

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
 Data File : BF130540.D
 Acq On : 05 Oct 2022 20:45
 Operator : CG\JU
 Sample : N4966-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 257248-5

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.804	458	462	474	rBV	140614	175973	6.87%	1.060%
2	5.234	532	535	554	rBV	903620	920552	35.93%	5.546%
3	5.640	600	604	613	rVB	29022	29755	1.16%	0.179%
4	6.275	709	712	726	rBV	532072	528156	20.61%	3.182%
5	6.634	769	773	778	rBV	664614	591296	23.08%	3.562%
6	7.204	865	870	873	rBV	1510469	1440027	56.20%	8.675%
7	7.281	879	883	893	rBV2	24802	53419	2.08%	0.322%
8	7.834	973	977	987	rBV	114211	320883	12.52%	1.933%
9	7.916	987	991	999	rVB	603540	552977	21.58%	3.331%
10	8.545	1095	1098	1110	rBV	58344	87198	3.40%	0.525%
11	8.992	1170	1174	1177	rBV	3007243	2358506	92.05%	14.208%
12	9.628	1279	1282	1285	rBV	557852	537910	20.99%	3.240%
13	9.663	1285	1288	1298	rVB	613672	511458	19.96%	3.081%
14	10.451	1419	1422	1437	rVB	1251294	1220598	47.64%	7.353%
15	10.598	1444	1447	1458	rVB	742903	652688	25.47%	3.932%
16	10.716	1464	1467	1479	rBV	252314	256515	10.01%	1.545%
17	11.145	1536	1540	1547	rBV	554005	443448	17.31%	2.671%
18	11.475	1593	1596	1599	rBV	102129	81623	3.19%	0.492%
19	11.563	1605	1611	1617	rBV	777003	724754	28.29%	4.366%
20	11.686	1629	1632	1634	rBV	162125	154518	6.03%	0.931%
21	11.716	1634	1637	1640	rVB	758489	586588	22.89%	3.534%
22	12.333	1738	1742	1750	rBV2	435503	511330	19.96%	3.080%
23	12.469	1762	1765	1768	rBV	51032	49951	1.95%	0.301%
24	12.733	1805	1810	1813	rBV	3070661	2562175	100.00%	15.435%
25	13.098	1866	1872	1876	rBV	154412	129971	5.07%	0.783%
26	13.463	1927	1934	1936	rBV4	17679	31959	1.25%	0.193%
27	13.774	1983	1987	1999	rBV	610821	662021	25.84%	3.988%
28	13.880	2002	2005	2011	rVB	31669	36005	1.41%	0.217%
29	15.163	2218	2223	2227	rBV	332743	387484	15.12%	2.334%

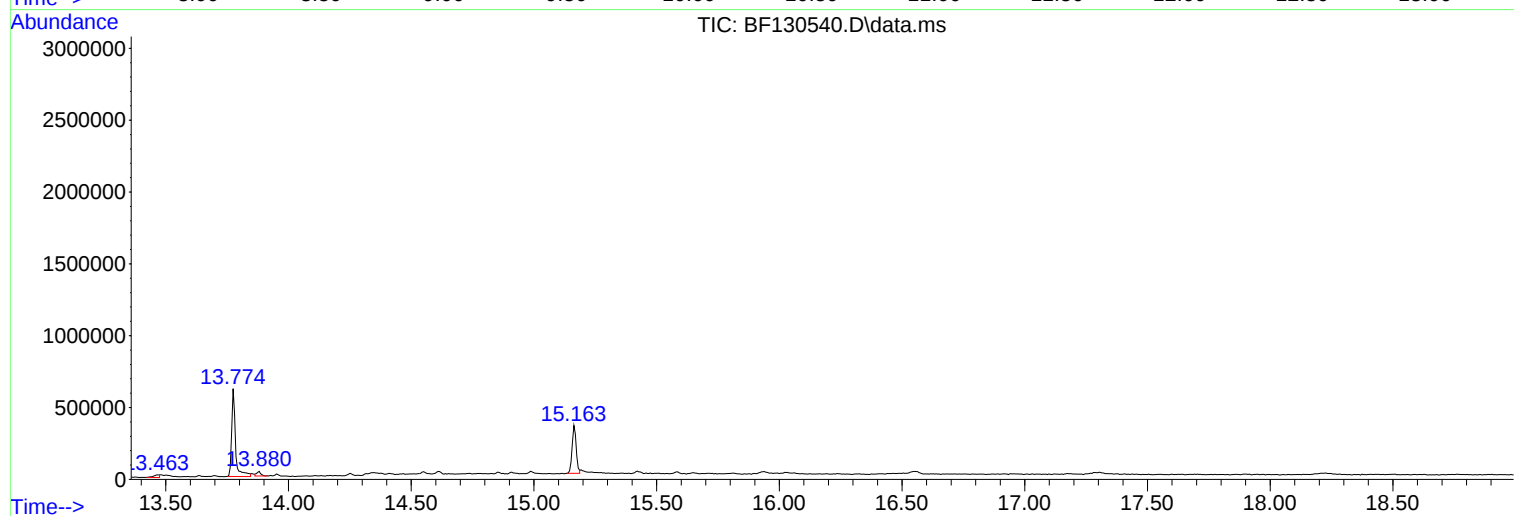
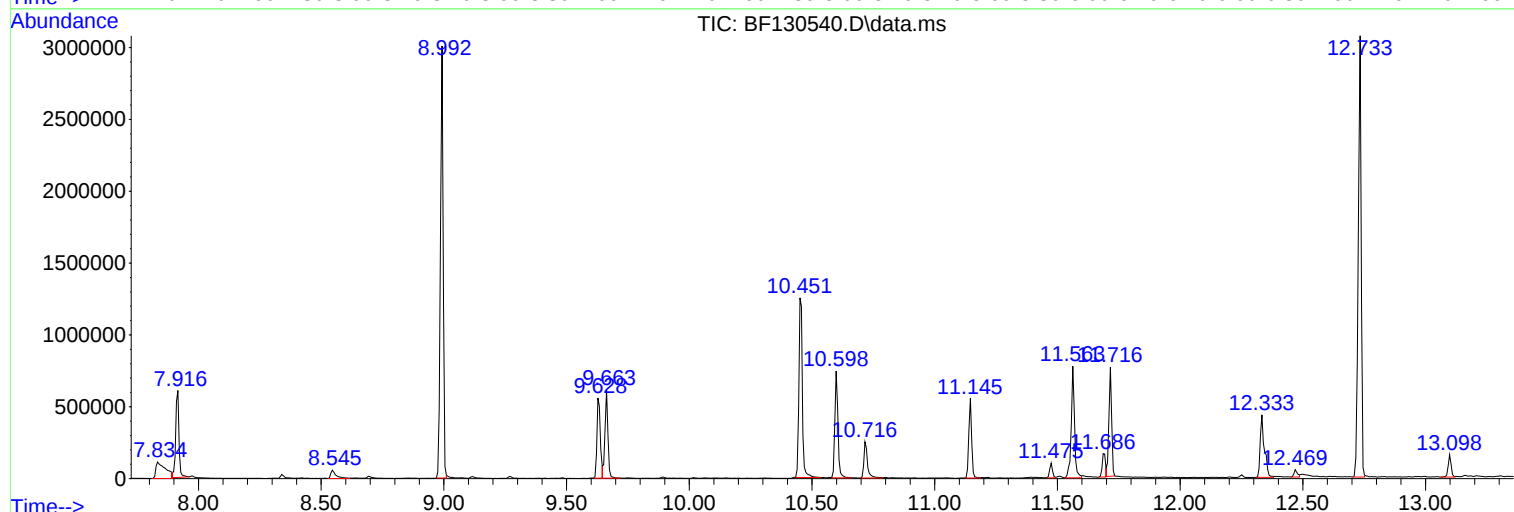
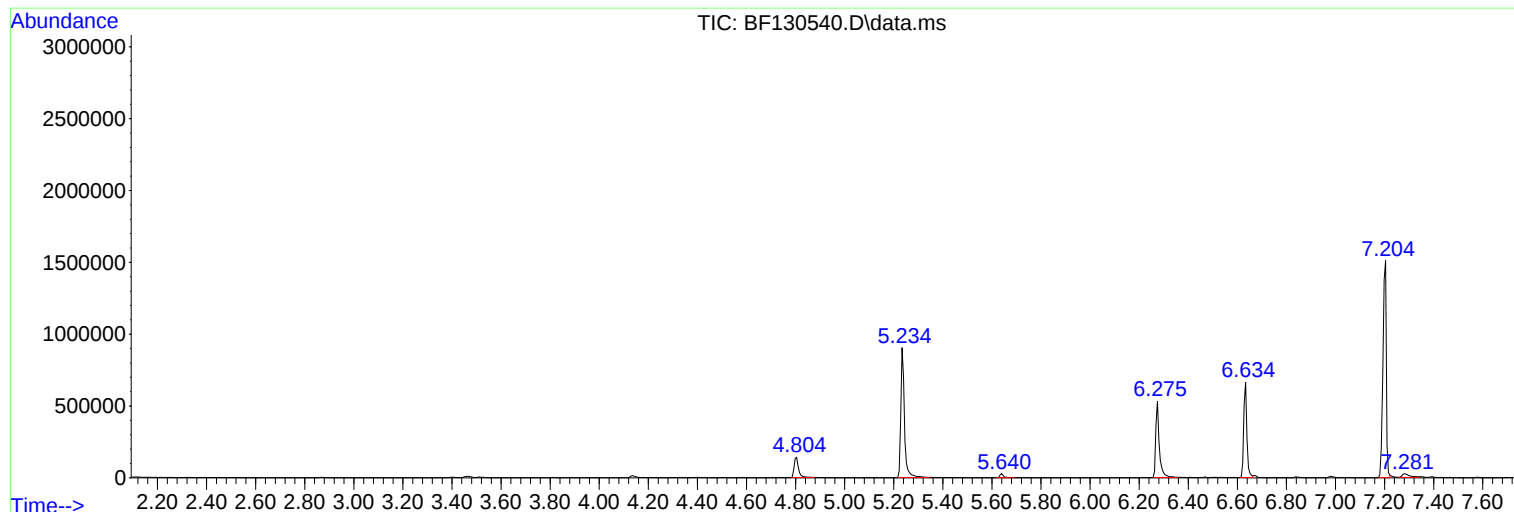
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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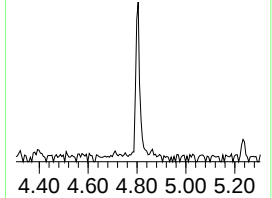
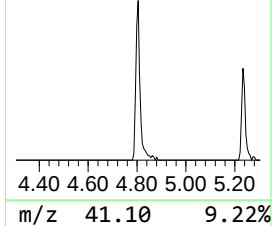
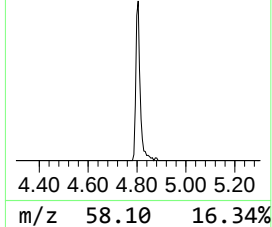
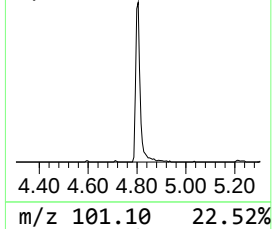
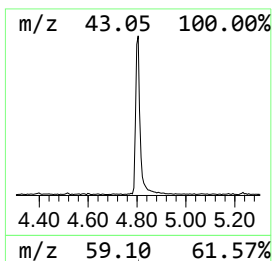
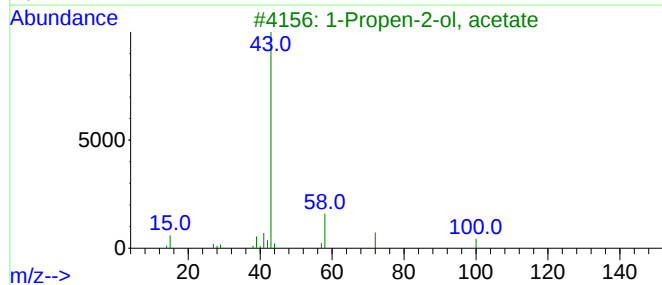
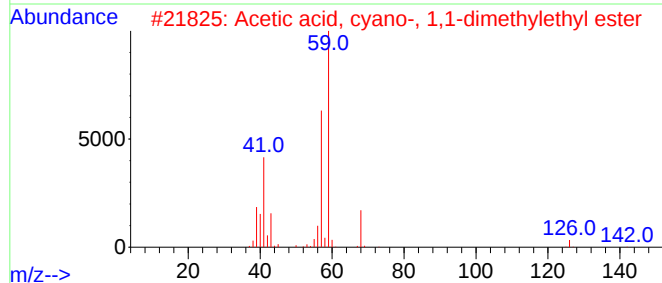
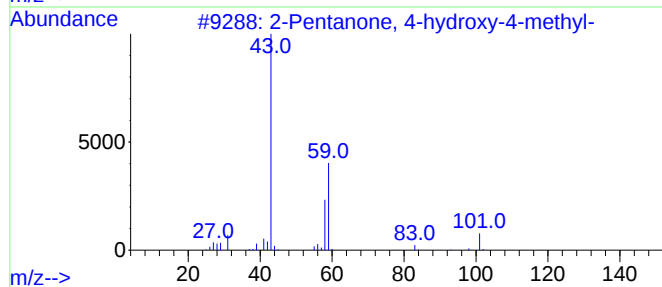
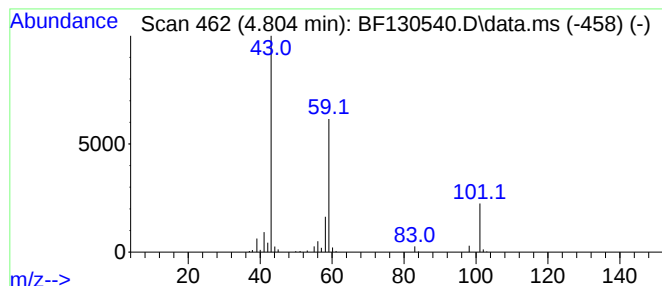
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.804	5.95 ng	175973	1,4-Dichlorobenzene-d4	6.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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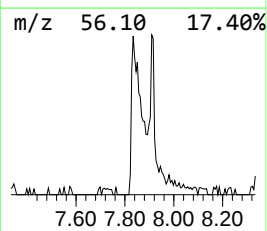
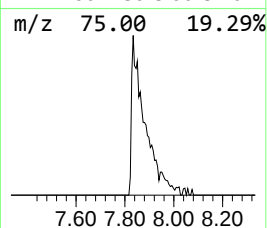
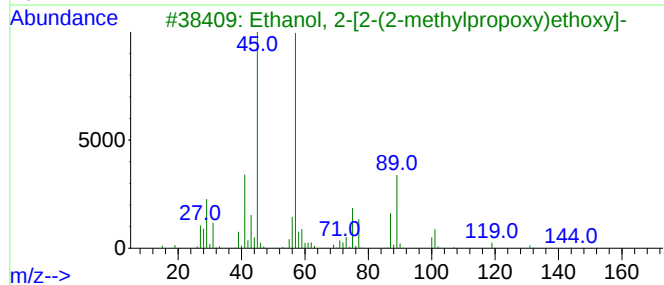
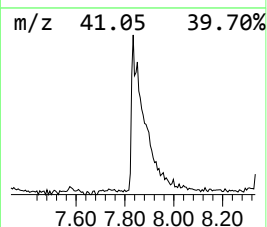
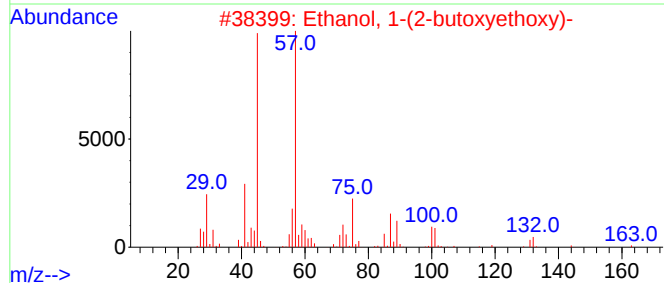
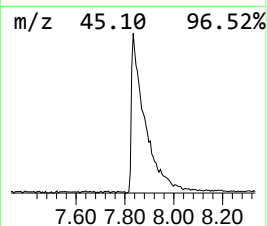
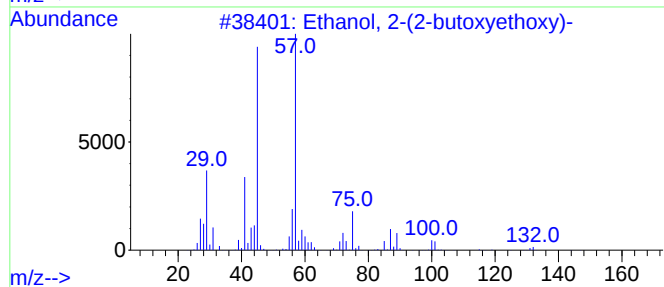
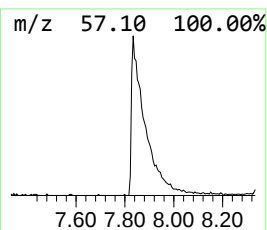
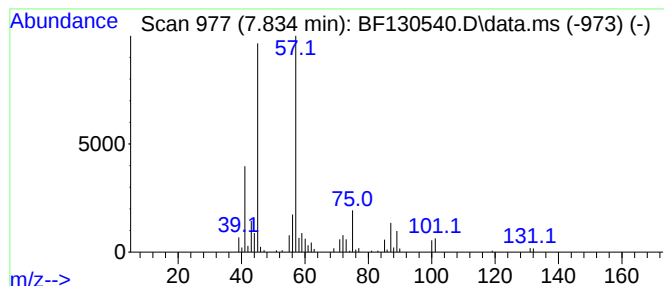
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.834	11.61 ng	320883	Naphthalene-d8	7.916

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	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53



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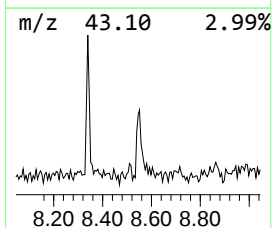
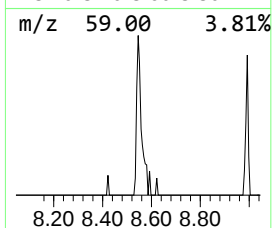
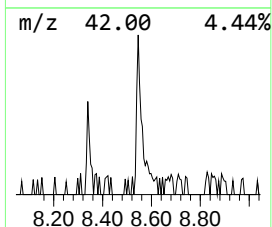
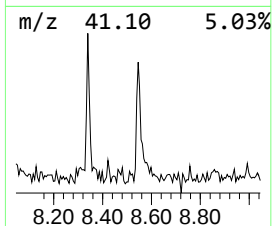
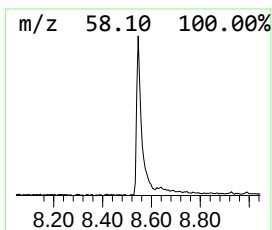
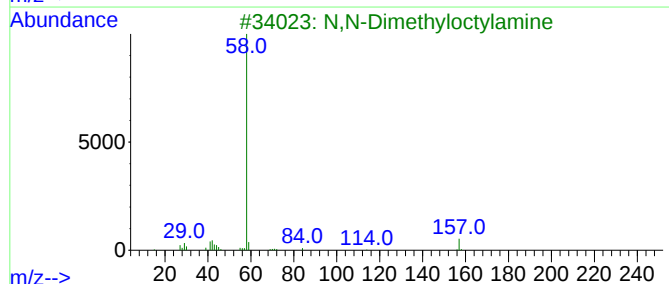
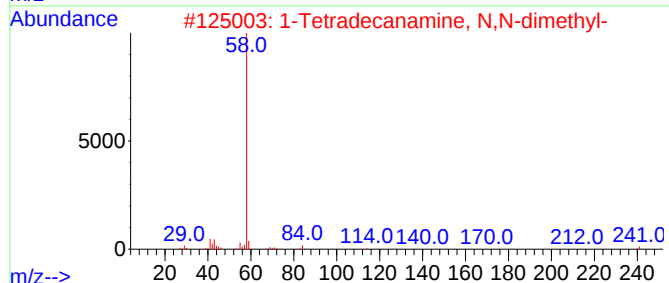
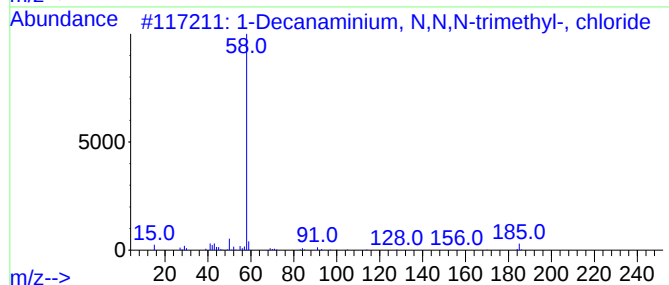
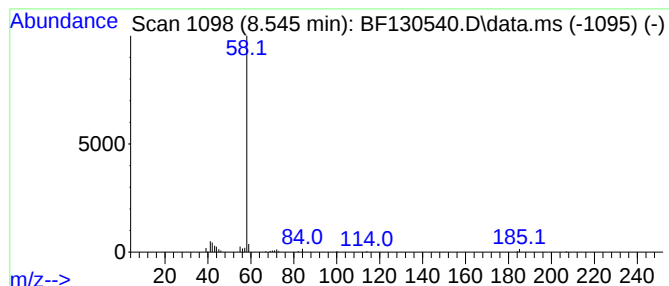
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Decanaminium, N,N,N-trime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	3.15 ng	87198	Naphthalene-d8	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanaminium, N,N,N-trimethyl-...	235	C13H30ClN	010108-87-9	78		
2	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	78		
3	N,N-Dimethyloctylamine	157	C10H23N	007378-99-6	78		
4	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78		
5	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	72		



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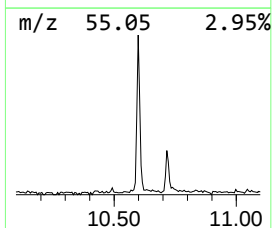
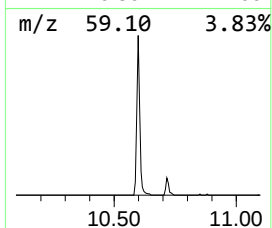
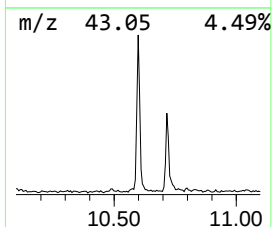
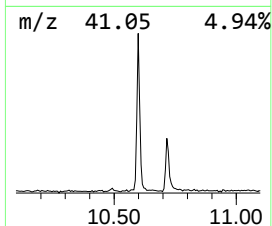
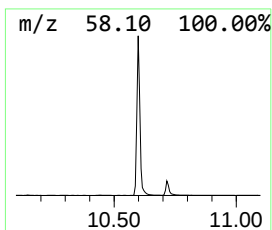
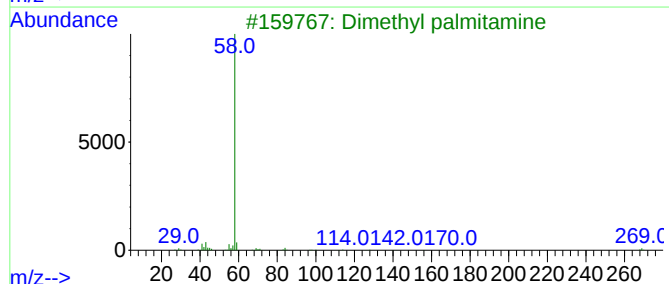
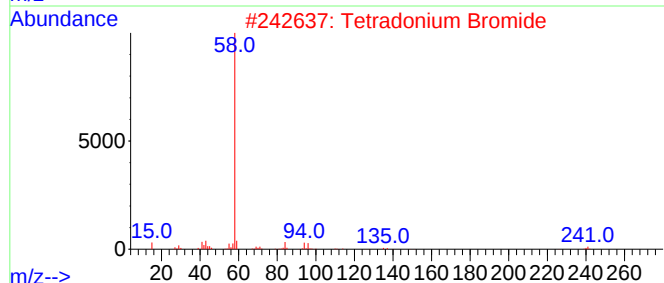
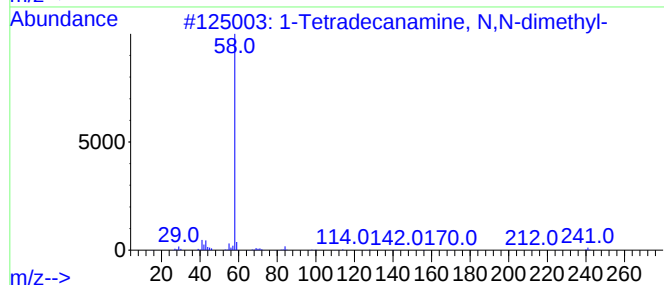
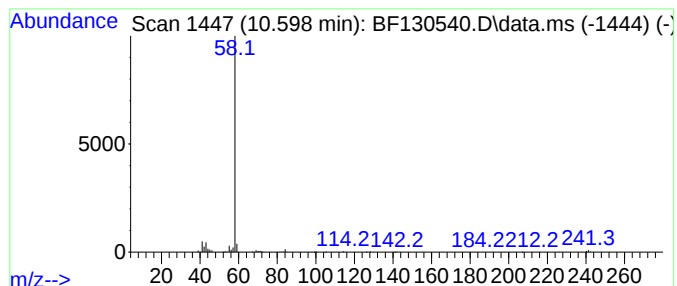
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Peak Number 4 1-Tetradecanamine, N,N-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	29.44 ng	652688	Phenanthrene-d10	11.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	91
2			Tetradonium Bromide	335	C17H38BrN	001119-97-7	78
3			Dimethyl palmitamine	269	C18H39N	000112-69-6	78
4			1-Decanaminium, N,N,N-trimethyl-...	235	C13H30ClN	010108-87-9	72
5			1-Heptadecanamine, N,N-dimethyl-	283	C19H41N	003002-57-1	72



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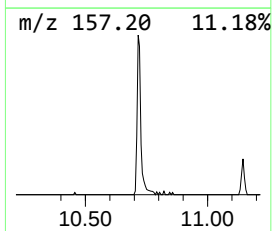
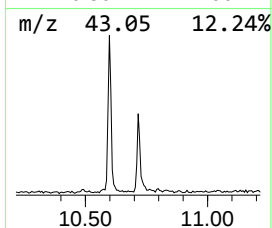
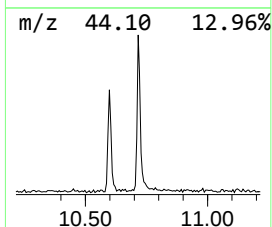
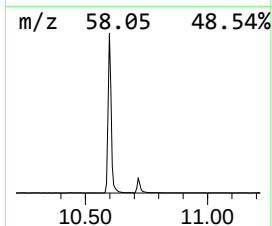
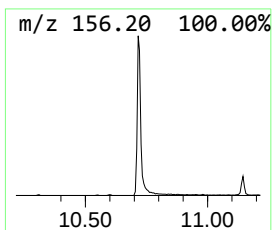
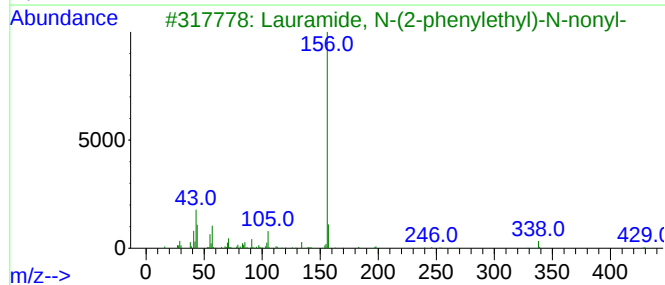
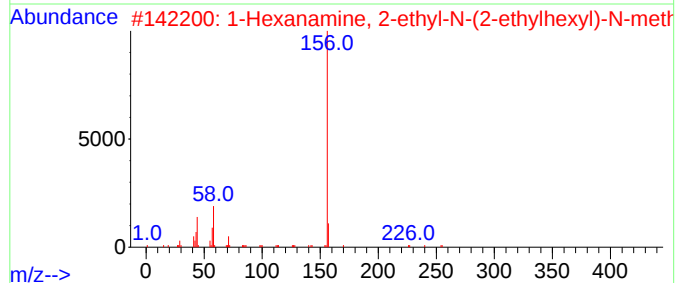
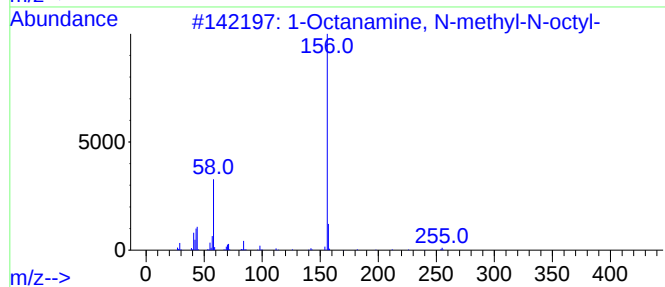
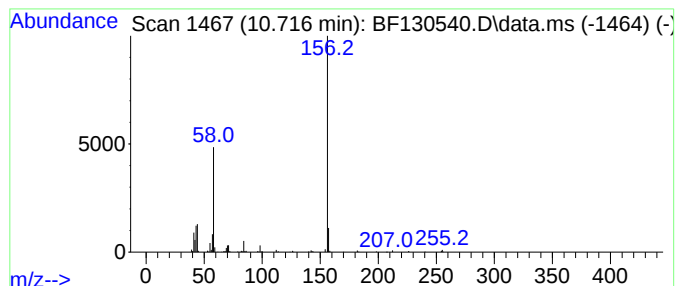
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Peak Number 5 1-Octanamine, N-methyl-N-oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.716	11.57 ng	256515	Phenanthrene-d10	11.145	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanamine, N-methyl-N-octyl-	255	C17H37N	004455-26-9	95
2	1-Hexanamine, 2-ethyl-N-(2-ethyl...	255	C17H37N	039168-98-4	58
3	Lauramide, N-(2-phenylethyl)-N-n...	429	C29H51NO	1000490-84-2	50
4	DL-Alanyl-DL-alanine, N,N'-dimet...	482	C27H50N2O5	1000392-74-9	50
5	l-Valine, N-allyloxycarbonyl-, h...	299	C16H29NO4	1000323-39-1	47



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257248-5

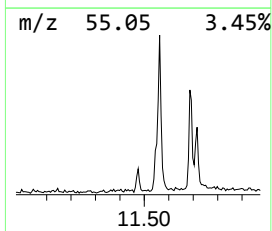
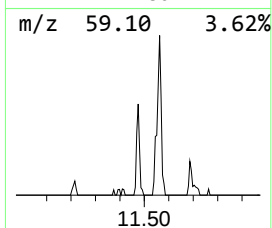
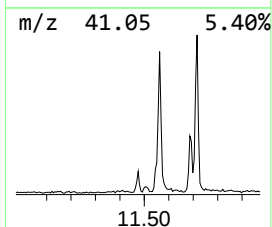
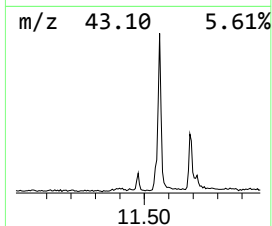
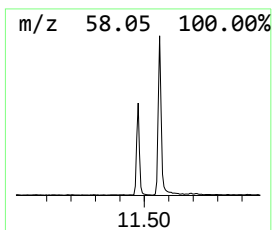
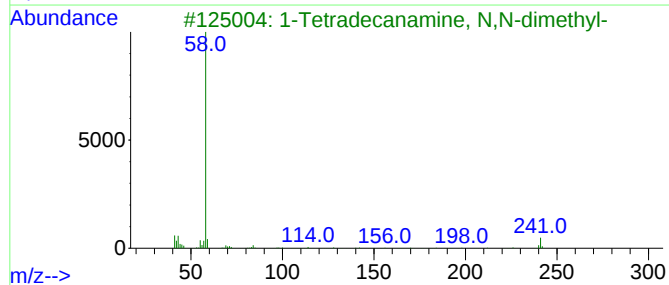
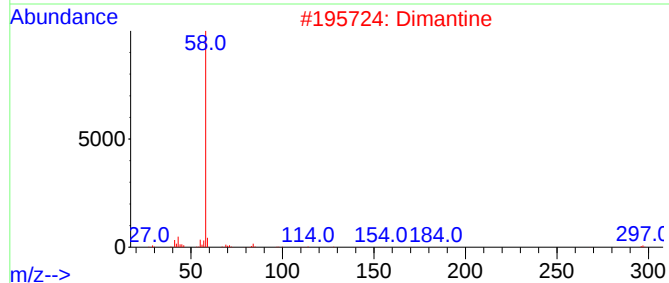
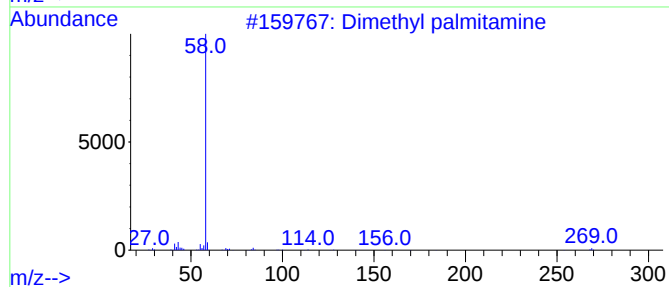
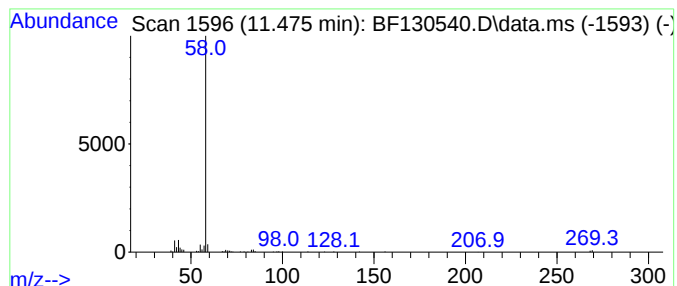
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dimethyl palmitamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	3.68 ng	81623	Phenanthrene-d10	11.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl palmitamine	269	C18H39N	000112-69-6	91
2			Dimantine	297	C20H43N	000124-28-7	78
3			1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	78
4			Cetrimonium Bromide	363	C19H42BrN	000057-09-0	78
5			Docosylamine, N,N-dimethyl-	353	C24H51N	1000406-30-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130540.D
Acq On : 05 Oct 2022 20:45
Operator : CG\JU
Sample : N4966-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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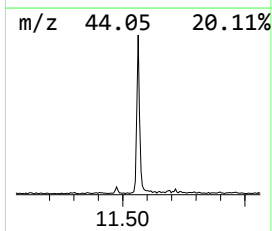
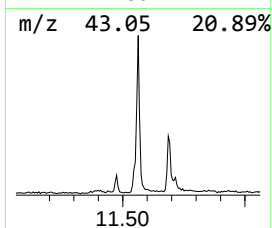
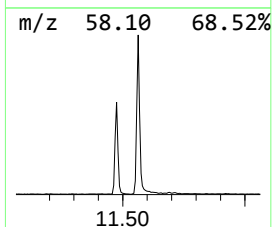
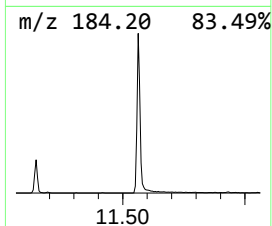
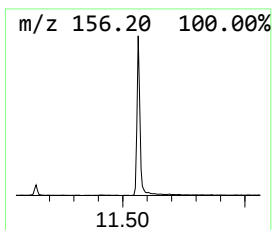
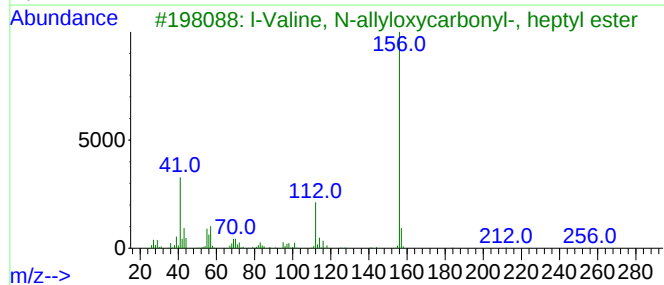
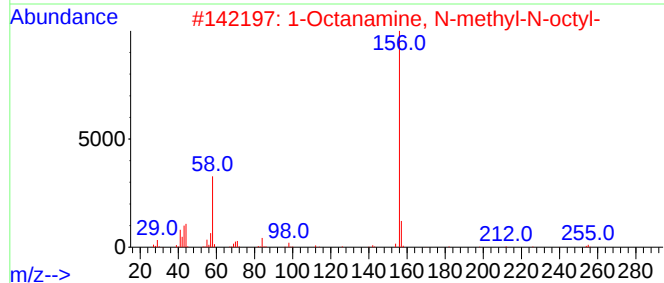
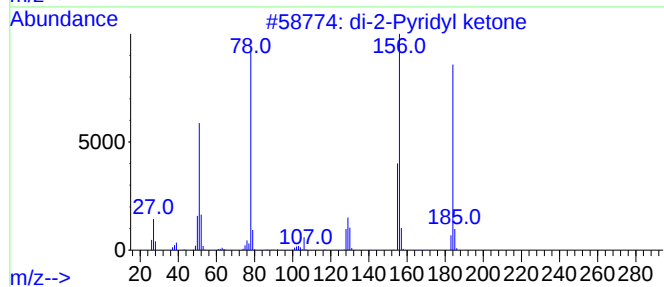
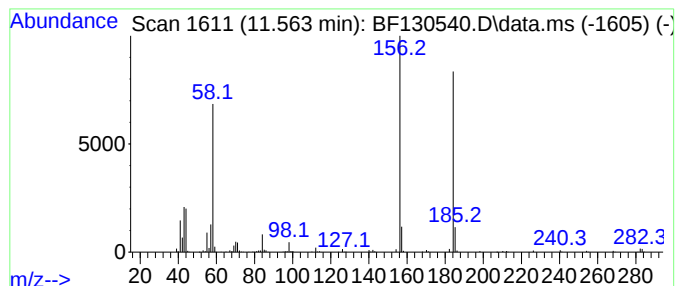
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 di-2-Pyridyl ketone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.563	32.69 ng	724754	Phenanthrene-d10	11.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-2-Pyridyl ketone	184	C11H8N2O	019437-26-4	50
2			1-Octanamine, N-methyl-N-octyl-	255	C17H37N	004455-26-9	38
3			l-Valine, N-allyloxycarbonyl-, h...	299	C16H29NO4	1000323-39-1	27
4			Lauramide, N-(2-phenylethyl)-N-n...	429	C29H51NO	1000490-84-2	27
5			1-Aminocyclopentanecarboxylic ac...	425	C25H47NO4	1010328-98-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130540.D
Acq On : 05 Oct 2022 20:45
Operator : CG\JU
Sample : N4966-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

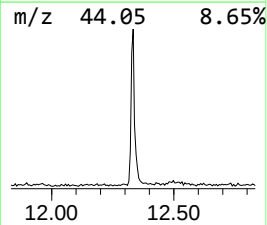
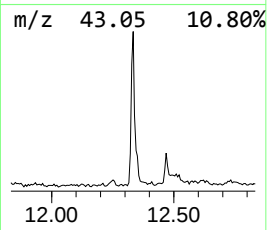
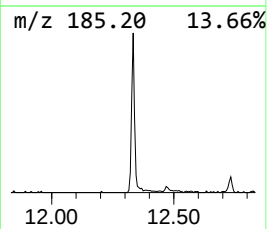
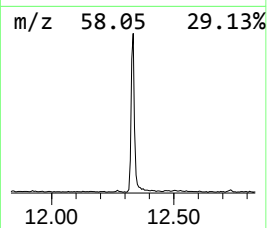
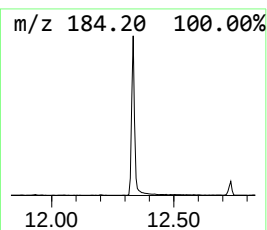
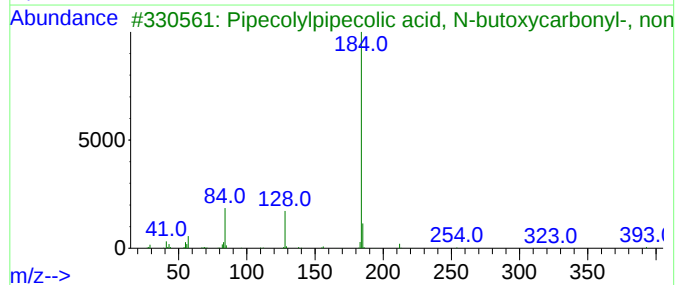
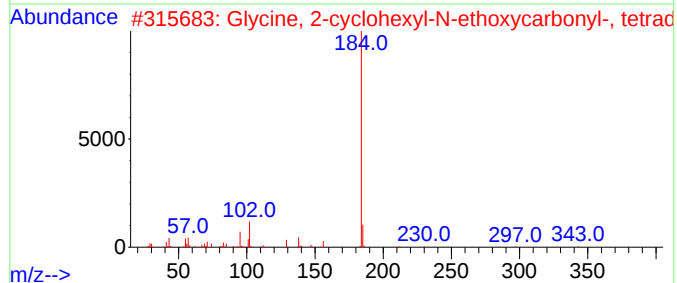
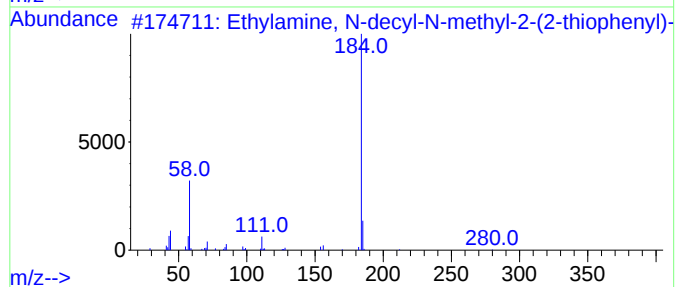
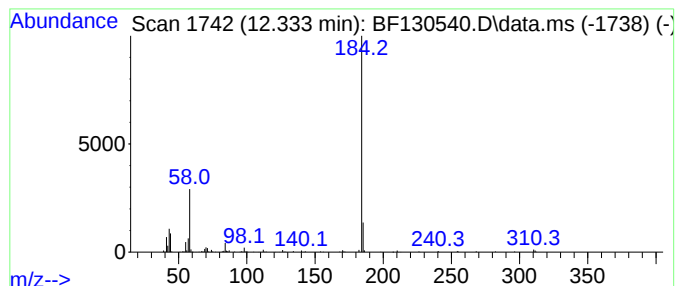
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethylamine, N-decyl-N-methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.333	23.06 ng	511330	Phenanthrene-d10	11.145	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylamine, N-decyl-N-methyl-2-(...	281	C17H31NS	1000310-34-4	72
2	Glycine, 2-cyclohexyl-N-ethoxyca...	425	C25H47NO4	1000383-09-0	53
3	Pipecolylpipecolic acid, N-butox...	466	C26H46N2O5	1000393-07-0	53
4	Pipecolic acid, N-butoxycarbonyl...	355	C20H37NO4	1000393-05-5	53
5	Pipecolic acid, N-butoxycarbonyl...	341	C19H35NO4	1010393-05-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130540.D
Acq On : 05 Oct 2022 20:45
Operator : CG\JU
Sample : N4966-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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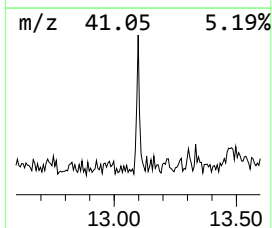
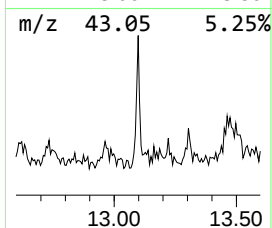
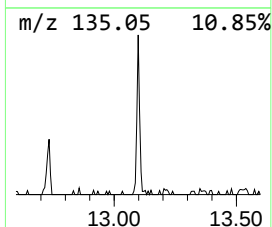
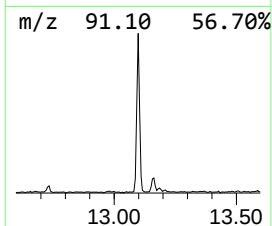
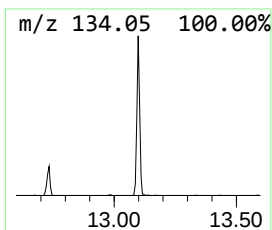
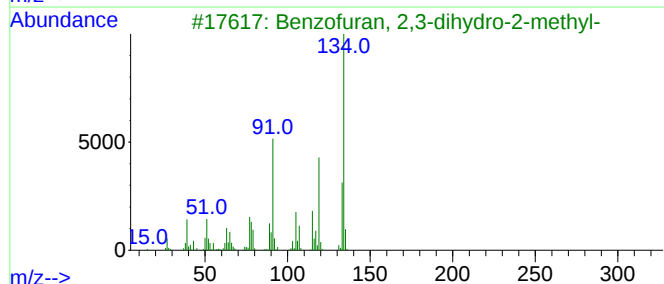
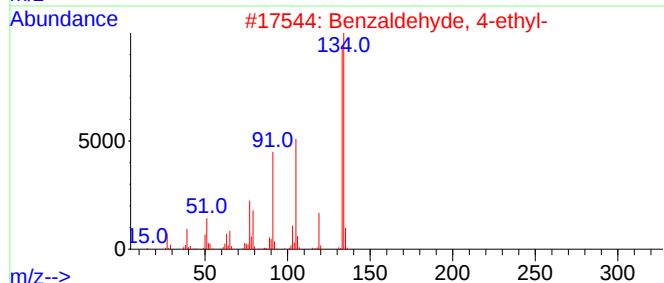
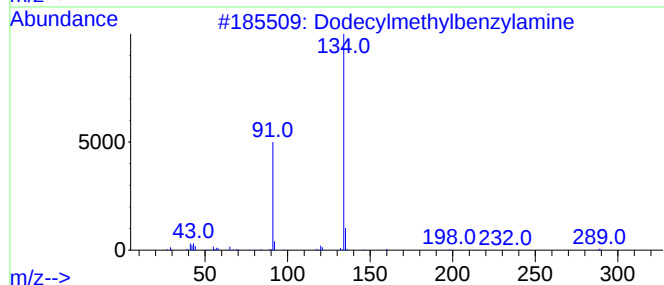
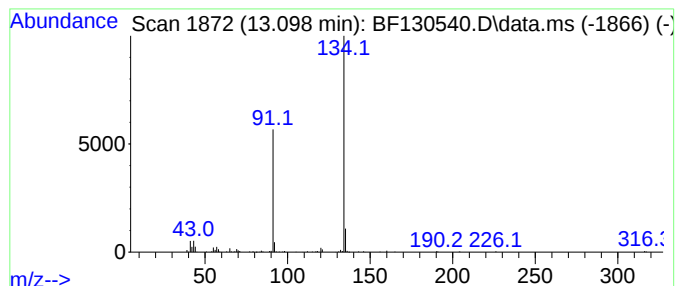
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecylmethylbenzylamine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	3.93 ng	129971	Chrysene-d12	13.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecylmethylbenzylamine	289	C20H35N	068397-57-9	86
2			Benzaldehyde, 4-ethyl-	134	C9H10O	004748-78-1	78
3			Benzofuran, 2,3-dihydro-2-methyl-	134	C9H10O	001746-11-8	72
4			2-[Benzyl(methyl)amino]ethanol, ...	279	C16H29NOSi	1000481-09-4	64
5			N-Methyl-N-benzyltetradecanamine	317	C22H39N	083690-72-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130540.D
Acq On : 05 Oct 2022 20:45
Operator : CG\JU
Sample : N4966-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.804	6.0	ng	175973	1	6.634	591296	20.0
Ethanol, 2-(2-b...	7.834	11.6	ng	320883	2	7.916	552977	20.0
1-Decanaminium,...	8.545	3.1	ng	87198	2	7.916	552977	20.0
1-Tetradecanami...	10.598	29.4	ng	652688	4	11.145	443448	20.0
1-Octanamine, N...	10.716	11.6	ng	256515	4	11.145	443448	20.0
Dimethyl palmit...	11.475	3.7	ng	81623	4	11.145	443448	20.0
di-2-Pyridyl ke...	11.563	32.7	ng	724754	4	11.145	443448	20.0
Ethylamine, N-d...	12.333	23.1	ng	511330	4	11.145	443448	20.0
Dodecylmethylbe...	13.098	3.9	ng	129971	5	13.774	662021	20.0