

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
 Data File : BF128240.D
 Acq On : 13 May 2022 15:44
 Operator : CG\JU
 Sample : N2823-12
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SC-12

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-BF050922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.504	543	547	561	rVB	1158810	1296992	20.88%	5.660%
2	5.851	599	606	609	rBV	1439431	2082678	33.52%	9.089%
3	6.516	715	719	730	rBV	1086105	1363633	21.95%	5.951%
4	6.887	778	782	785	rBV	372218	331227	5.33%	1.445%
5	6.963	787	795	798	rBV	4354193	6213002	100.00%	27.113%
6	7.292	846	851	854	rBV	309125	236065	3.80%	1.030%
7	7.422	870	873	875	rBV	263085	227108	3.66%	0.991%
8	7.451	875	878	881	rVB	1051127	879064	14.15%	3.836%
9	8.169	996	1000	1003	rBV	506884	429266	6.91%	1.873%
10	9.245	1178	1183	1186	rBV	1715822	1605723	25.84%	7.007%
11	9.922	1295	1298	1302	rVB	545320	482259	7.76%	2.105%
12	10.716	1429	1433	1442	rBV	1199199	1029417	16.57%	4.492%
13	10.828	1447	1452	1454	rBV	148215	163992	2.64%	0.716%
14	11.263	1523	1526	1529	rBV	273609	215416	3.47%	0.940%
15	11.292	1529	1531	1537	rVB	98758	98804	1.59%	0.431%
16	11.416	1548	1552	1555	rBV	660805	546028	8.79%	2.383%
17	13.004	1818	1822	1825	rVB	1657399	1387875	22.34%	6.057%
18	13.857	1965	1967	1971	rBV	75087	88104	1.42%	0.384%
19	14.033	1992	1997	1999	rBV	2703359	2543241	40.93%	11.098%
20	14.063	1999	2002	2006	rVB	389866	326457	5.25%	1.425%
21	15.551	2251	2255	2262	rVB	284143	371287	5.98%	1.620%
22	16.180	2358	2362	2367	rVB	68628	97237	1.57%	0.424%
23	16.562	2421	2427	2433	rVB	339669	573388	9.23%	2.502%
24	16.704	2447	2451	2458	rVB3	52693	96643	1.56%	0.422%
25	17.104	2513	2519	2527	rVB2	113939	230518	3.71%	1.006%

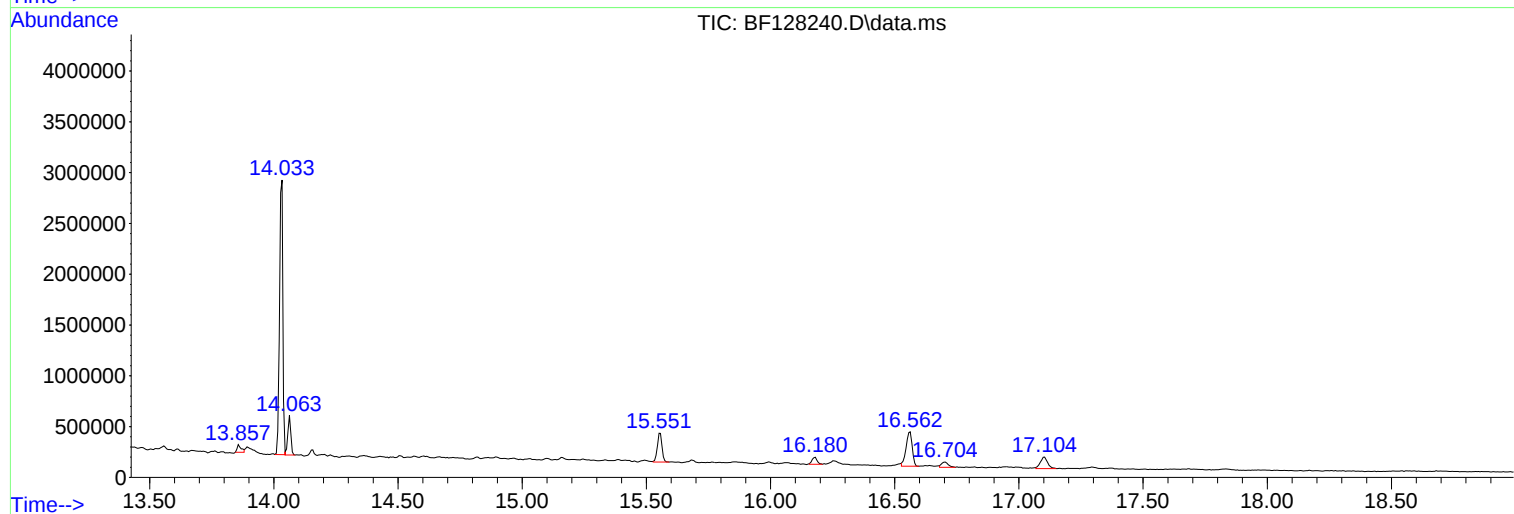
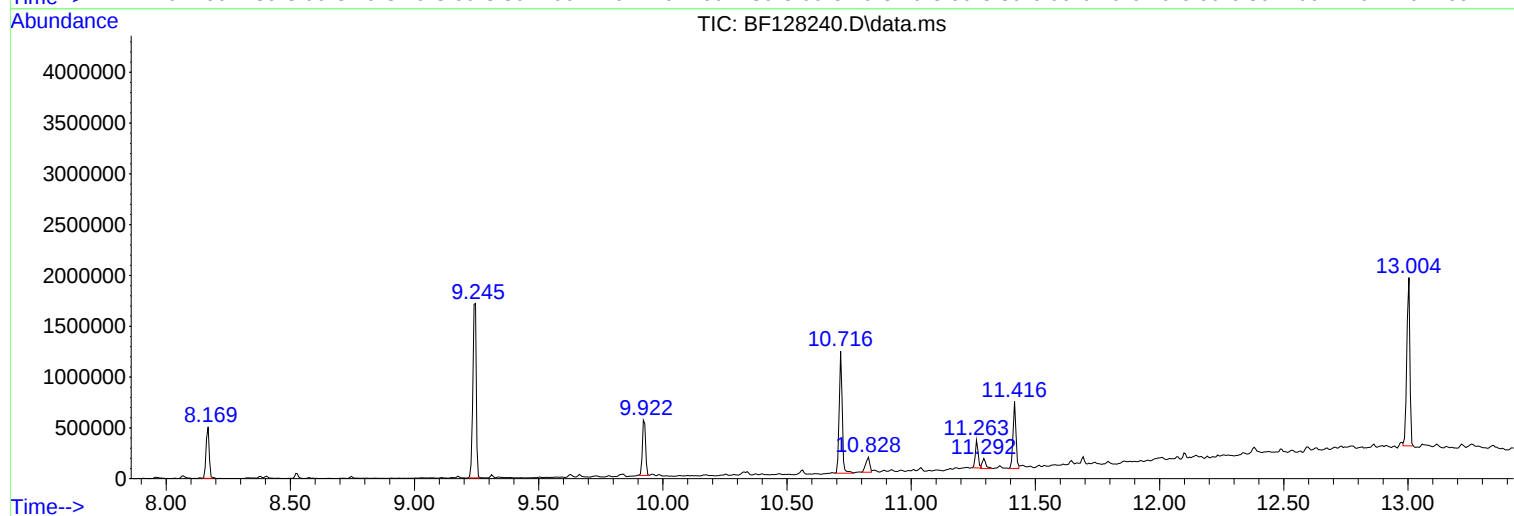
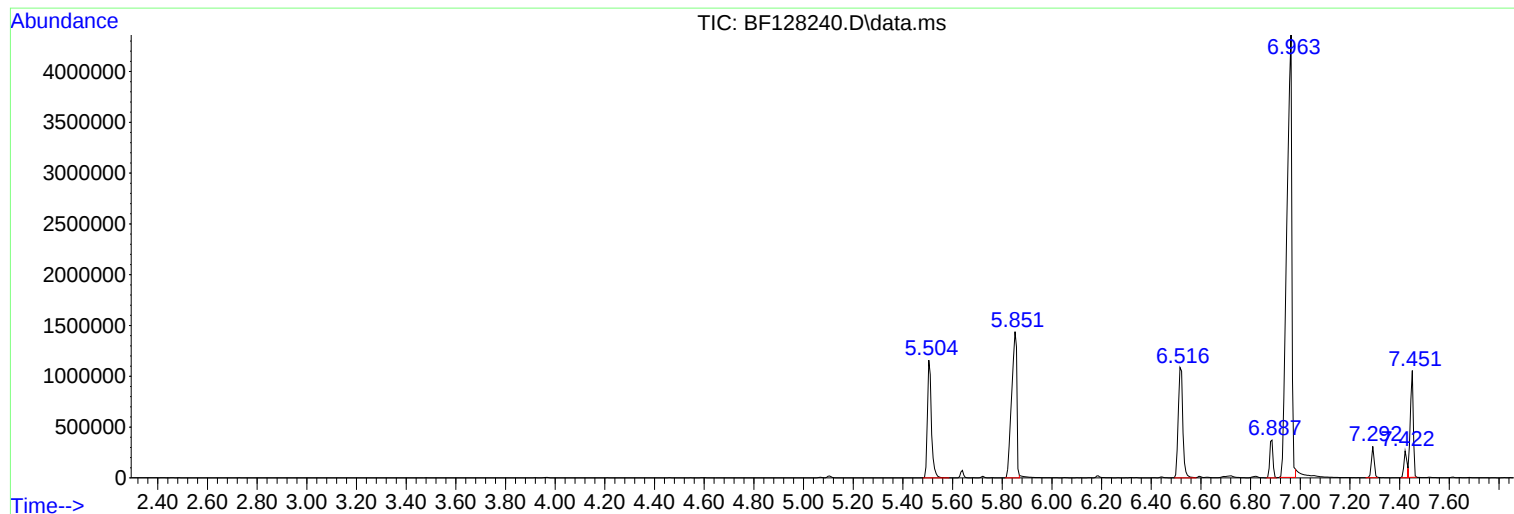
Sum of corrected areas: 22915424

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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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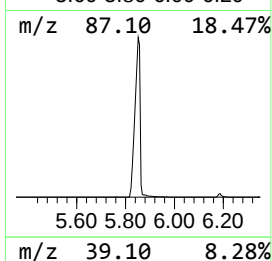
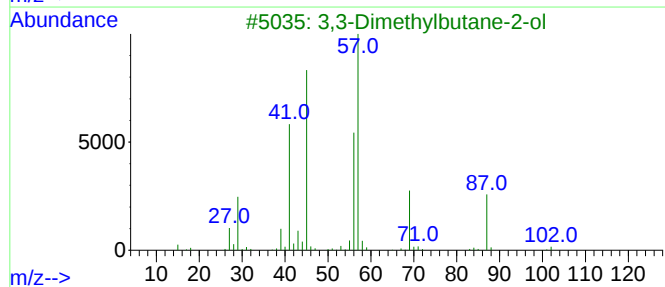
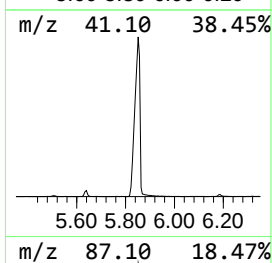
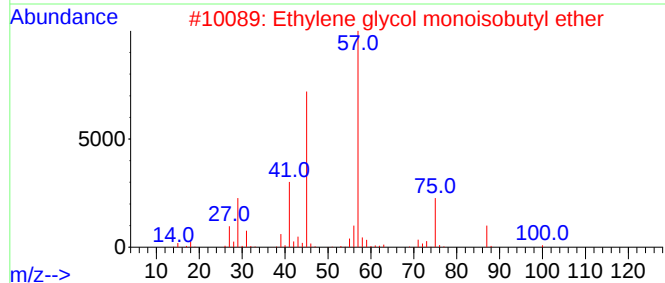
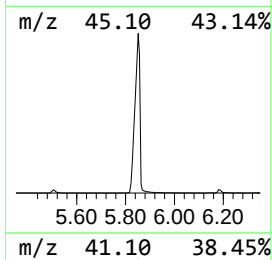
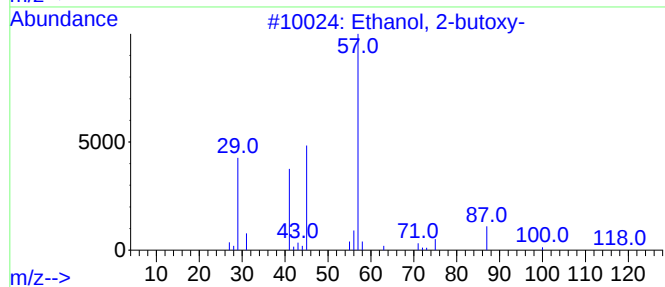
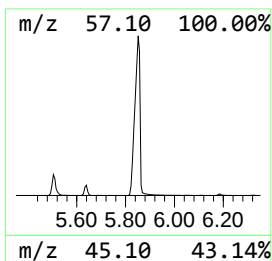
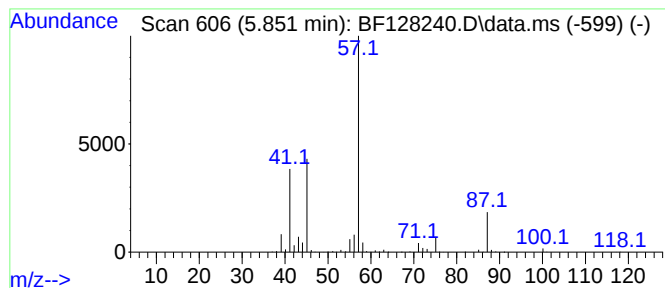
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	125.76 ng	2082680	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	25
5			n-Butyl ether	130	C8H18O	000142-96-1	16



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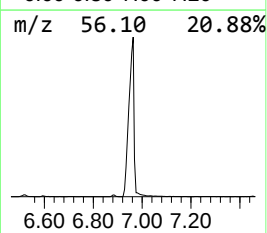
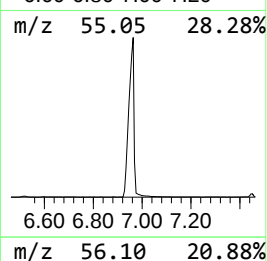
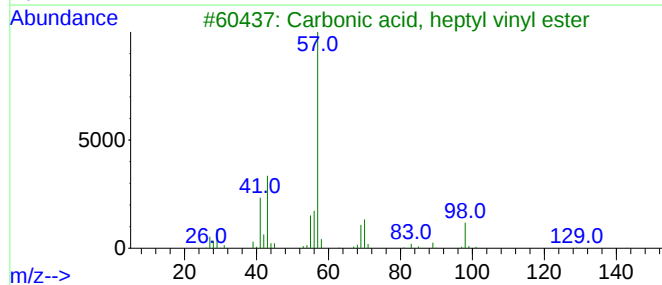
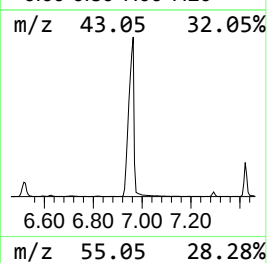
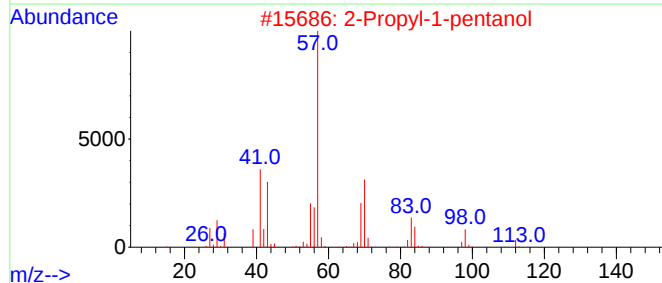
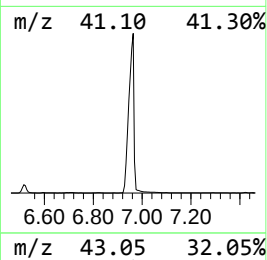
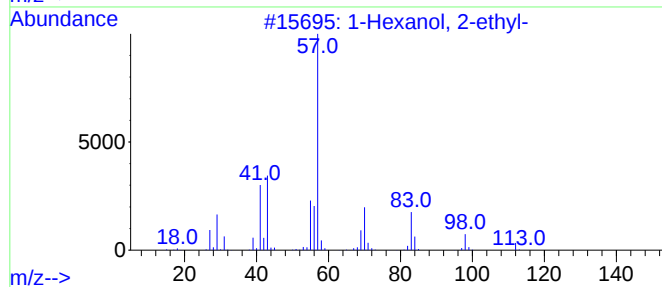
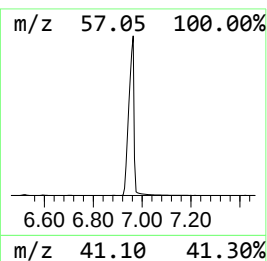
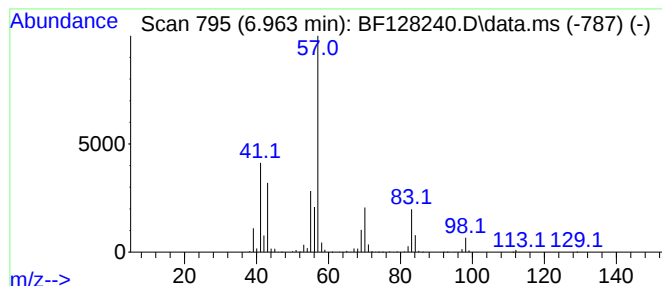
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	375.15 ng	6213000	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50
3	Carbonic acid, heptyl vinyl ester			186	C10H18O3	1010383-25-4	47
4	Oxalic acid, isobutyl octyl ester			258	C14H26O4	1000309-37-3	47
5	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	45



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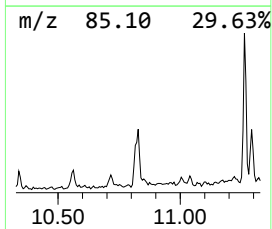
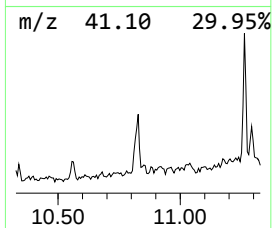
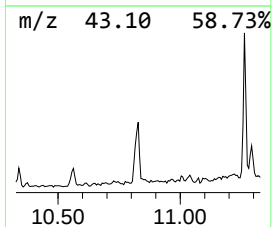
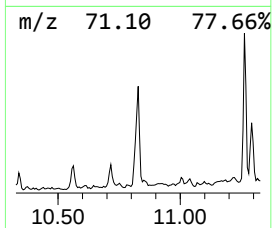
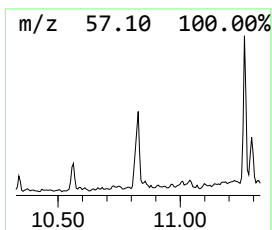
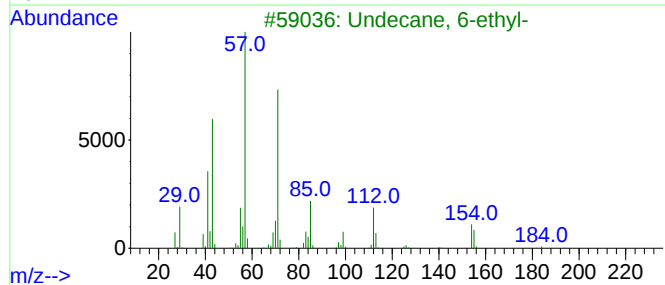
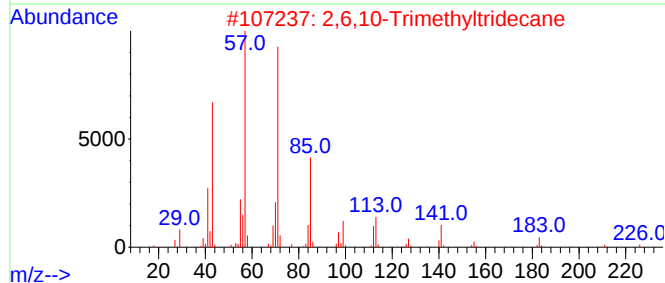
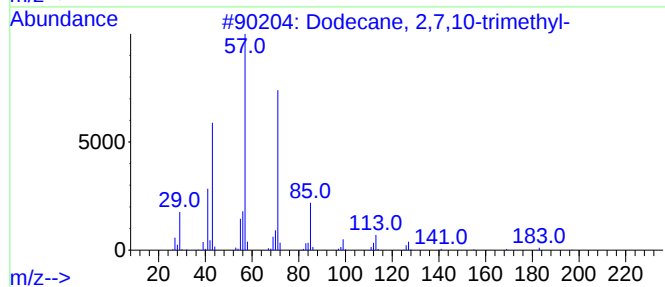
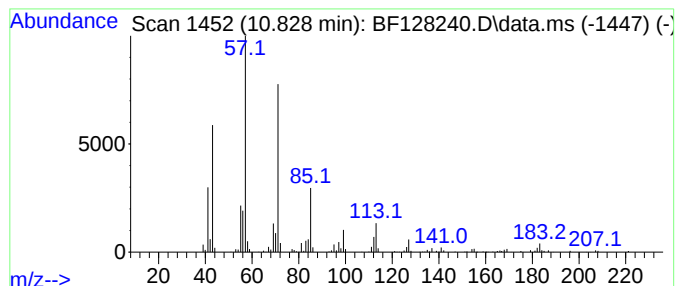
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Peak Number 3 Dodecane, 2,7,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	6.01 ng	163992	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	91
2			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	90
3			Undecane, 6-ethyl-	184	C13H28	017312-60-6	87
4			Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	80
5			Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	72



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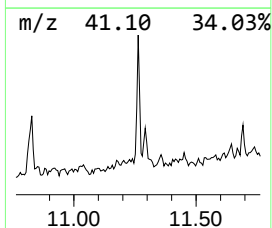
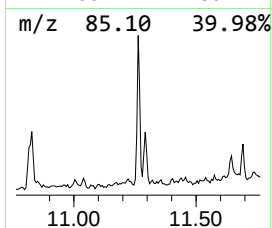
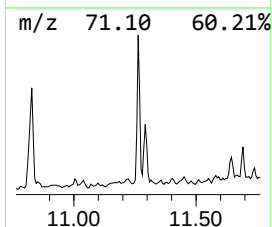
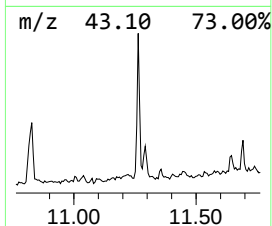
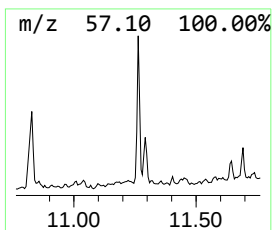
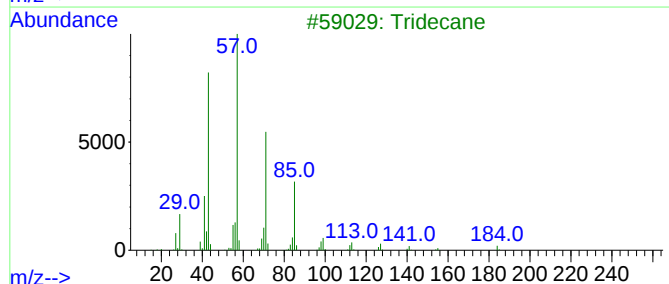
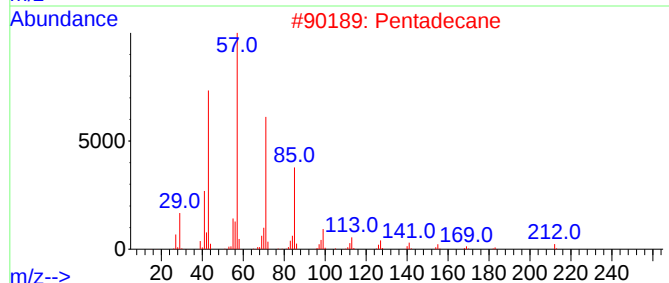
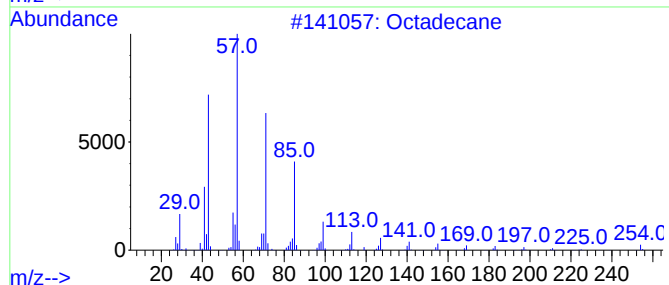
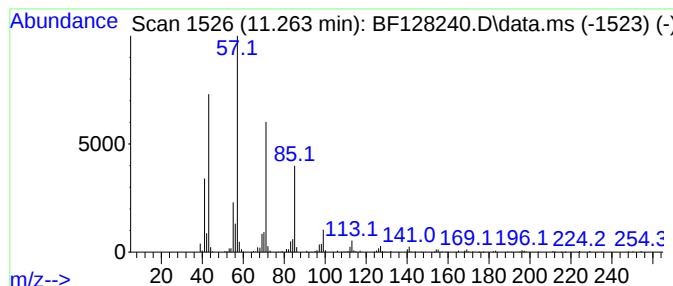
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	7.89 ng	215416	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	93
2		Pentadecane	212	C15H32	000629-62-9	91
3		Tridecane	184	C13H28	000629-50-5	90
4		Eicosane	282	C20H42	000112-95-8	86
5		Tetradecane	198	C14H30	000629-59-4	86



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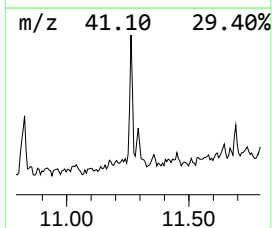
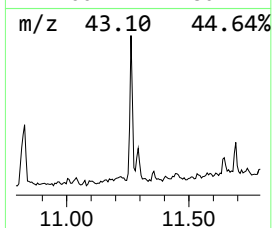
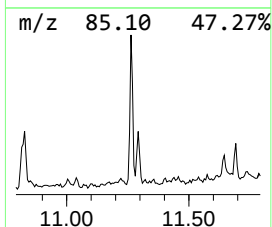
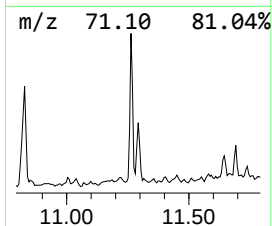
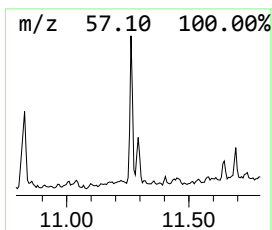
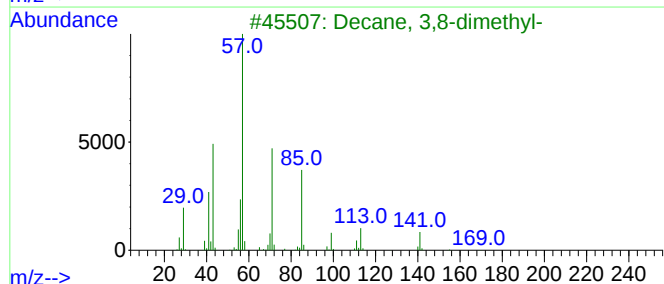
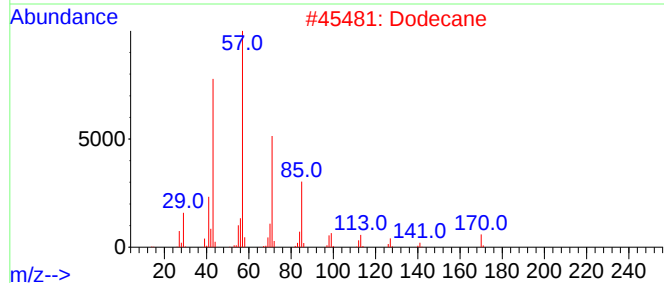
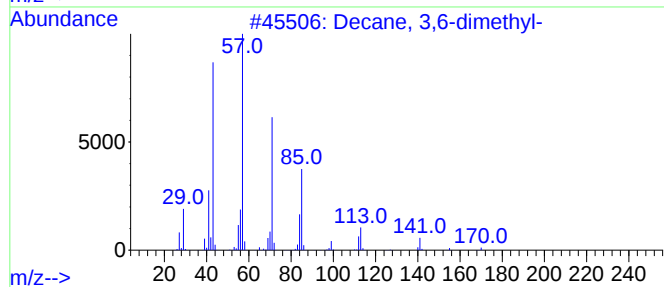
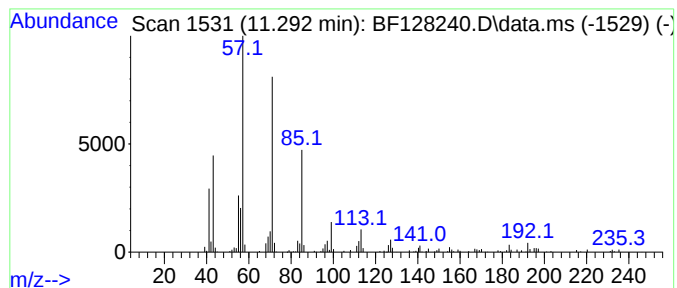
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Peak Number 5 Decane, 3,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.292	3.62 ng	98804	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	90
2			Dodecane	170	C12H26	000112-40-3	87
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	86
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86



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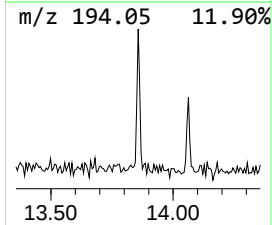
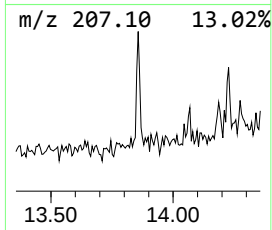
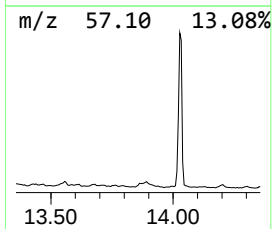
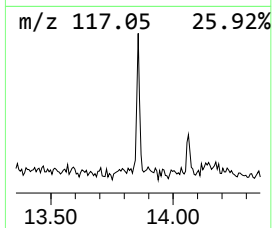
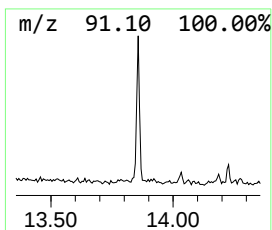
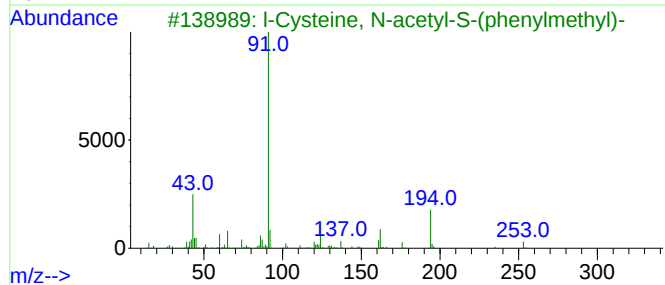
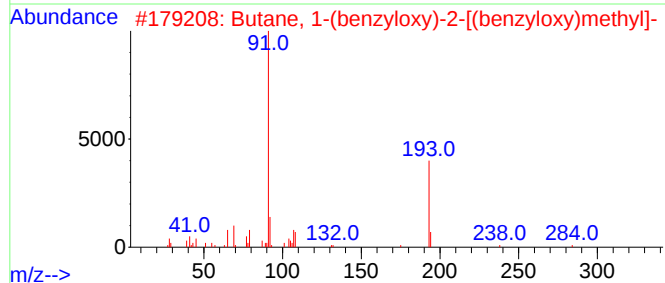
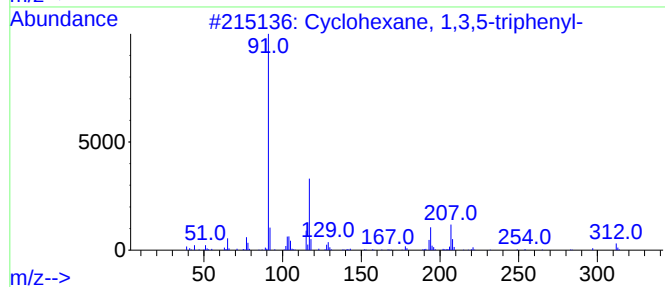
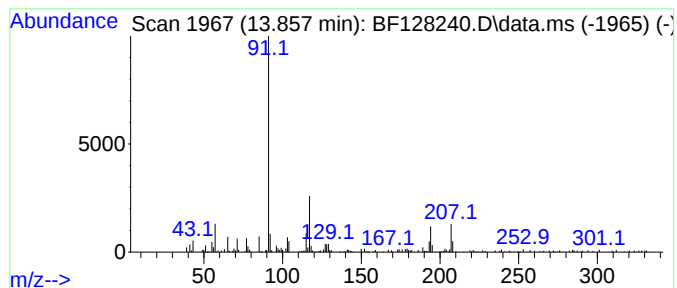
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BNA_F
ClientSampleId :
SC-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	5.40 ng	88104	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	64
2	Butane, 1-(benzyloxy)-2-[(benzyl...	284	C19H24O2	033498-90-7	27
3	L-Cysteine, N-acetyl-S-(phenylme...	253	C12H15NO3S	019542-77-9	22
4	N-Benzyl-N-methyl-5,7-dinitro-2,...	329	C14H11N5O5	1000387-18-5	12
5	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128240.D
Acq On : 13 May 2022 15:44
Operator : CG\JU
Sample : N2823-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-12

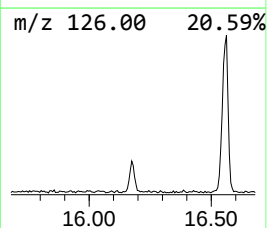
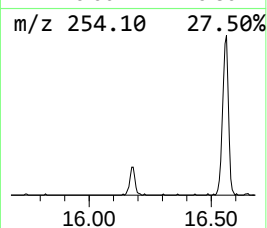
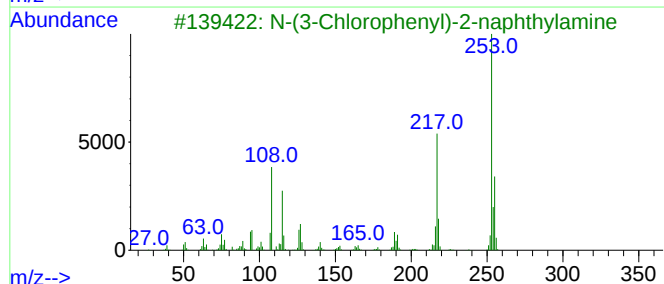
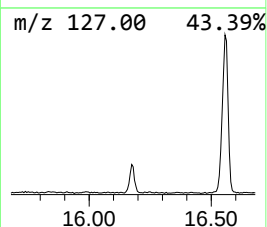
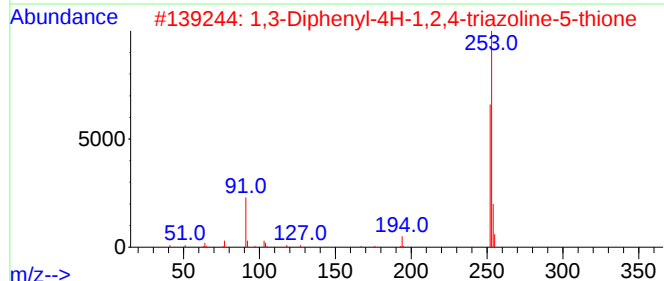
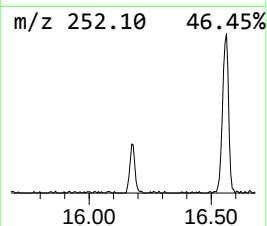
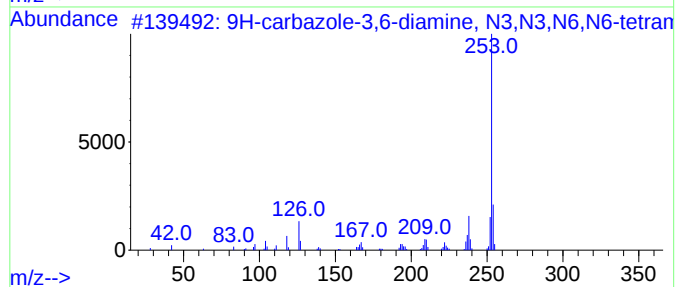
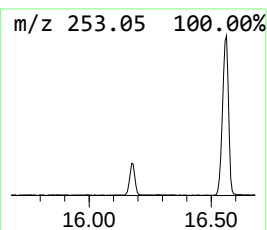
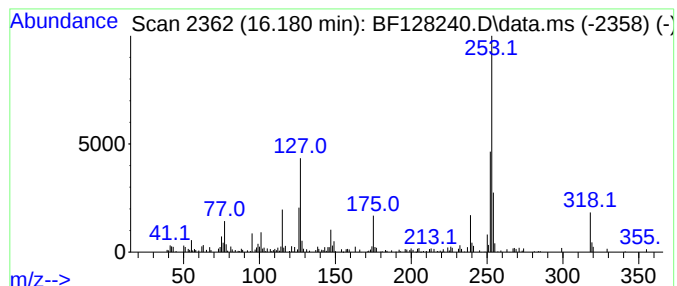
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.180 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	5.24 ng	97237	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-carbazole-3,6-diamine, N3,N3,...	253	C16H19N3	1010396-68-8	43		
2	1,3-Diphenyl-4H-1,2,4-triazoline...	253	C14H11N3S	005055-73-2	43		
3	N-(3-Chlorophenyl)-2-naphthylamine	253	C16H12ClN	1000446-91-1	35		
4	1,1-Dioxido-1,2-benzisothiazol-3...	254	C10H14N2O2SSi	1000479-94-7	35		
5	1,2-Dihydropyrido(3,2,1-kl)pheno...	253	C15H11NOS	069513-42-4	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128240.D
Acq On : 13 May 2022 15:44
Operator : CG\JU
Sample : N2823-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SC-12

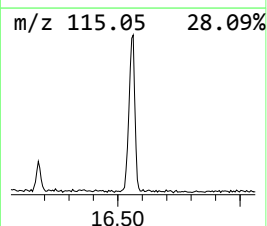
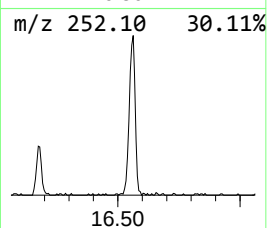
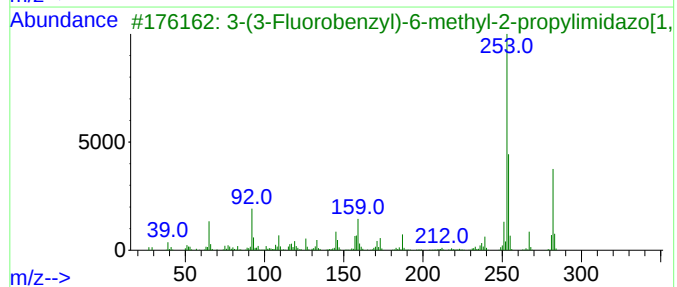
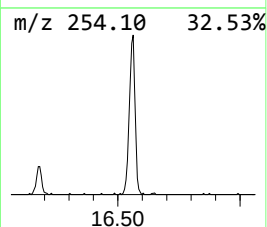
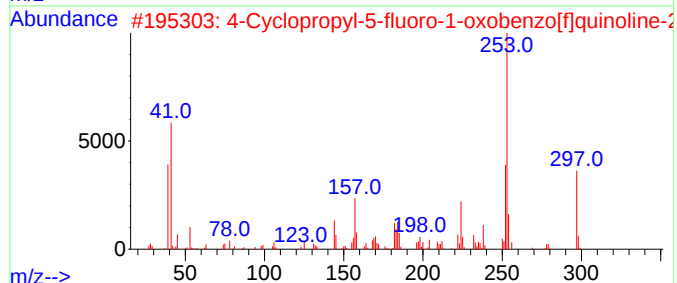
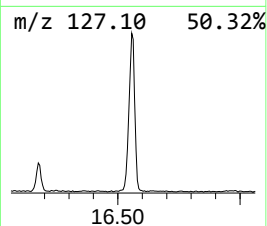
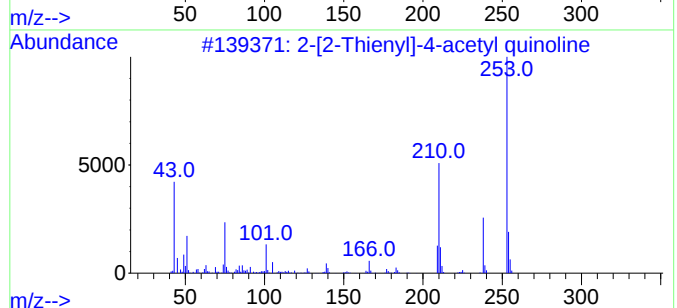
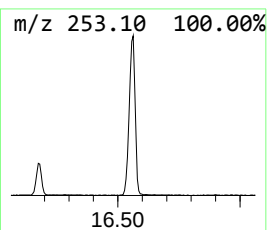
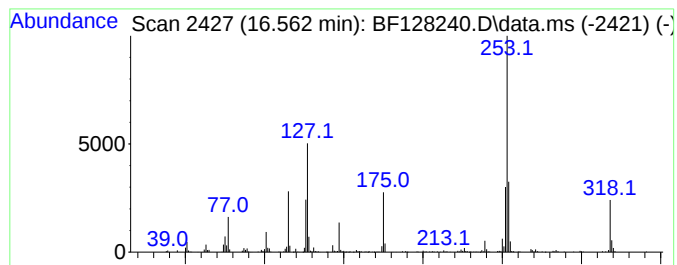
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.562 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.562	30.89 ng	573388	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		[2-Thienyl]-4-acetyl quinoline	253	C15H11NOS	027302-83-6	22
2	4		Cyclopropyl-5-fluoro-1-oxobenz...	297	C17H12FNO3	1000435-59-2	17
3	3		(3-Fluorobenzyl)-6-methyl-2-pr...	282	C18H19FN2	1000457-96-1	16
4	Benzimidazol-5-amine, 1-(4-ethox...	253	C15H15N3O	007104-62-3	16		
5	6-(2-Formylhydrazino)-N,N'-bis(i...	253	C10H19N7O	084305-82-8	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128240.D
Acq On : 13 May 2022 15:44
Operator : CG\JU
Sample : N2823-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SC-12

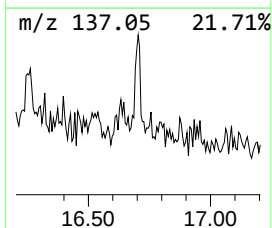
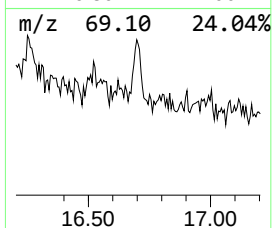
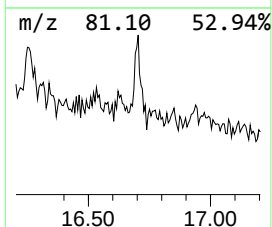
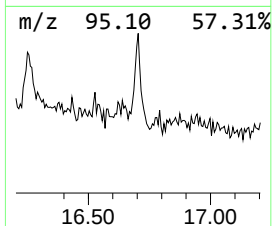
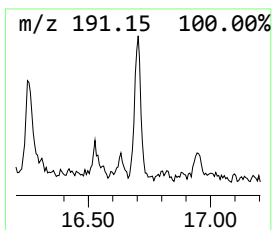
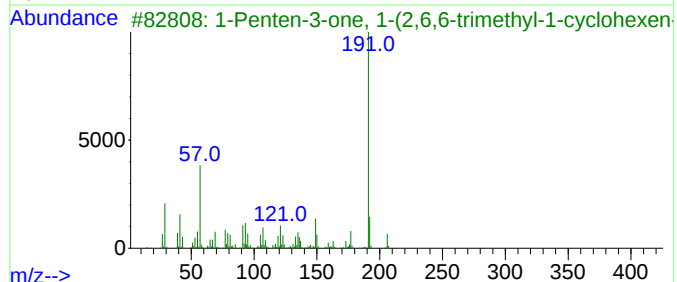
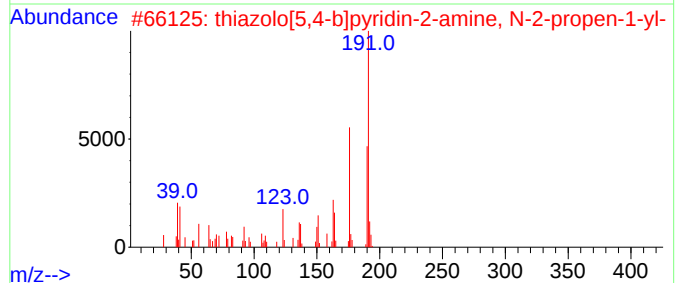
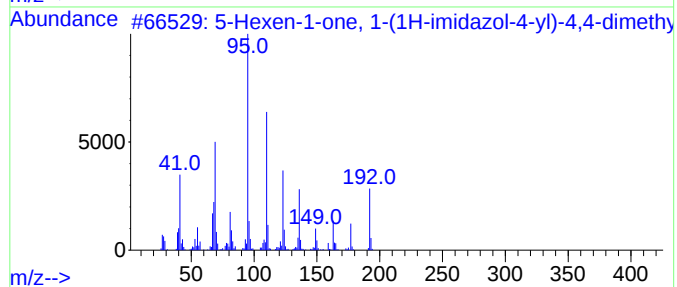
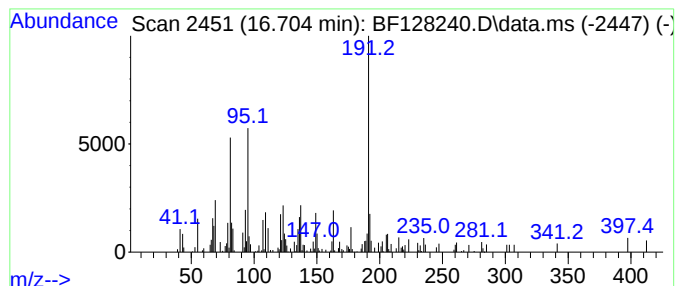
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5-Hexen-1-one, 1-(1H-imidaz... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.704	5.21 ng	96643	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	51
2			thiazolo[5,4-b]pyridin-2-amine, ...	191	C9H9N3S	1000400-23-3	50
3			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
4			4H-Benzo[def]carbazole	191	C14H9N	000203-65-6	43
5			4-Fluoro-3-trifluoromethylbenzoi...	418	C23H34F4O2	1000338-69-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128240.D
Acq On : 13 May 2022 15:44
Operator : CG\JU
Sample : N2823-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-12

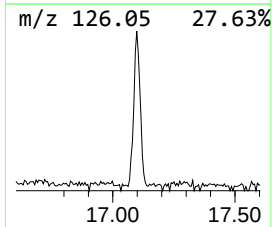
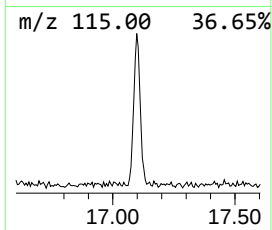
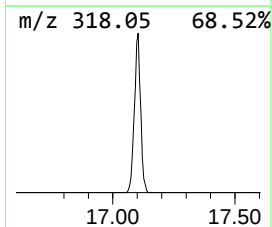
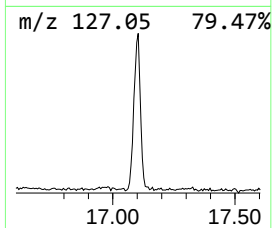
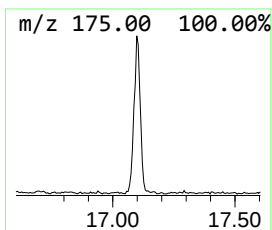
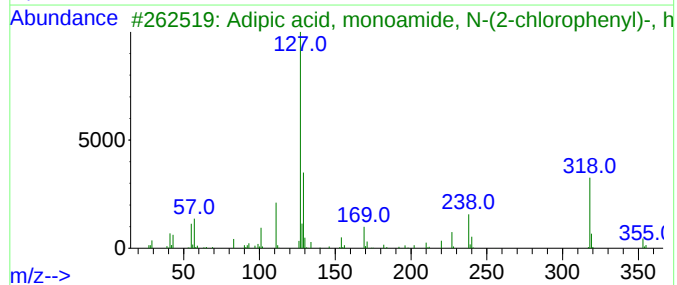
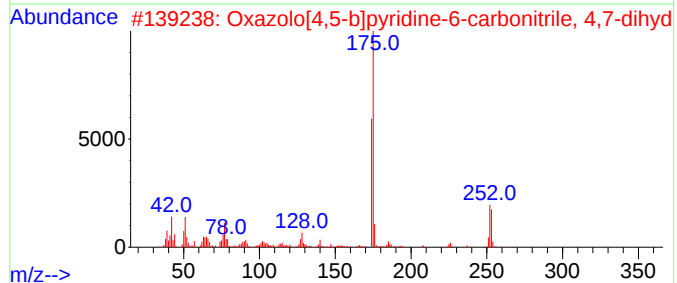
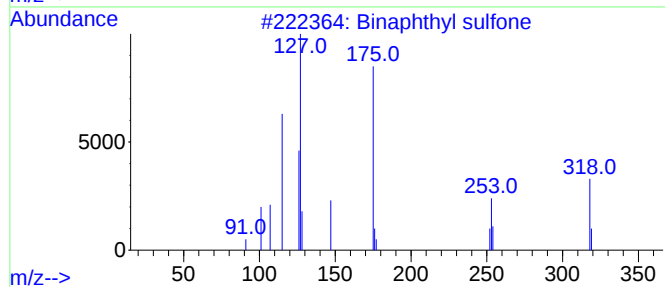
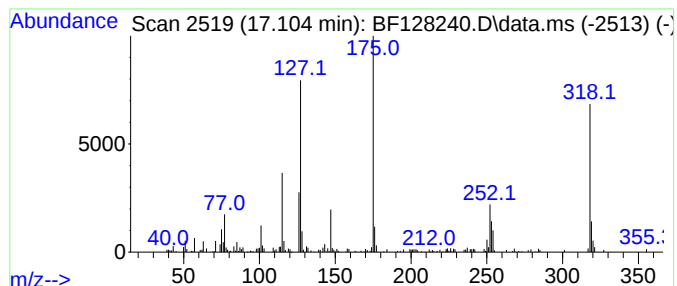
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Binaphthyl sulfone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.104	12.42 ng	230518	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Binaphthyl sulfone	318	C20H14O2S	032390-26-4	50
2			Oxazolo[4,5-b]pyridine-6-carboni...	253	C14H11N3O2	1000259-79-0	38
3			Adipic acid, monoamide, N-(2-chl...	353	C19H28ClNO3	1000324-08-6	35
4			2,2'-Dithiodi[3-pyridinol]	252	C10H8N2O2S2	068750-09-4	22
5			4H,7H-Pyrazolo[3,4-b]pyran-5-car...	253	C13H11N5O	132813-99-1	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128240.D
Acq On : 13 May 2022 15:44
Operator : CG\JU
Sample : N2823-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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
Ethanol, 2-butoxy-	5.851	125.8	ng	2082680	1	6.887	331227	20.0
1-Hexanol, 2-et...	6.963	375.1	ng	6213000	1	6.887	331227	20.0
Dodecane, 2,7,1...	10.828	6.0	ng	163992	4	11.416	546028	20.0
Octadecane	11.263	7.9	ng	215416	4	11.416	546028	20.0
Decane, 3,6-dim...	11.292	3.6	ng	98804	4	11.416	546028	20.0
Cyclohexane, 1,...	13.857	5.4	ng	88104	5	14.063	326457	20.0
unknown16.180	16.180	5.2	ng	97237	6	15.557	371287	20.0
unknown16.562	16.562	30.9	ng	573388	6	15.557	371287	20.0
5-Hexen-1-one, ...	16.704	5.2	ng	96643	6	15.557	371287	20.0
Binaphthyl sulfone	17.104	12.4	ng	230518	6	15.557	371287	20.0