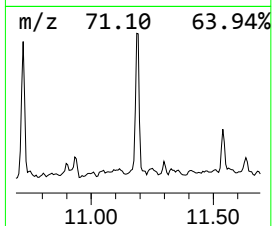
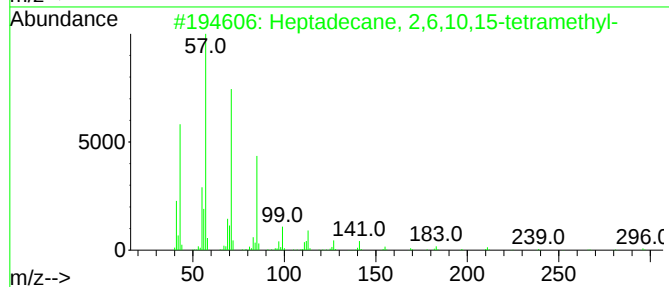
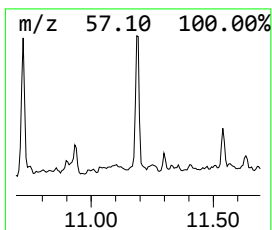
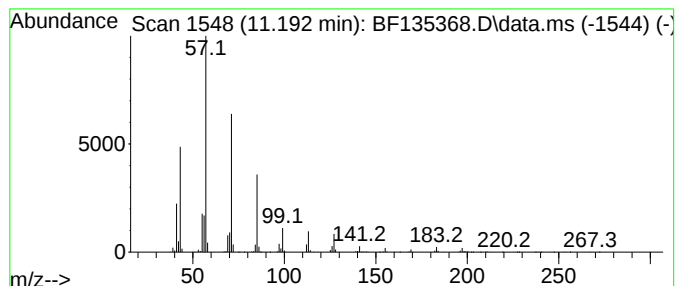
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.192	27.74 ng	1383480	Phenanthrene-d10	11.292	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	87
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86



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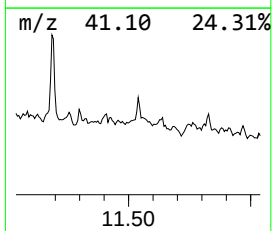
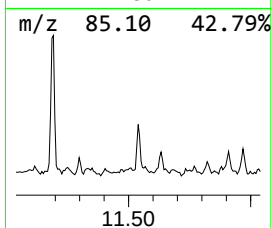
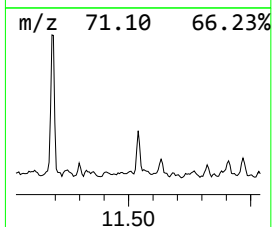
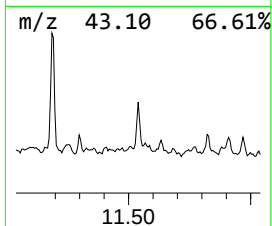
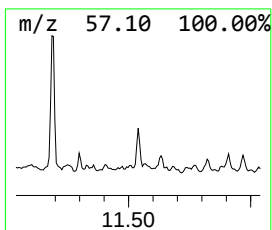
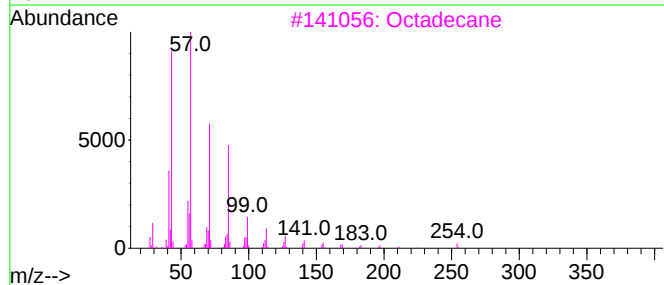
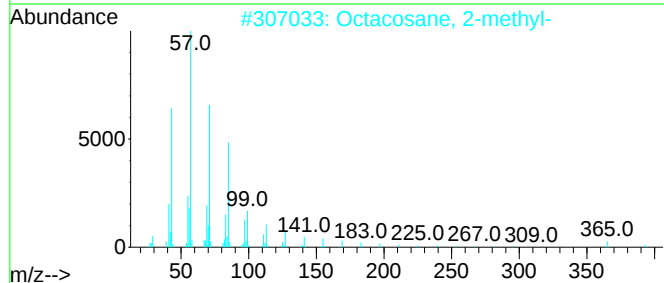
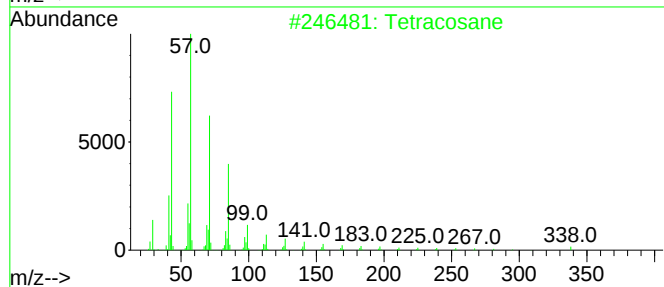
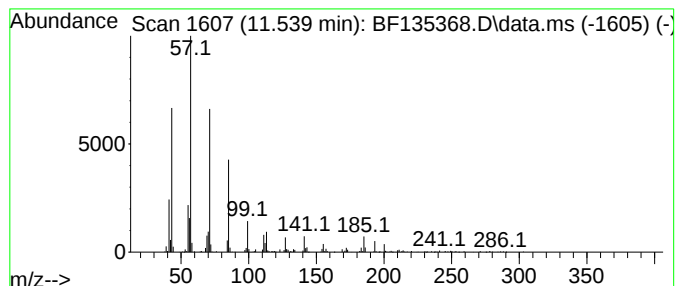
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.539	6.88 ng	342923	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	80
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	80
3			Octadecane	254	C18H38	000593-45-3	80
4			Heptacosane	380	C27H56	000593-49-7	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135368.D
Acq On : 20 Sep 2023 20:50
Operator : CG\JU
Sample : 04304-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

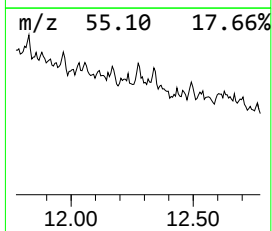
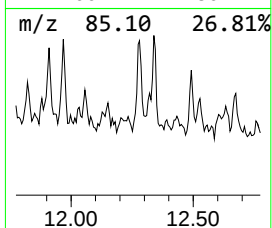
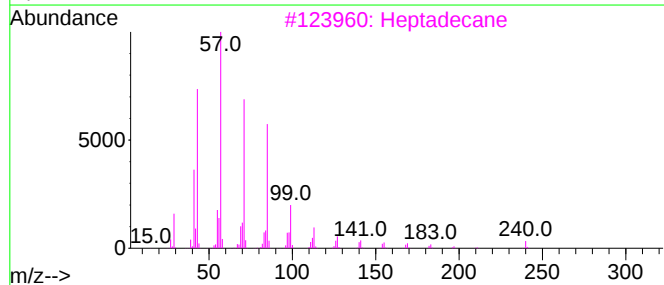
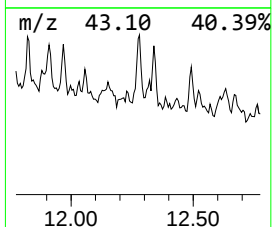
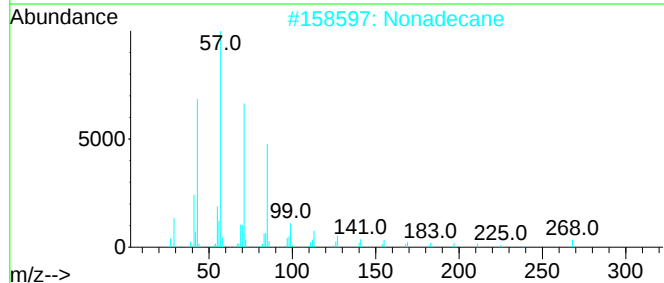
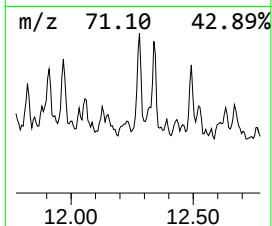
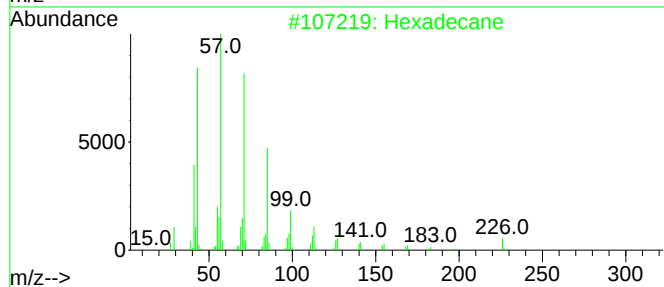
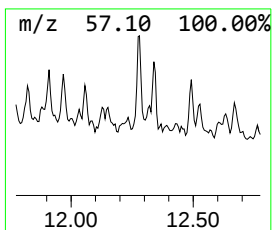
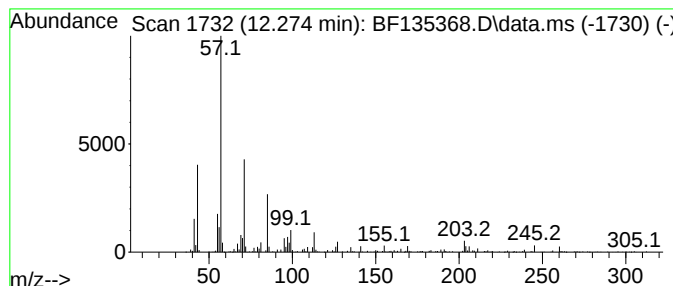
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.274	5.89 ng	293750	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	72
2			Nonadecane	268	C19H40	000629-92-5	72
3			Heptadecane	240	C17H36	000629-78-7	72
4			Docosane	310	C22H46	000629-97-0	72
5			Heneicosane	296	C21H44	000629-94-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135368.D
Acq On : 20 Sep 2023 20:50
Operator : CG\JU
Sample : 04304-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

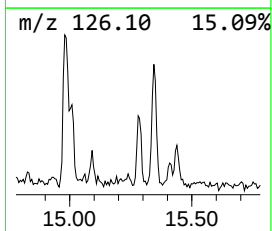
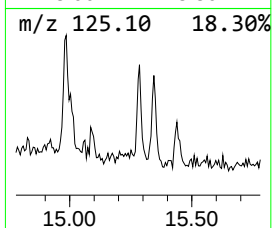
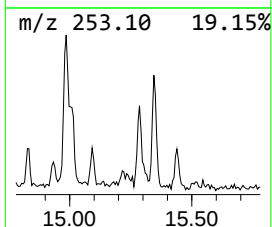
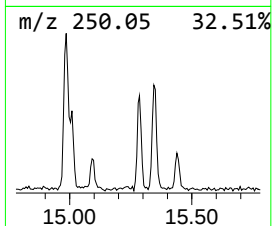
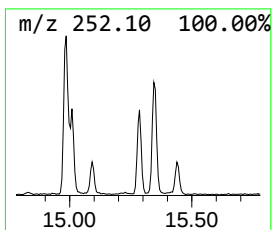
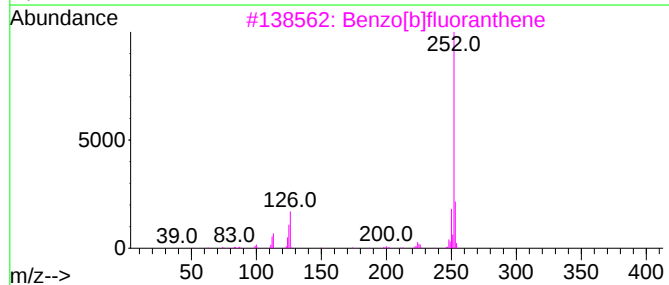
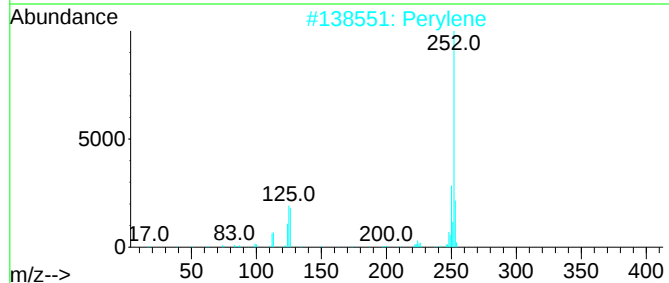
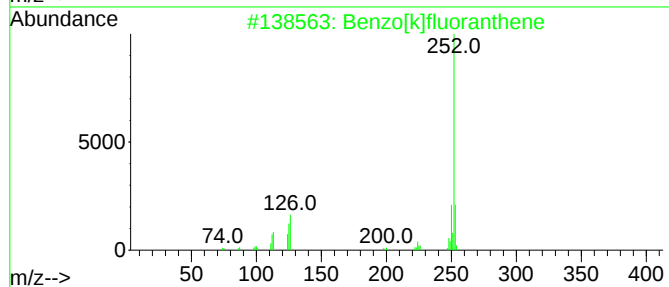
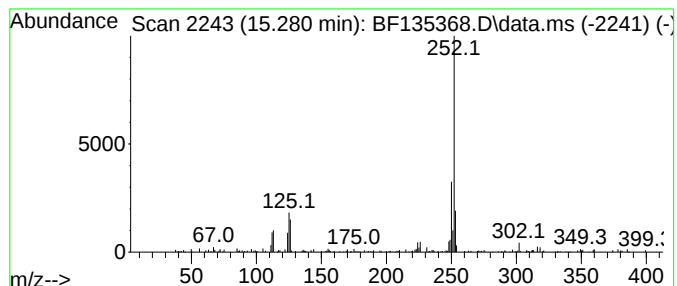
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Perylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	3.40 ng	97441	Perylene-d12	15.409

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2		Perylene	252	C20H12	000198-55-0	93
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4		Benzo[e]pyrene	252	C20H12	000192-97-2	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092023\
Data File : BF135368.D
Acq On : 20 Sep 2023 20:50
Operator : CG\JU
Sample : 04304-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	2.8	ng	102334	1	6.757	739459	20.0
Undecane, 3-cyc...	9.198	2.4	ng	103966	3	9.792	860070	20.0
unknown9.422	9.422	3.3	ng	139969	3	9.792	860070	20.0
Tetradecane, 1-...	9.516	4.5	ng	195766	3	9.792	860070	20.0
unknown9.657	9.657	5.9	ng	254429	3	9.792	860070	20.0
unknown9.698	9.698	4.6	ng	198878	3	9.792	860070	20.0
Tetradecane	10.051	4.9	ng	209550	3	9.792	860070	20.0
2,4,6-Trimethyl...	10.198	4.2	ng	181492	3	9.792	860070	20.0
Tetratetracontane	10.451	15.2	ng	652186	3	9.792	860070	20.0
Tridecane, 5-pr...	10.722	24.6	ng	1227720	4	11.292	997315	20.0
Heptadecane, 2,...	11.192	27.7	ng	1383480	4	11.292	997315	20.0
Tetracosane	11.539	6.9	ng	342923	4	11.292	997315	20.0
Hexadecane	12.274	5.9	ng	293750	4	11.292	997315	20.0
Perylene	15.280	3.4	ng	97441	6	15.409	573773	20.0