

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
 Data File : BF128609.D
 Acq On : 31 May 2022 22:33
 Operator : CG\JU
 Sample : N2952-13
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P037-SS001-1824-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128609.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	468	471	479	rVB	26612	30372	1.22%	0.183%
2	5.510	544	548	562	rBV	1962905	2185938	87.47%	13.193%
3	6.534	718	722	741	rVB	1755007	2171470	86.89%	13.106%
4	6.845	771	775	778	rBV	793529	662459	26.51%	3.998%
5	7.410	865	871	874	rBV	1637409	1459188	58.39%	8.807%
6	8.128	989	993	996	rBV	1003530	775028	31.01%	4.678%
7	9.204	1170	1176	1179	rBV	3107487	2498988	100.00%	15.082%
8	9.886	1288	1292	1295	rBV	855536	777654	31.12%	4.693%
9	10.680	1423	1427	1441	rBV	1453449	1305865	52.26%	7.881%
10	11.374	1541	1545	1548	rBV	762489	684653	27.40%	4.132%
11	11.910	1632	1636	1646	rBV2	127964	204438	8.18%	1.234%
12	12.574	1745	1749	1758	rVB2	130188	192717	7.71%	1.163%
13	12.692	1766	1769	1775	rBV4	30401	50905	2.04%	0.307%
14	12.963	1810	1815	1818	rBV	2270120	1916319	76.68%	11.566%
15	13.351	1877	1881	1885	rVB2	97196	127899	5.12%	0.772%
16	13.598	1918	1923	1930	rVB	54089	89503	3.58%	0.540%
17	13.898	1970	1974	1979	rBV3	58077	84523	3.38%	0.510%
18	14.015	1990	1994	1997	rBV	567675	519507	20.79%	3.135%
19	14.057	1997	2001	2006	rVV2	81595	118827	4.76%	0.717%
20	14.115	2007	2011	2018	rVB	183210	201414	8.06%	1.216%
21	14.721	2110	2114	2120	rVB6	50882	76744	3.07%	0.463%
22	15.486	2240	2244	2255	rVB	325346	434600	17.39%	2.623%

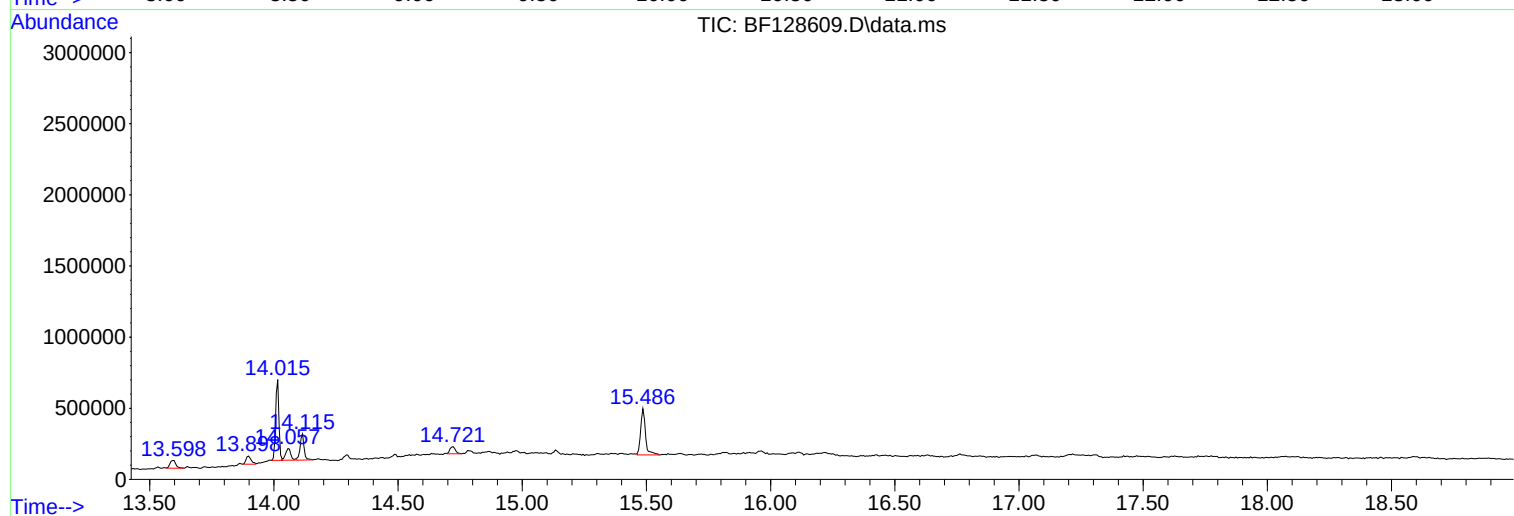
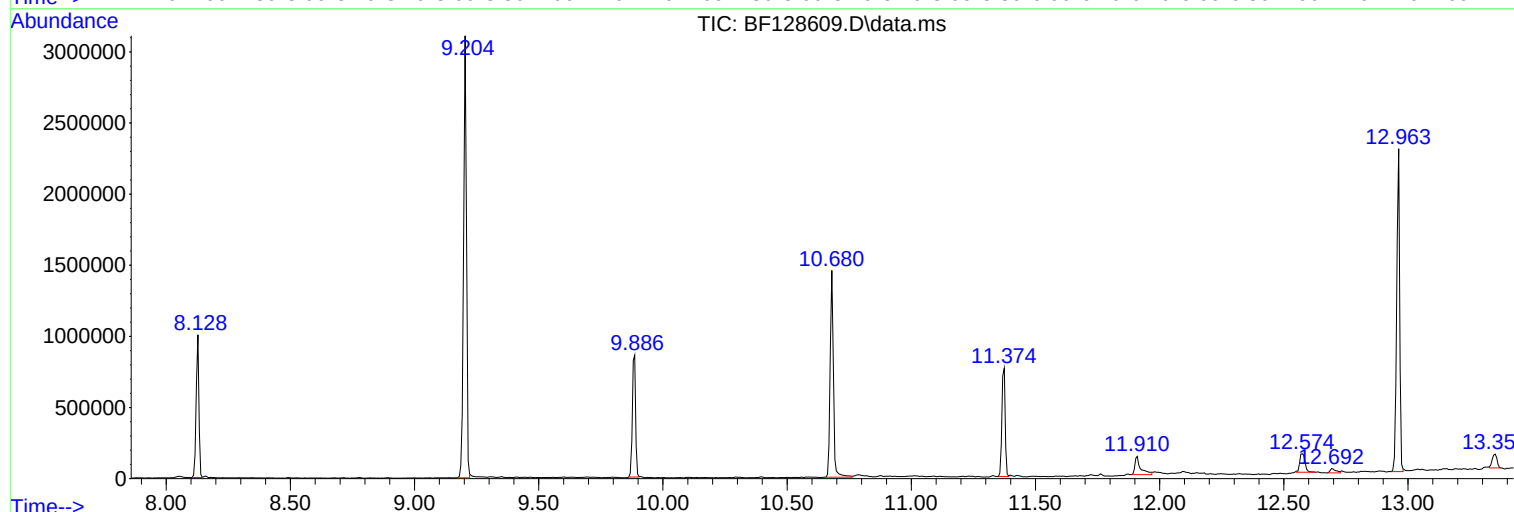
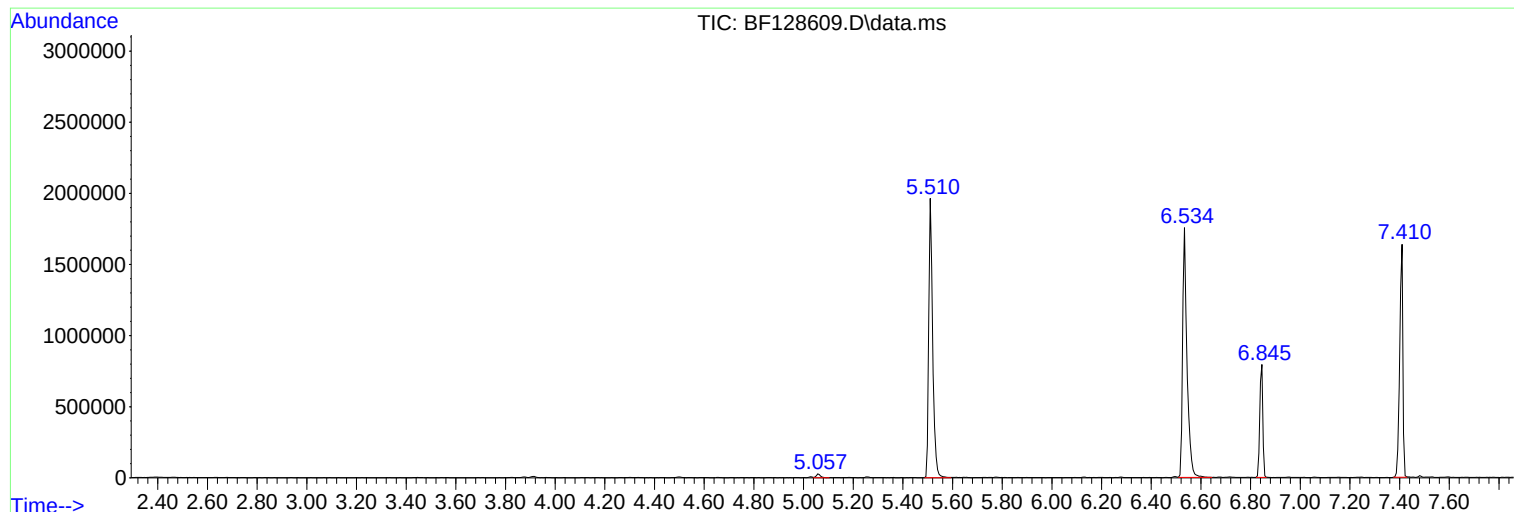
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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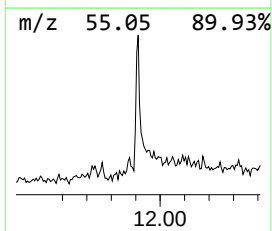
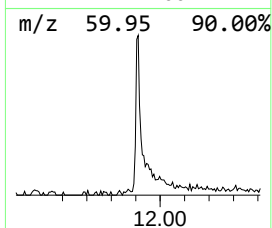
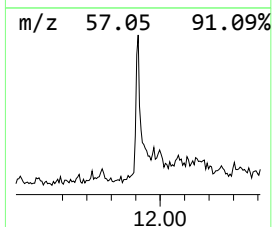
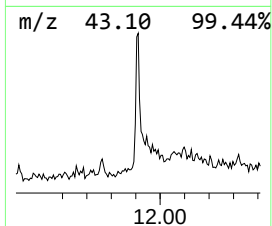
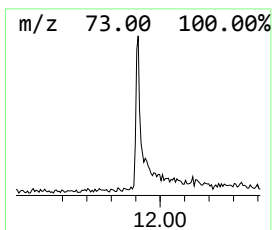
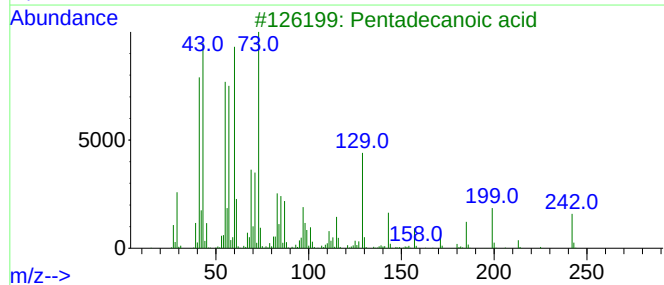
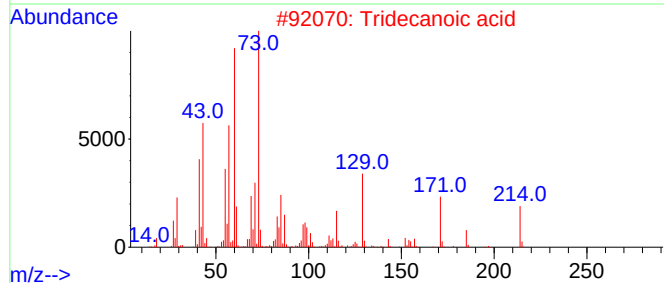
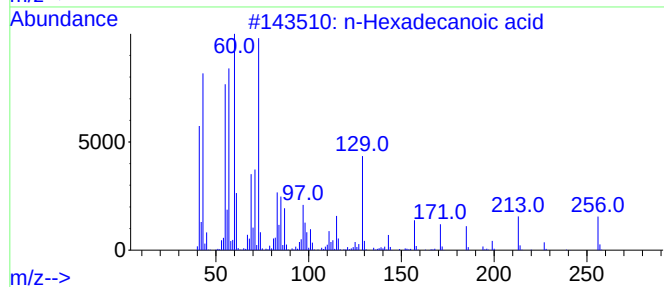
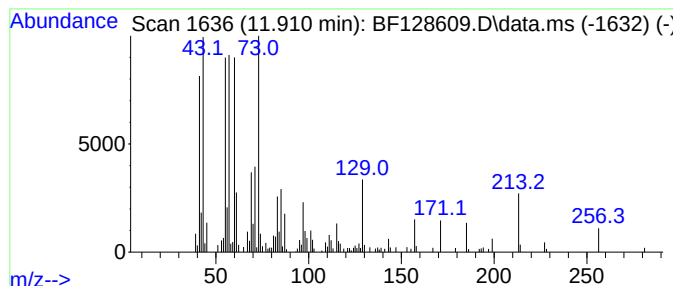
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.97 ng	204438	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	20



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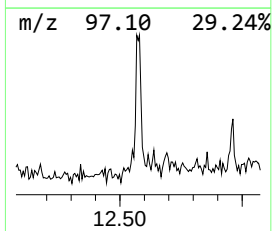
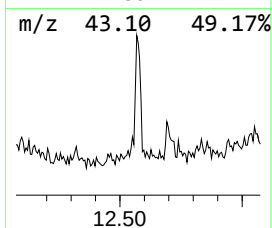
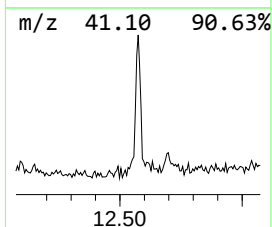
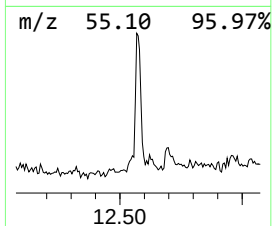
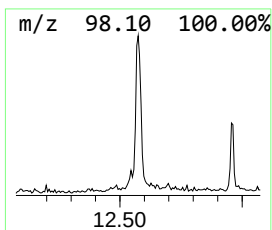
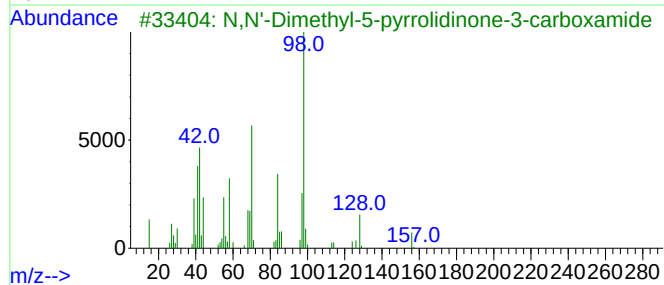
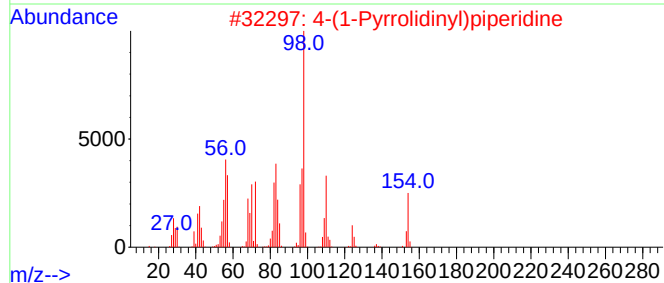
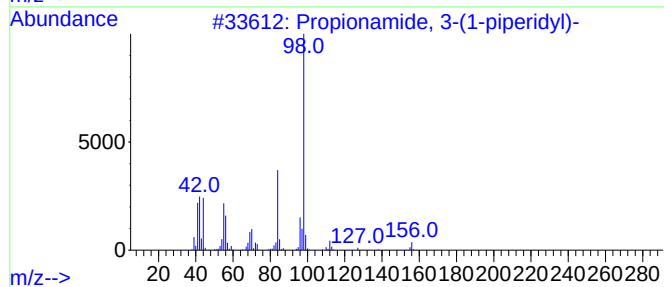
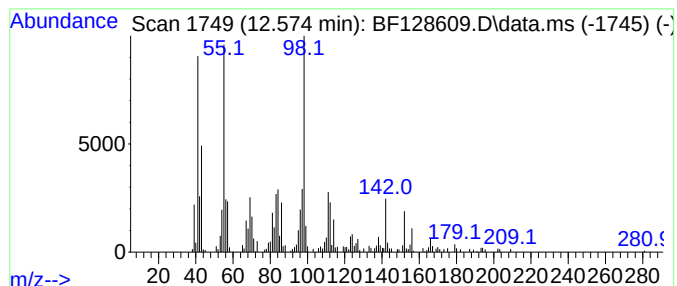
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Peak Number 2 unknown12.574 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	5.63 ng	192717	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propionamide, 3-(1-piperidyl)-	156	C8H16N2O	004269-30-1	47
2			4-(1-Pyrrolidinyl)piperidine	154	C9H18N2	005004-07-9	46
3			N,N'-Dimethyl-5-pyrrolidinone-3-...	156	C7H12N2O2	089851-99-0	43
4			n-Heptylamine, N-acetyl-1-cyano-	182	C10H18N2O	1000227-03-9	43
5			2-Dodecylcyclobutanone	238	C16H30O	035493-46-0	43



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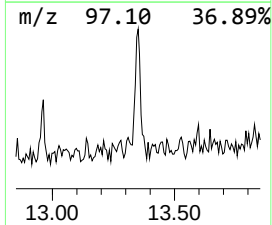
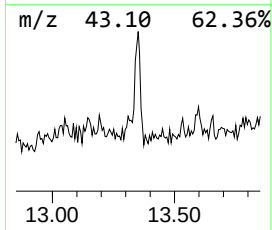
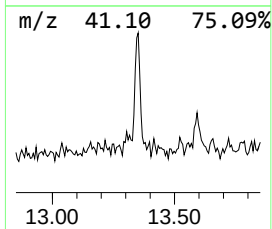
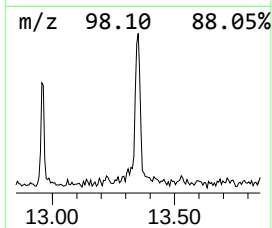
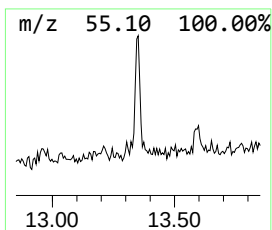
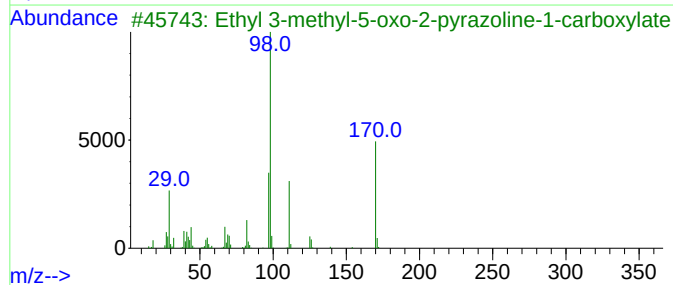
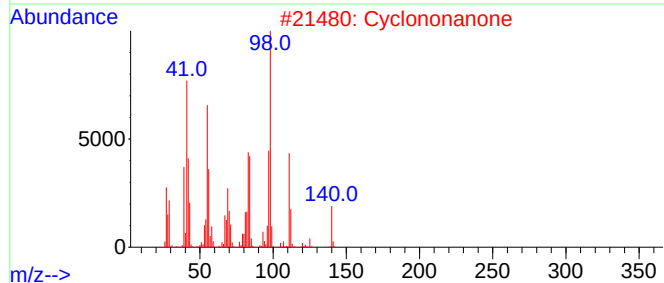
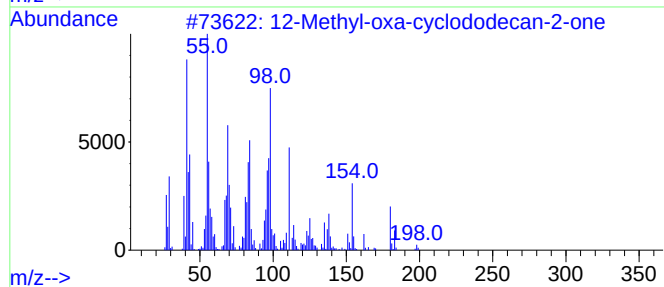
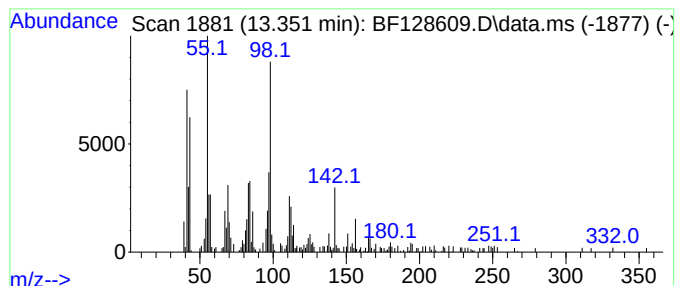
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Peak Number 3 12-Methyl-oxa-cyclododecan-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	4.92 ng	127899	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			12-Methyl-oxa-cyclododecan-2-one	198	C12H22O2	1000193-59-0	55
2			Cyclononanone	140	C9H16O	003350-30-9	52
3			Ethyl 3-methyl-5-oxo-2-pyrazolin...	170	C7H10N2O3	089943-54-4	46
4			2-Thiopheneacetamide, N-(2-ethyl...	253	C14H23NOS	1010407-01-1	45
5			Pentylamine, N-acetyl-1-cyano-	154	C8H14N2O	027395-08-0	43



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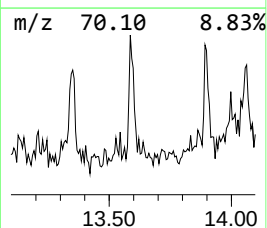
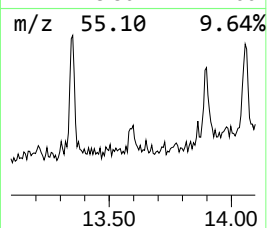
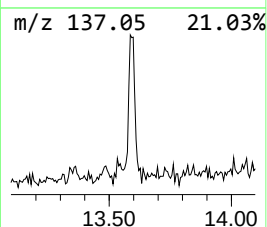
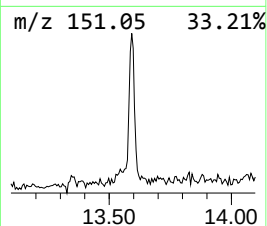
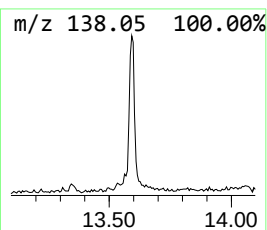
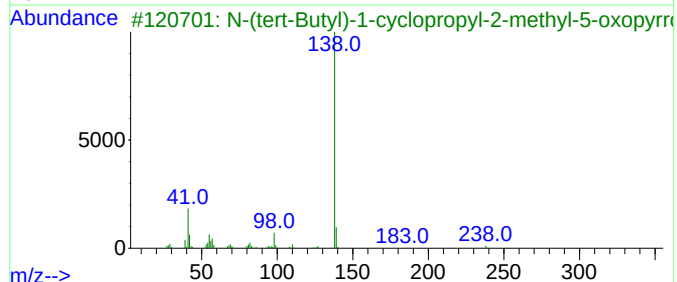
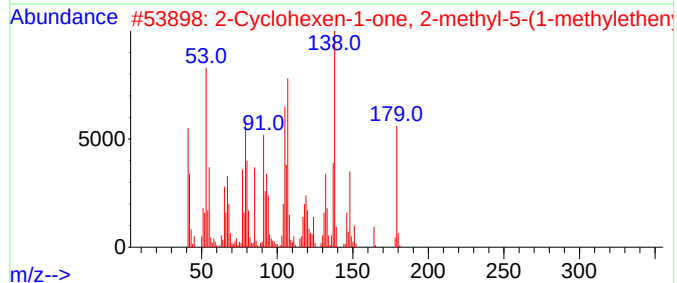
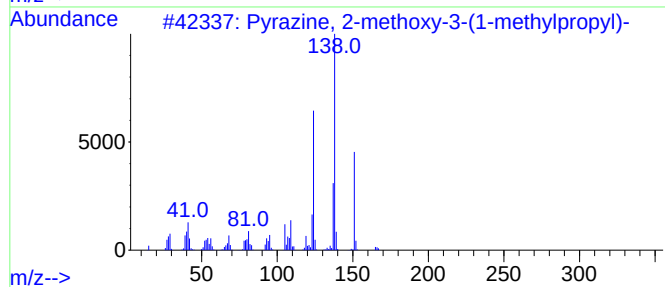
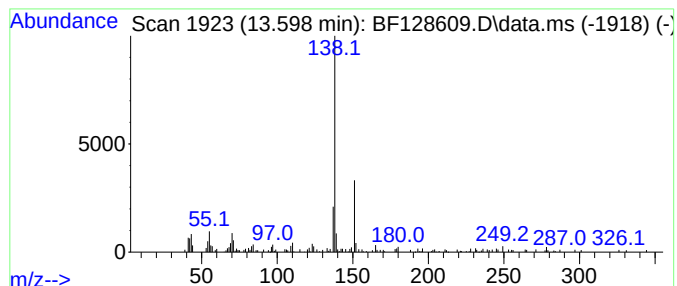
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Peak Number 4 Pyrazine, 2-methoxy-3-(1-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	3.45 ng	89503	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrazine, 2-methoxy-3-(1-methylp...	166	C9H14N2O	024168-70-5	72
2			2-Cyclohexen-1-one, 2-methyl-5-(...	179	C11H17NO	057397-12-3	53
3			N-(tert-Butyl)-1-cyclopropyl-2-m...	238	C13H22N2O2	1000458-30-5	43
4			N-Benzyl-1-cyclopropyl-2-methyl-...	272	C16H20N2O2	1000458-29-7	43
5			2-Propenoic acid, 2-methyl-, 1,2...	239	C14H25NO2	068548-08-3	43



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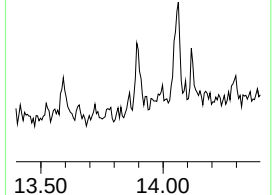
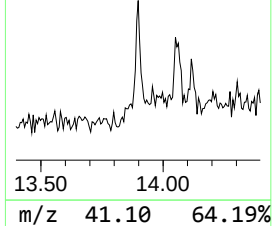
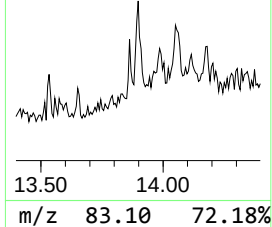
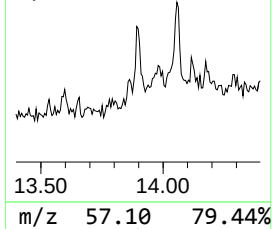
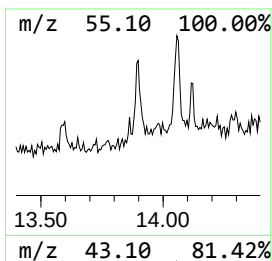
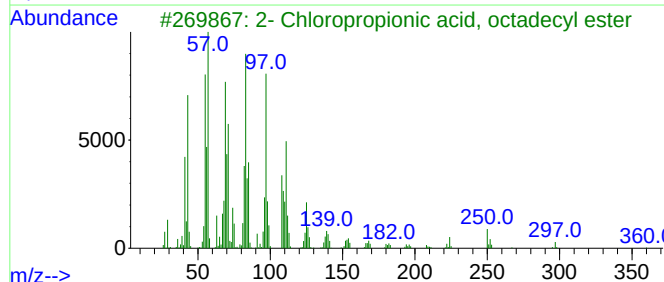
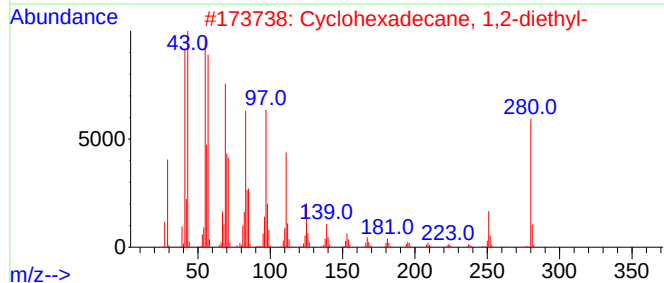
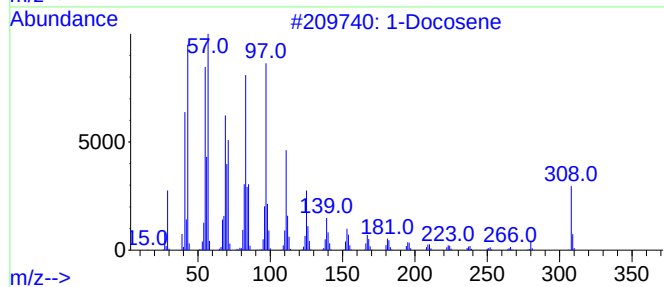
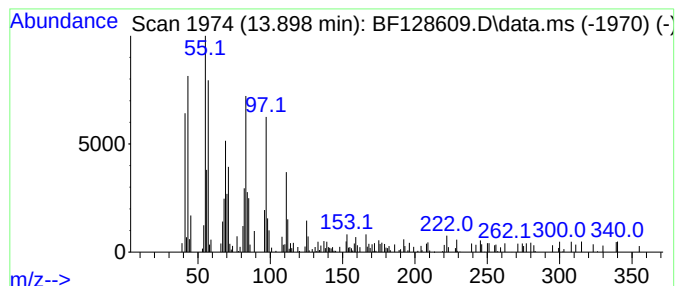
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.25 ng	84523	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	91
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
5			2- Bromopropionic acid, hexadecy...	376	C19H37BrO2	063966-83-6	87



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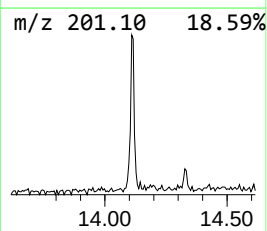
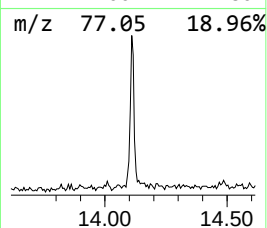
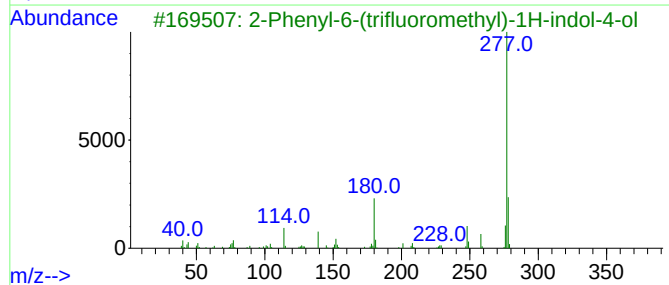
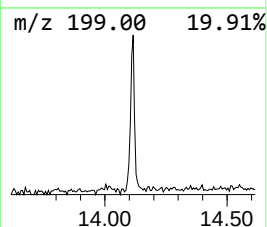
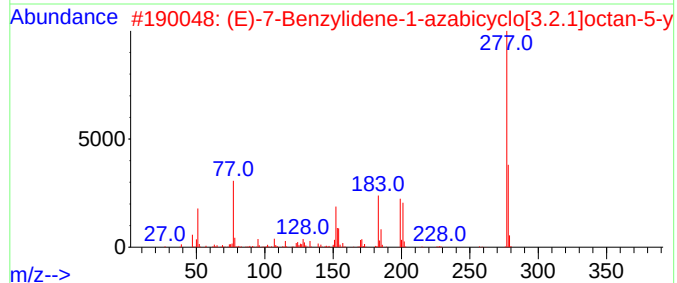
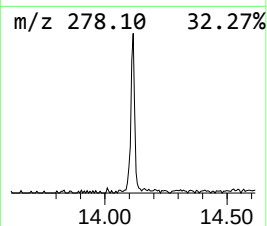
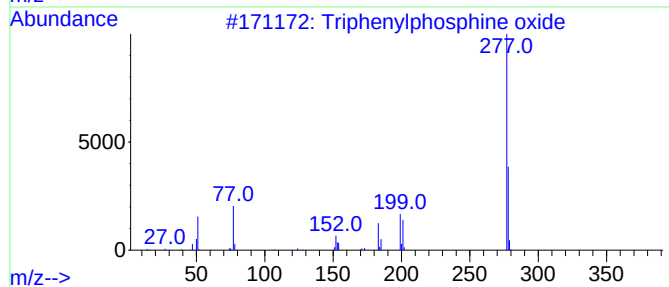
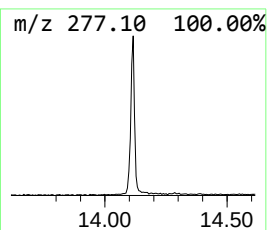
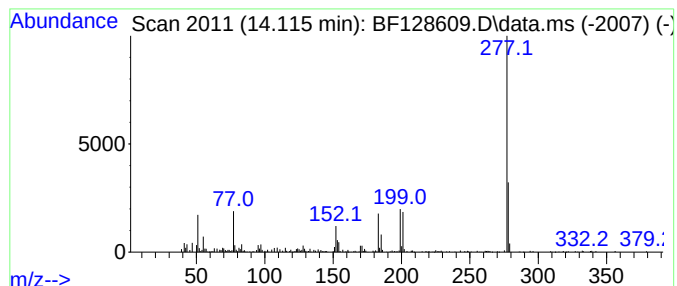
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.115	7.75 ng	201414	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	87
3			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	47
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128609.D
Acq On : 31 May 2022 22:33
Operator : CG\JU
Sample : N2952-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-1824-01

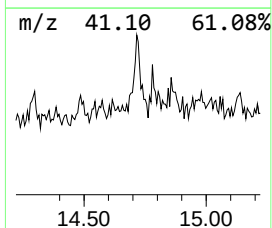
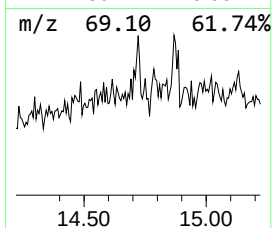
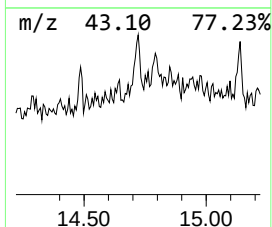
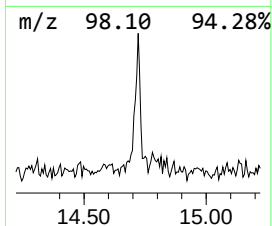
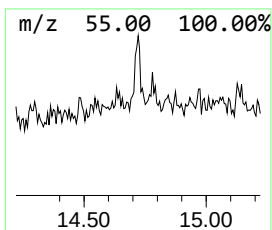
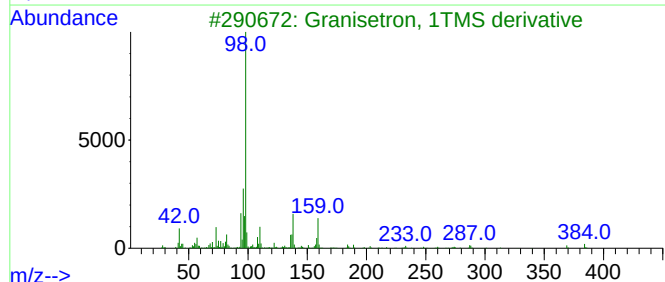
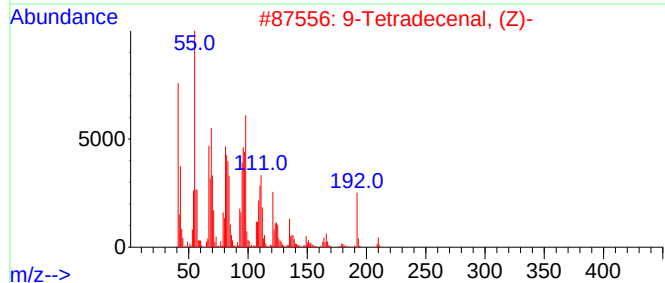
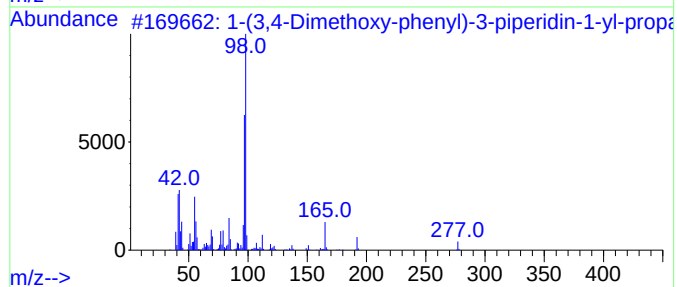
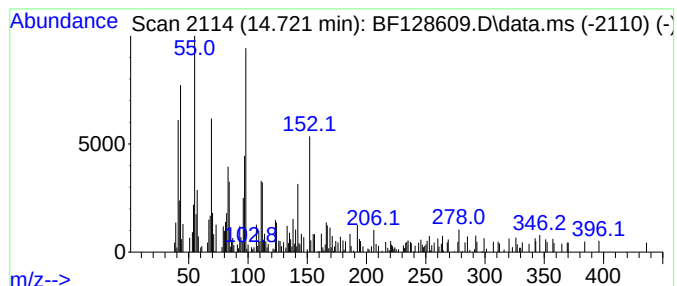
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.721 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.95 ng	76744	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	-(3,4-Dimethoxy-phenyl)-3-piper...	277	C16H23NO3	1000295-21-6	43	
2	9-Tetradecenal, (Z)-	210	C14H26O	053939-27-8	38		
3	Granisetron, 1TMS derivative	384	C21H32N4OSi	1000485-88-8	30		
4	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	30		
5	1-[2-(2-Piperidinoethoxy)ethoxy]...	337	C19H31NO4	1000215-99-3	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128609.D
Acq On : 31 May 2022 22:33
Operator : CG\JU
Sample : N2952-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
n-Hexadecanoic ...	11.910	6.0	ng	204438	4	11.374	684653	20.0
unknown12.574	12.574	5.6	ng	192717	4	11.374	684653	20.0
12-Methyl-oxa-c...	13.351	4.9	ng	127899	5	14.015	519507	20.0
Pyrazine, 2-met...	13.598	3.5	ng	89503	5	14.015	519507	20.0
1-Docosene	13.898	3.3	ng	84523	5	14.015	519507	20.0
Triphenylphosph...	14.115	7.8	ng	201414	5	14.015	519507	20.0
unknown14.721	14.721	3.0	ng	76744	5	14.015	519507	20.0