

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
 Data File : BF125824.D
 Acq On : 13 Oct 2021 13:43
 Operator : JU/CG
 Sample : M4127-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-27080

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	494	505	512	rBV	50519	66962	1.73%	0.226%
2	5.457	568	573	577	rBV	3339310	3414313	88.44%	11.513%
3	6.469	740	745	748	rBV	3571812	3382480	87.61%	11.406%
4	6.845	805	809	812	rBV	1176219	1024890	26.55%	3.456%
5	6.904	816	819	828	rBV	65958	58708	1.52%	0.198%
6	7.404	899	904	907	rBV	2294165	2219469	57.49%	7.484%
7	8.022	1006	1009	1022	rBV	661696	630281	16.33%	2.125%
8	8.122	1022	1026	1030	rBV	1725221	1362630	35.29%	4.595%
9	9.151	1198	1201	1205	rBV4	51887	68627	1.78%	0.231%
10	9.198	1205	1209	1212	rBV	4897369	3860787	100.00%	13.019%
11	9.316	1226	1229	1231	rBV4	47193	61377	1.59%	0.207%
12	9.398	1241	1243	1246	rBV3	51140	58307	1.51%	0.197%
13	9.475	1254	1256	1258	rBV	67487	52723	1.37%	0.178%
14	9.516	1261	1263	1265	rBV2	105274	83780	2.17%	0.283%
15	9.563	1268	1271	1273	rBV4	60281	65962	1.71%	0.222%
16	9.586	1273	1275	1277	rBV2	146330	163215	4.23%	0.550%
17	9.792	1308	1310	1312	rBV2	157469	112919	2.92%	0.381%
18	9.875	1321	1324	1328	rVB	1622645	1394769	36.13%	4.703%
19	10.139	1367	1369	1371	rBV3	276937	246903	6.40%	0.833%
20	10.192	1376	1378	1382	rBV3	297986	437717	11.34%	1.476%
21	10.292	1392	1395	1399	rBV5	390723	573925	14.87%	1.935%
22	10.663	1455	1458	1461	rBV2	1707646	1588576	41.15%	5.357%
23	10.869	1490	1493	1495	rBV2	598781	602937	15.62%	2.033%
24	11.269	1558	1561	1565	rVB2	1024329	1177926	30.51%	3.972%
25	11.363	1575	1577	1580	rBV	1005373	911077	23.60%	3.072%
26	12.951	1844	1847	1850	rBV	2523571	2110165	54.66%	7.116%
27	13.998	2021	2025	2028	rVB	1276625	1161915	30.10%	3.918%
28	14.492	2106	2109	2121	rVB	414034	564806	14.63%	1.905%
29	14.845	2167	2169	2177	rVB3	67861	85119	2.20%	0.287%
30	15.021	2196	2199	2203	rBV	176561	274133	7.10%	0.924%
31	15.110	2211	2214	2216	rBV	79413	76827	1.99%	0.259%
32	15.327	2247	2251	2257	rVB	112736	149858	3.88%	0.505%
33	15.386	2257	2261	2266	rBV	141383	163736	4.24%	0.552%
34	15.451	2267	2272	2276	rBV	997333	1195613	30.97%	4.032%
35	15.921	2349	2352	2357	rVB2	37829	50677	1.31%	0.171%
36	16.886	2512	2516	2523	rVB3	64686	123476	3.20%	0.416%

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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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.321	2588	2590	2600	rVB	39708	77442	2.01%	0.261%
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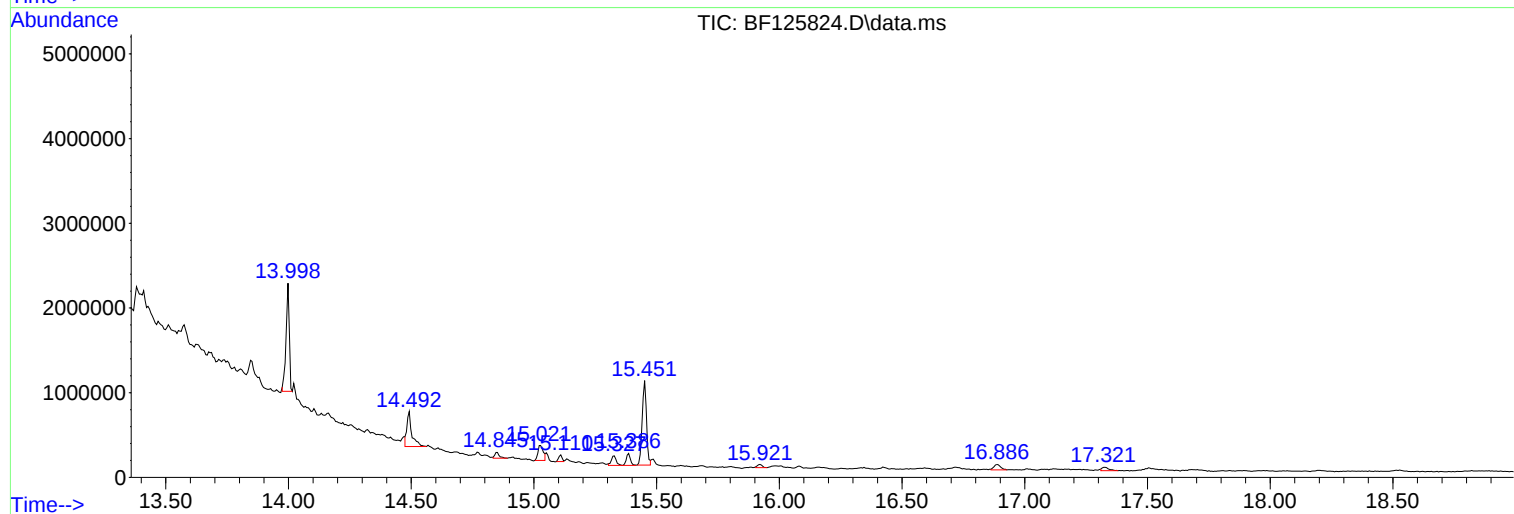
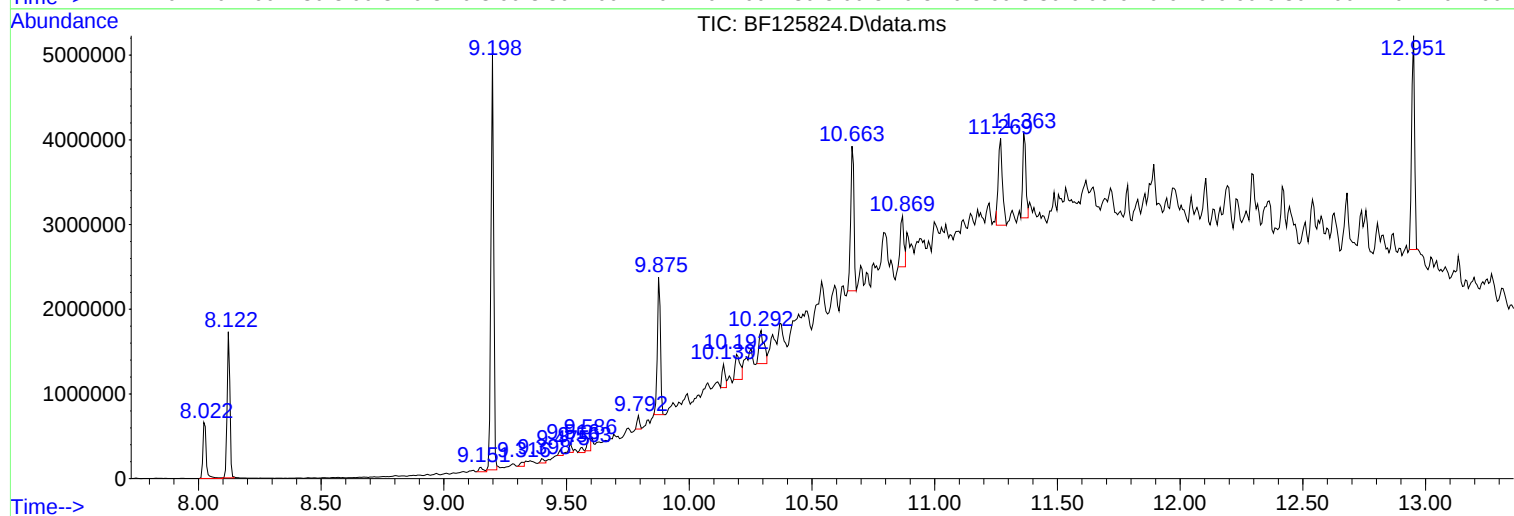
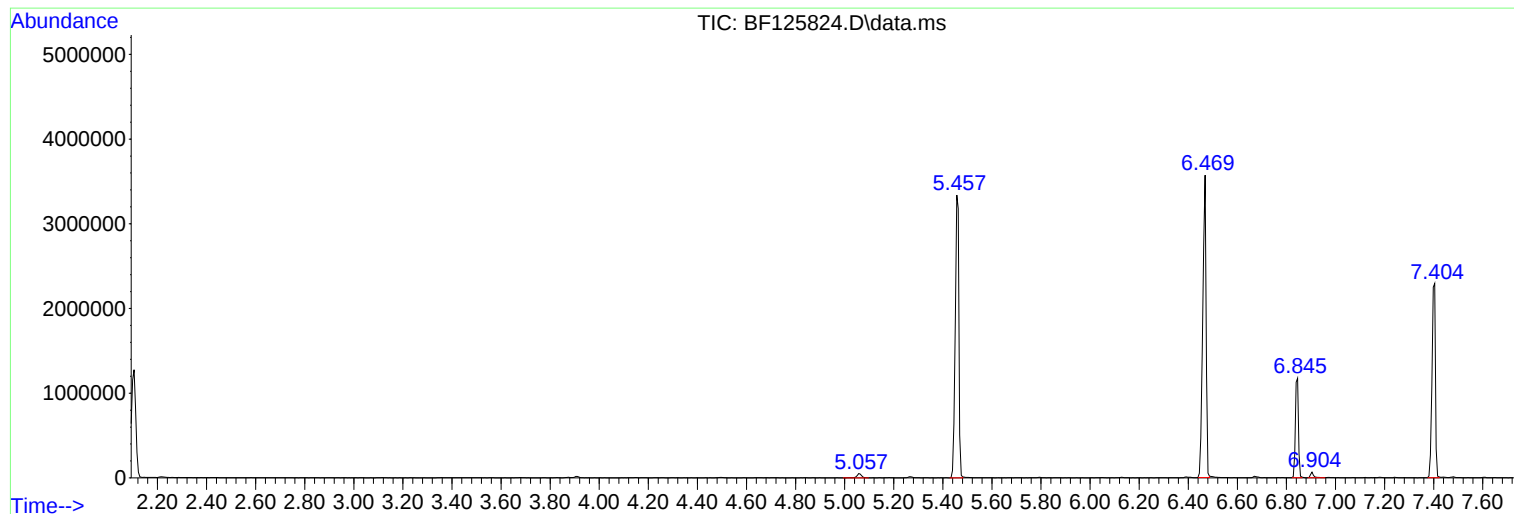
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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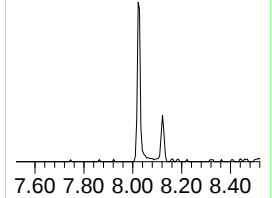
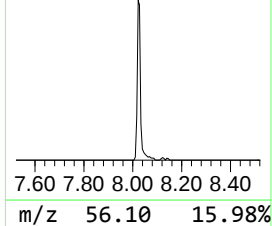
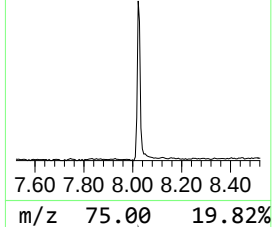
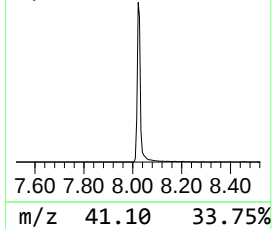
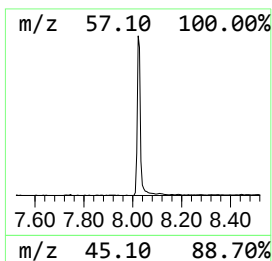
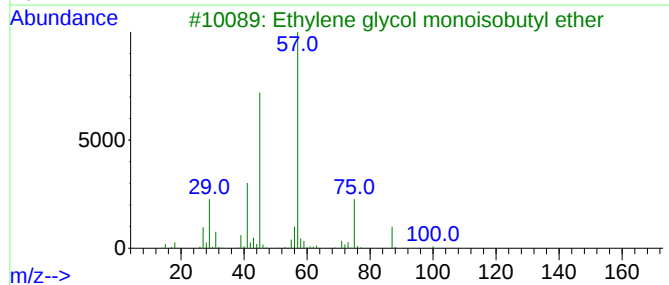
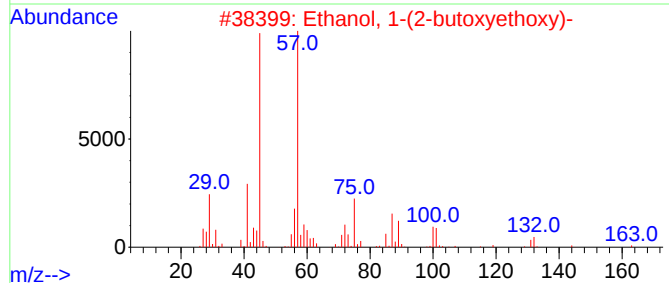
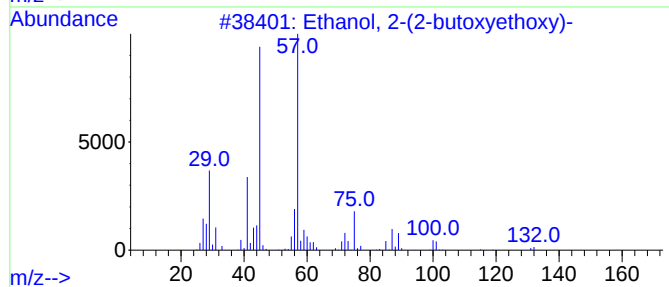
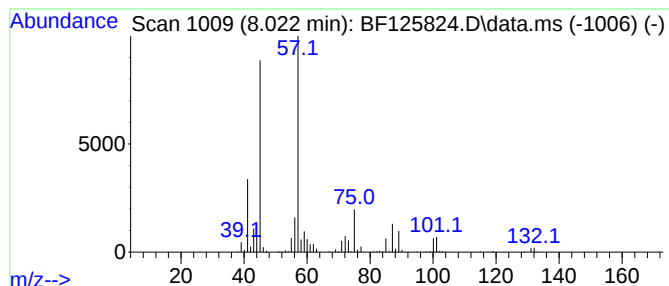
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	9.25 ng	630281	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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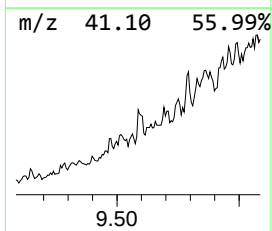
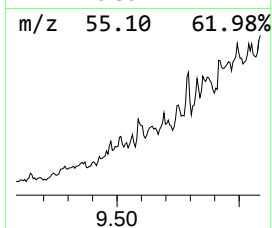
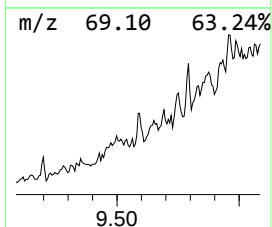
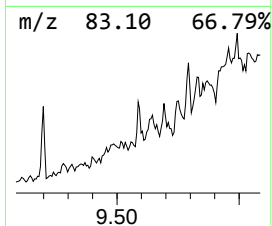
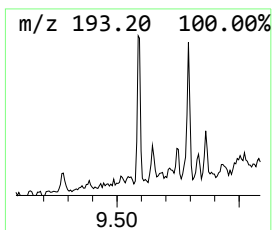
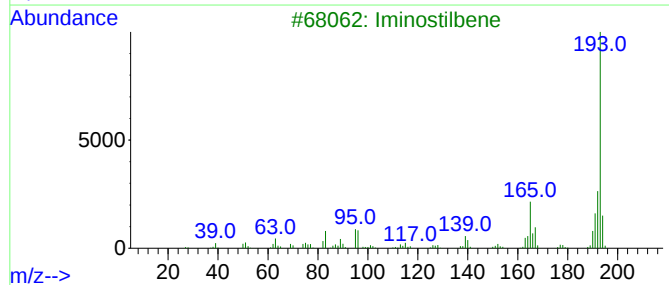
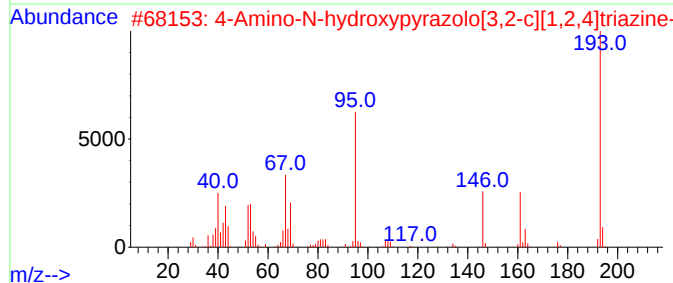
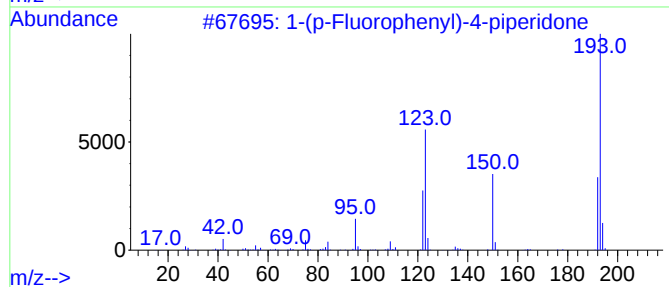
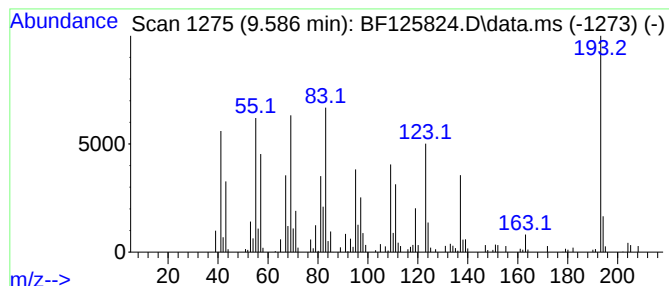
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.586 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	2.34 ng	163215	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
2	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	30		
3	Iminostilbene	193	C14H11N	000256-96-2	27		
4	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	18		
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	18		



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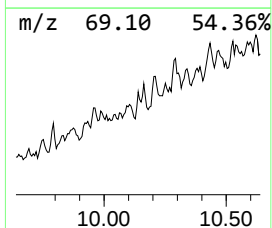
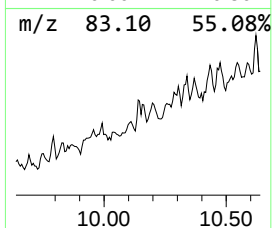
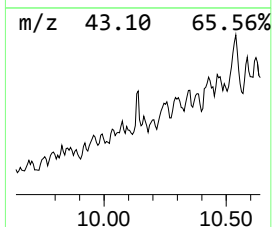
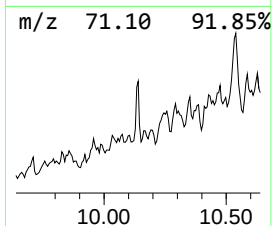
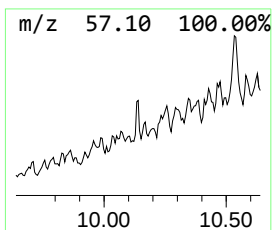
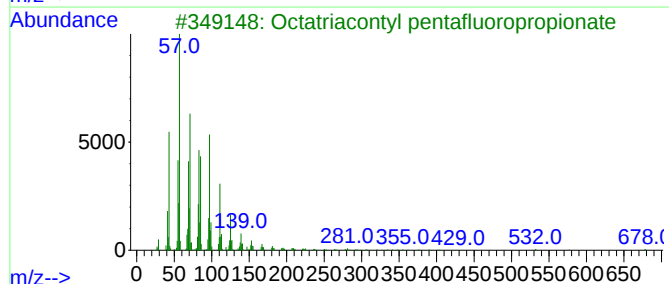
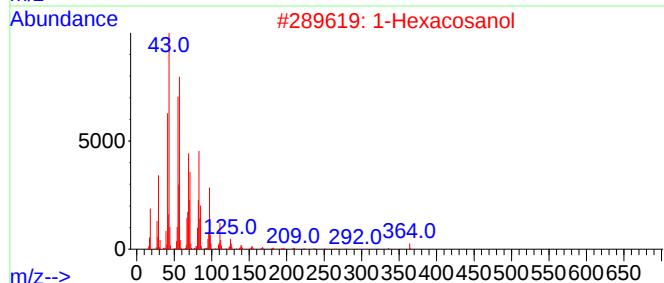
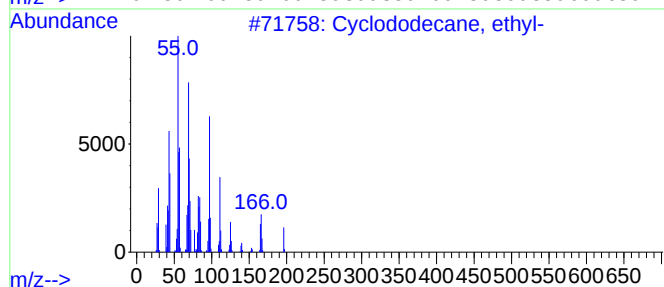
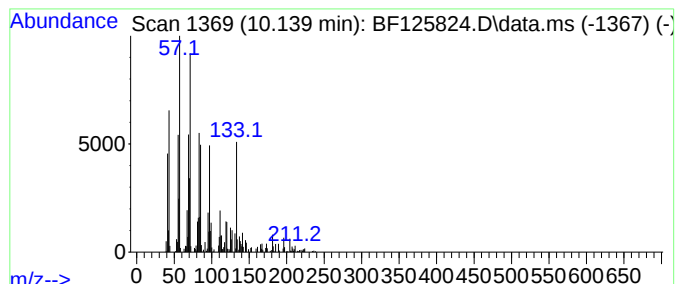
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclododecane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.139	3.54 ng	246903	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane, ethyl-	196	C14H28	028981-49-9	62
2			1-Hexacosanol	382	C26H54O	000506-52-5	49
3			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	46
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	41
5			1-Hexacosene	364	C26H52	018835-33-1	41



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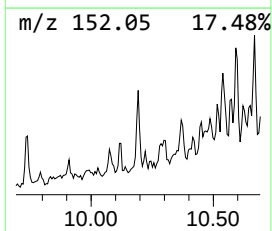
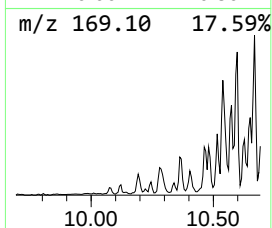
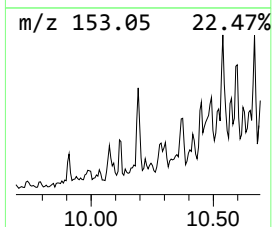
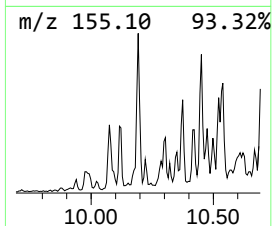
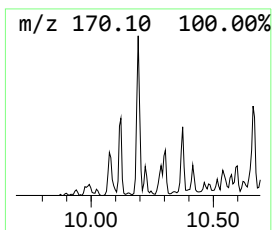
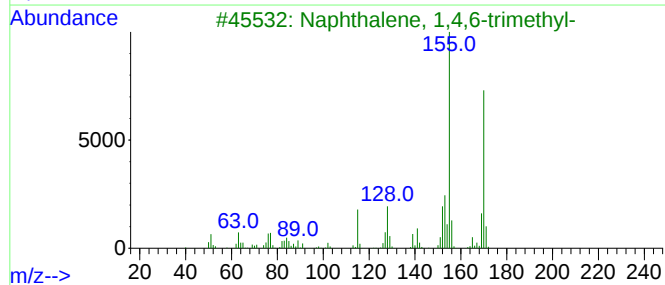
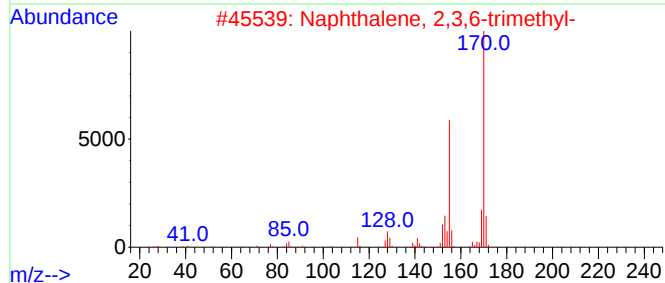
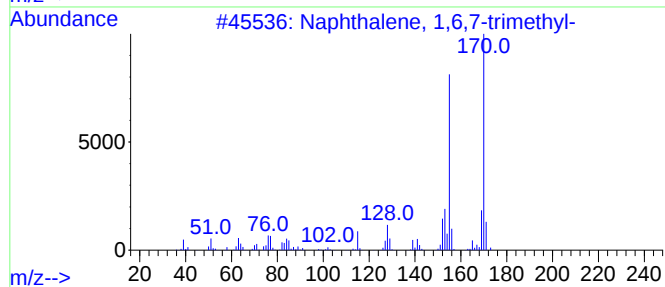
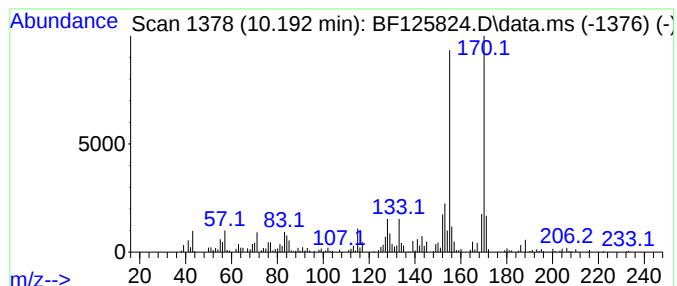
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,6,7-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.192	6.28 ng	437717	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	98
2			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	95
3			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	93
4			Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	93
5			1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	87



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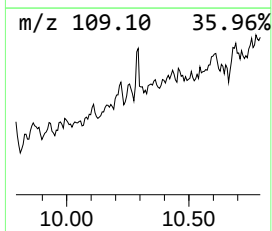
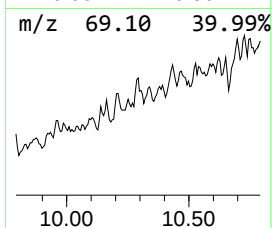
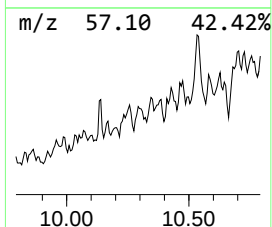
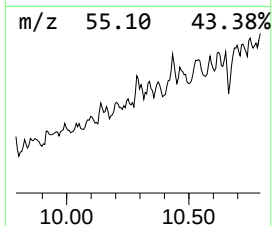
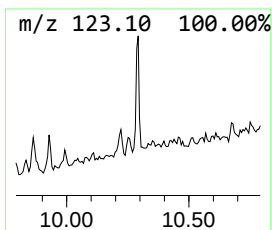
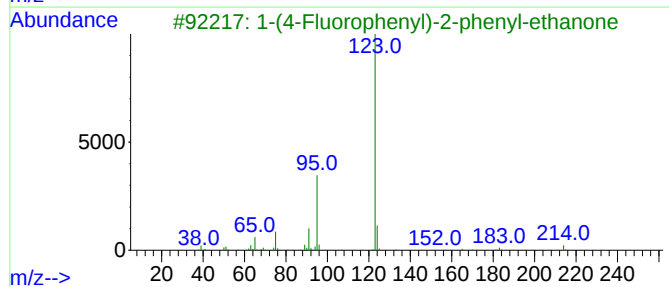
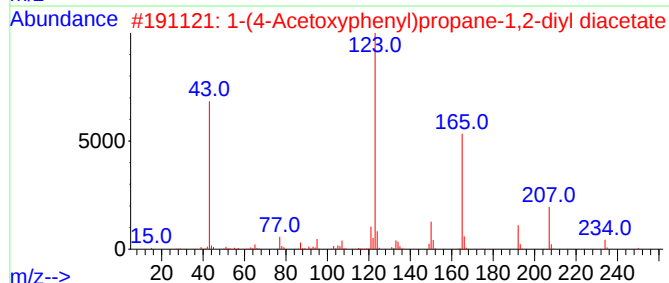
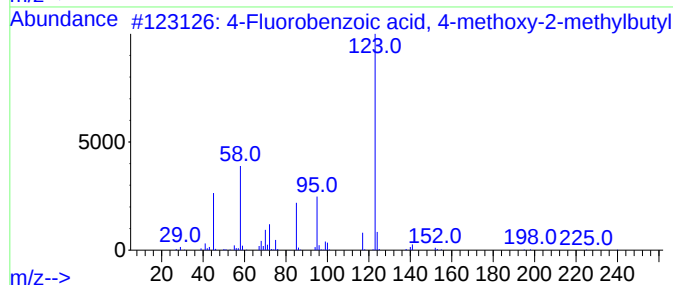
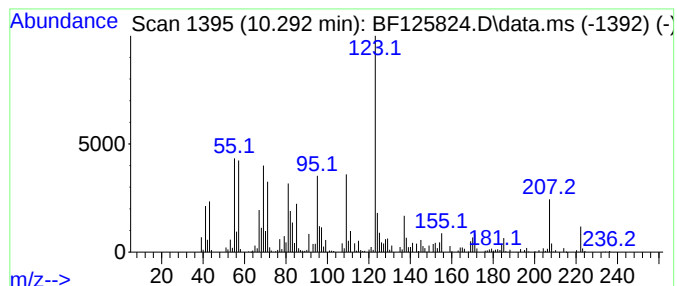
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown10.292 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.292	8.23 ng	573925	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Fluorobenzoic acid, 4-methoxy-...	240	C13H17F03	1000355-67-7	47
2			1-(4-Acetoxyphenyl)propane-1,2-d...	294	C15H18O6	1000495-87-2	43
3			1-(4-Fluorophenyl)-2-phenyl-etha...	214	C14H11FO	000347-84-2	43
4			Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	43
5			4-Fluorobenzoic acid, 2,2-dimeth...	210	C12H15FO2	069912-03-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
Acq On : 13 Oct 2021 13:43
Operator : JU/CG
Sample : M4127-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

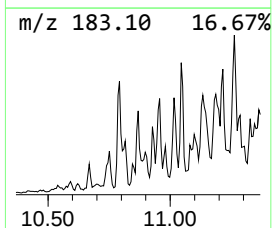
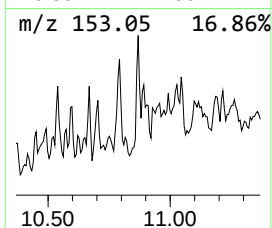
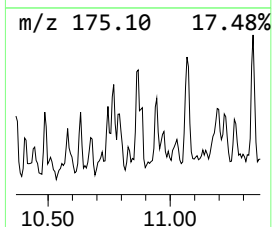
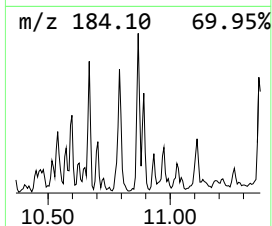
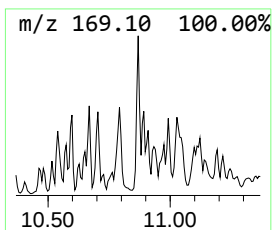
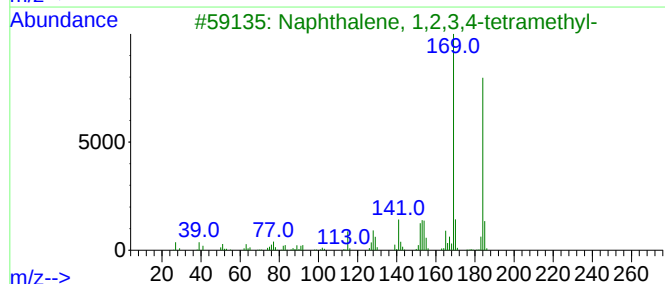
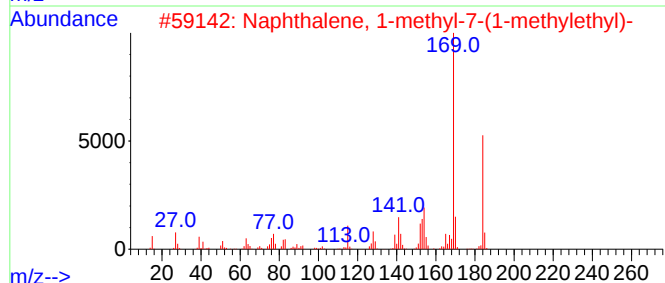
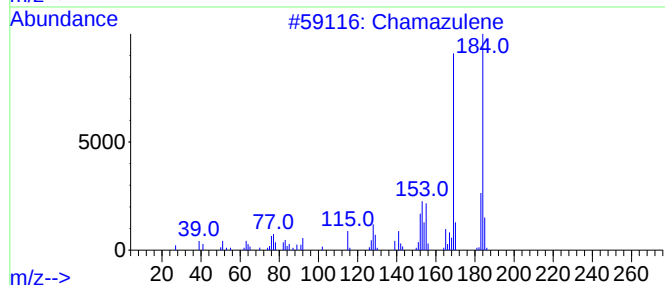
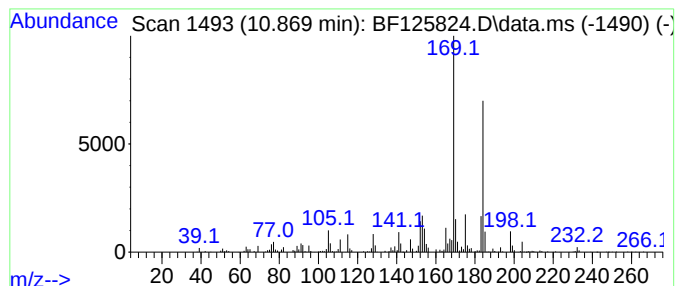
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Chamazulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.869	13.24 ng	602937	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chamazulene	184	C14H16	000529-05-5	93
2	Naphthalene, 1-methyl-7-(1-methy...	184	C14H16	000490-65-3	90
3	Naphthalene, 1,2,3,4-tetramethyl-	184	C14H16	003031-15-0	83
4	1,4,5,8-Tetramethylnaphthalene	184	C14H16	002717-39-7	83
5	Cyclopentene, 1,2-dimethyl-4-met...	184	C14H16	1000152-22-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
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Sample : M4127-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
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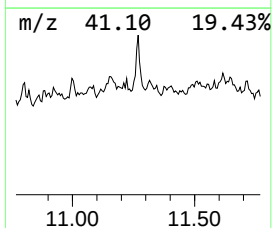
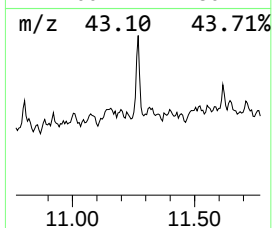
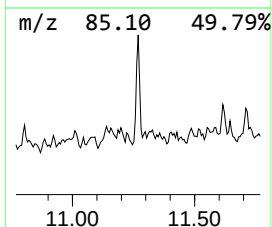
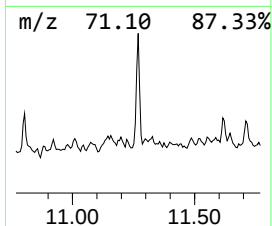
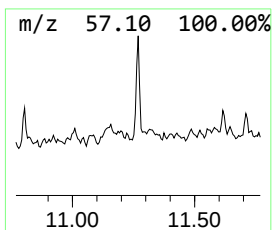
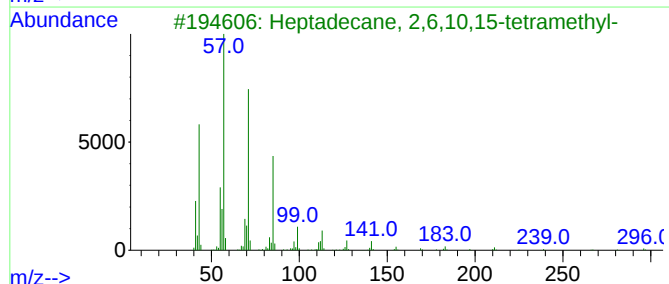
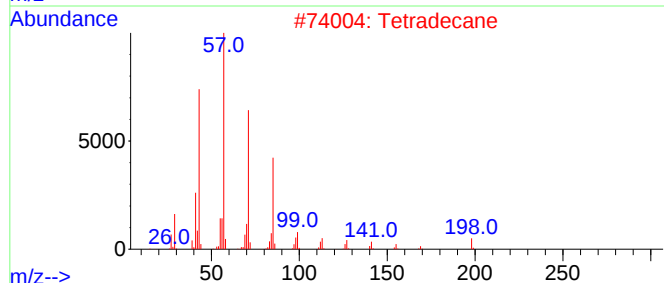
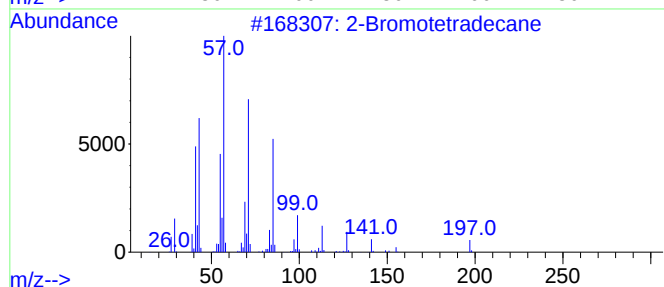
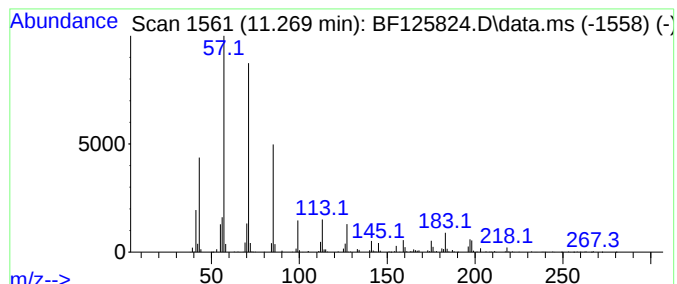
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromotetradecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	25.86 ng	1177930	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Bromotetradecane	276	C14H29Br	074036-95-6	91
2		Tetradecane	198	C14H30	000629-59-4	90
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4		Pentacosane	352	C25H52	000629-99-2	86
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
Acq On : 13 Oct 2021 13:43
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Sample : M4127-01
Misc :
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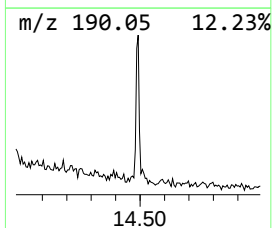
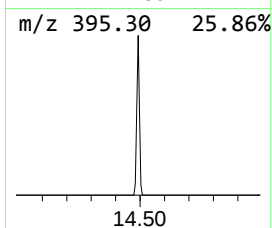
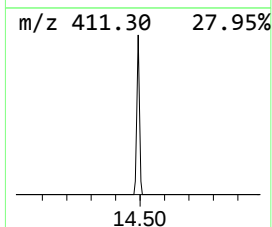
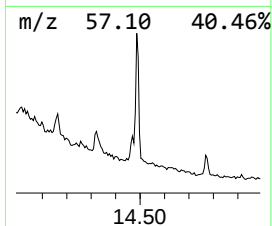
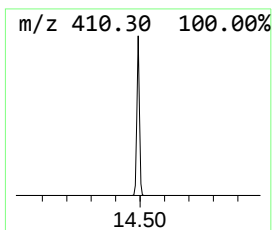
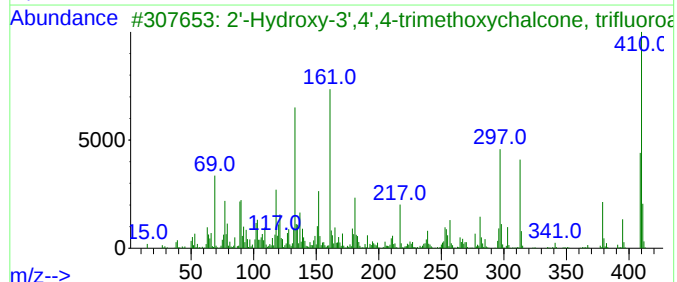
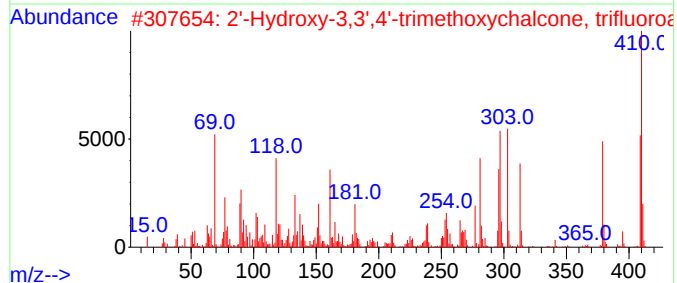
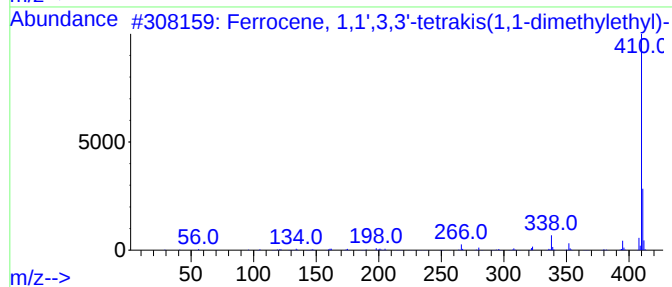
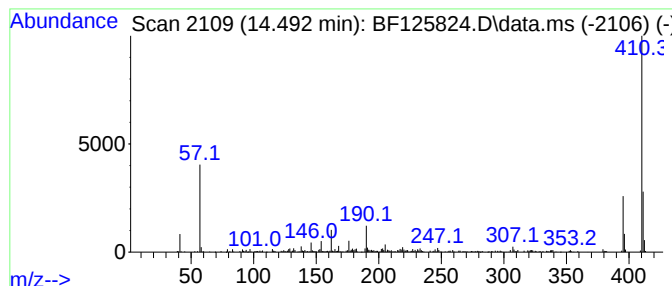
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ferrocene, 1,1',3,3'-tetrak... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	9.72 ng	564806	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	58
2			2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	50
3			2'-Hydroxy-3',4',4'-trimethoxycha...	410	C20H17F3O6	1000449-45-6	42
4			Stigmasta-4,6,22-trien-3.alpha.-ol	410	C29H46O	1000103-93-1	40
5			6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
Acq On : 13 Oct 2021 13:43
Operator : JU/CG
Sample : M4127-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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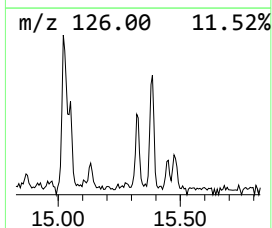
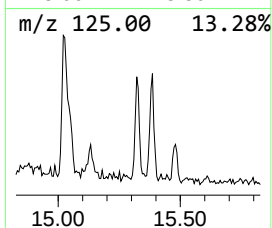
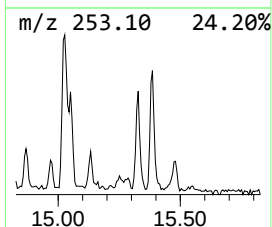
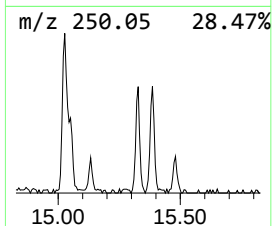
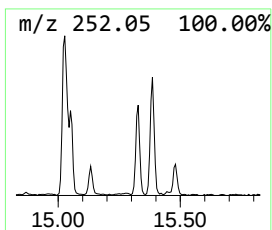
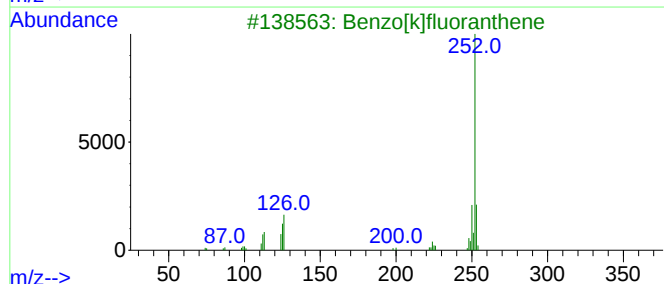
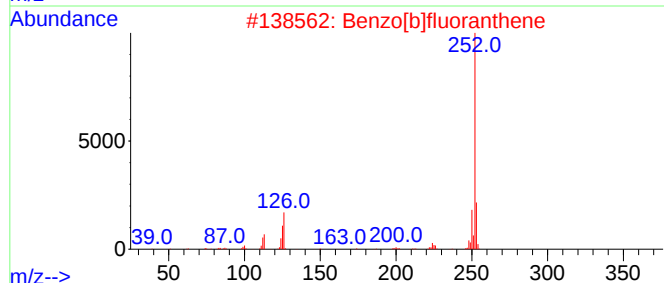
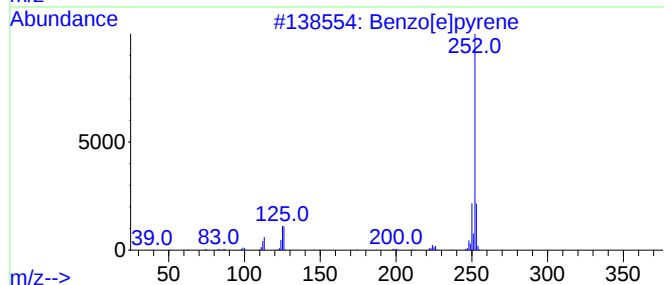
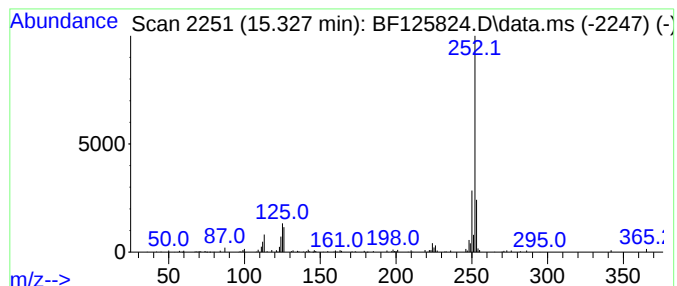
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	2.51 ng	149858	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
Acq On : 13 Oct 2021 13:43
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Sample : M4127-01
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ClientSampleId :
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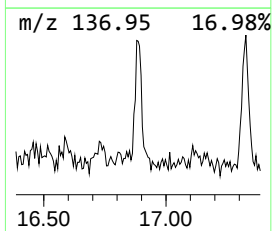
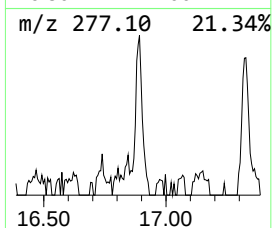
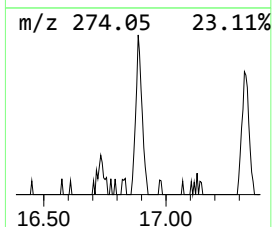
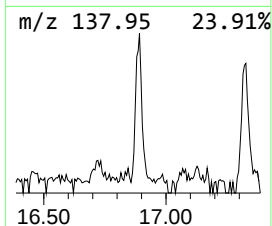
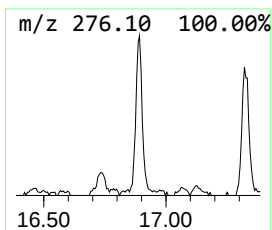
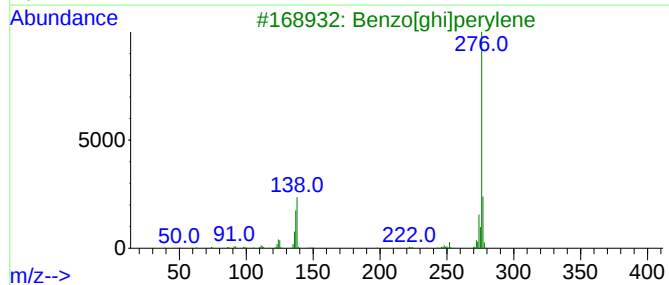
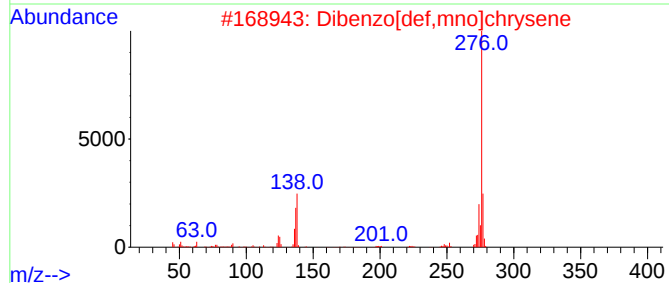
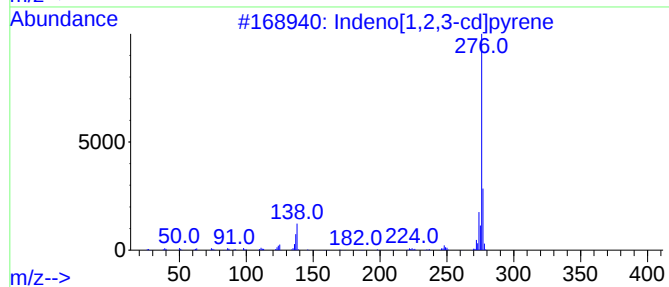
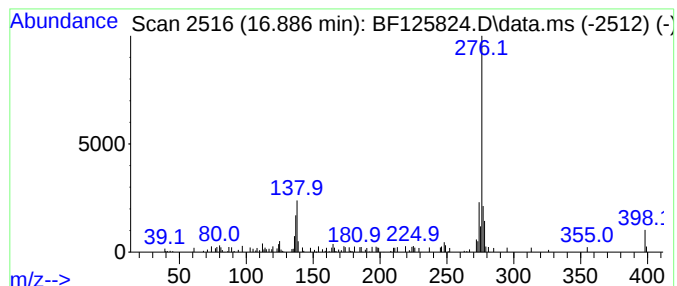
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dibenzo[def,mno]chrysene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.886	2.07 ng	123476	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	96
2			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	95
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	95
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	89
5			2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125824.D
Acq On : 13 Oct 2021 13:43
Operator : JU/CG
Sample : M4127-01
Misc :
ALS Vial : 9 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown9.586	9.586	2.3	ng	163215	3	9.875	1394770	20.0
Cyclododecane, ...	10.139	3.5	ng	246903	3	9.875	1394770	20.0
Naphthalene, 1,...	10.192	6.3	ng	437717	3	9.875	1394770	20.0
unknown10.292	10.292	8.2	ng	573925	3	9.875	1394770	20.0
Chamazulene	10.869	13.2	ng	602937	4	11.363	911077	20.0
2-Bromotetradecane	11.269	25.9	ng	1177930	4	11.363	911077	20.0
Ferrocene, 1,1'...	14.492	9.7	ng	564806	5	13.998	1161920	20.0
Benzo[e]pyrene	15.327	2.5	ng	149858	6	15.451	1195610	20.0
Dibenzo[def,mno...	16.886	2.1	ng	123476	6	15.451	1195610	20.0