

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
 Data File : BF124851.D
 Acq On : 29 Jul 2021 15:03
 Operator : JU/CG
 Sample : M3206-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210590-AMENDED-COM-4

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124851.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	11	rBB	9978	11003	4.04%	0.720%
2	5.087	506	510	514	rBB	14245	15674	5.75%	1.026%
3	5.487	574	578	581	rBV	135887	130567	47.94%	8.546%
4	6.504	745	751	754	rBB	146590	162139	59.53%	10.613%
5	6.869	811	813	816	rBB	37848	29431	10.81%	1.926%
6	7.434	905	909	912	rBV	109736	109136	40.07%	7.143%
7	7.592	933	936	938	rBB	9484	8237	3.02%	0.539%
8	8.057	1011	1015	1018	rBV	69104	54199	19.90%	3.548%
9	8.151	1028	1031	1035	rBB	51397	42602	15.64%	2.788%
10	9.234	1210	1215	1218	rBV	241523	206415	75.78%	13.511%
11	9.304	1224	1227	1230	rBB	6339	5043	1.85%	0.330%
12	9.339	1231	1233	1236	rBB	5769	4455	1.64%	0.292%
13	9.875	1321	1324	1327	rBV	13825	16886	6.20%	1.105%
14	9.910	1327	1330	1333	rVB	69670	54154	19.88%	3.545%
15	10.704	1461	1465	1468	rBV	141200	127824	46.93%	8.367%
16	10.828	1482	1486	1489	rBB	40796	32545	11.95%	2.130%
17	11.269	1558	1561	1568	rBB	19408	17135	6.29%	1.122%
18	11.398	1579	1583	1586	rBV	80141	60580	22.24%	3.965%
19	11.786	1646	1649	1651	rVB	8653	6841	2.51%	0.448%
20	11.916	1669	1671	1674	rBV2	13980	11410	4.19%	0.747%
21	12.492	1766	1769	1772	rBV	19382	14490	5.32%	0.948%
22	12.575	1781	1783	1787	rVB2	4033	3085	1.13%	0.202%
23	12.698	1800	1804	1810	rBV3	3393	3988	1.46%	0.261%
24	12.986	1849	1853	1856	rBV	288811	272380	100.00%	17.828%
25	13.533	1943	1946	1947	rBV3	3204	2888	1.06%	0.189%
26	13.880	2001	2005	2017	rBV2	13211	24746	9.09%	1.620%
27	14.010	2024	2027	2029	rBV	3038	3007	1.10%	0.197%
28	14.039	2029	2032	2035	rVB	63711	49313	18.10%	3.228%
29	14.498	2107	2110	2113	rBV	3147	3251	1.19%	0.213%
30	14.804	2158	2162	2166	rBV2	3049	3775	1.39%	0.247%
31	15.515	2278	2283	2288	rBB2	32341	40606	14.91%	2.658%

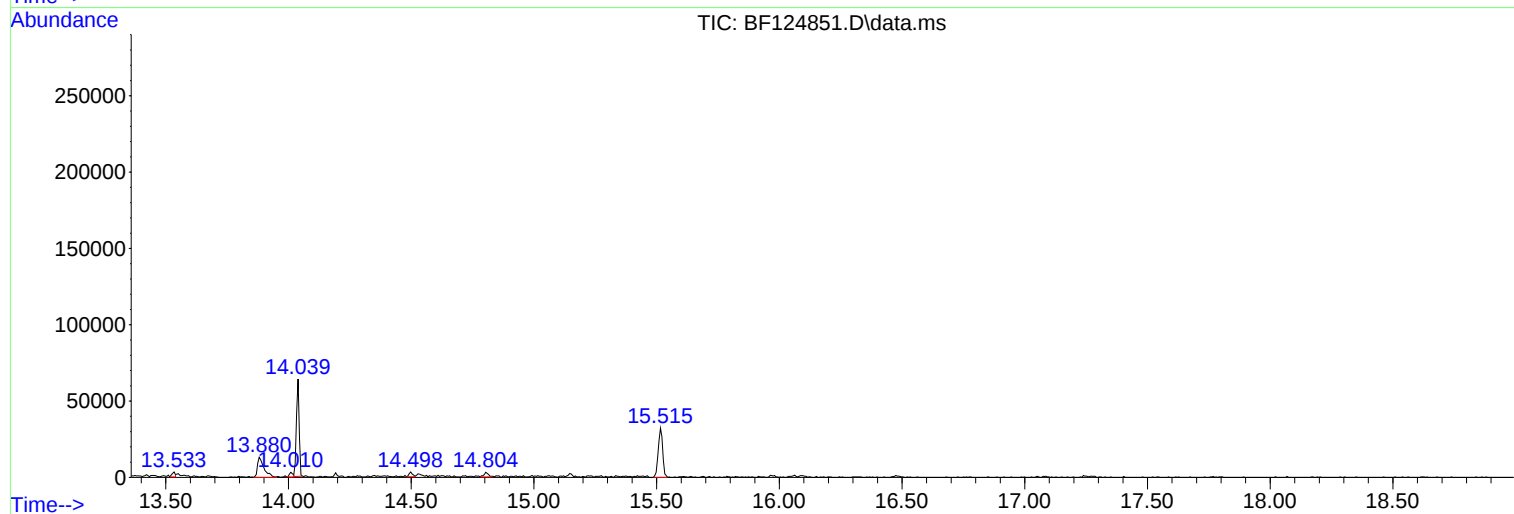
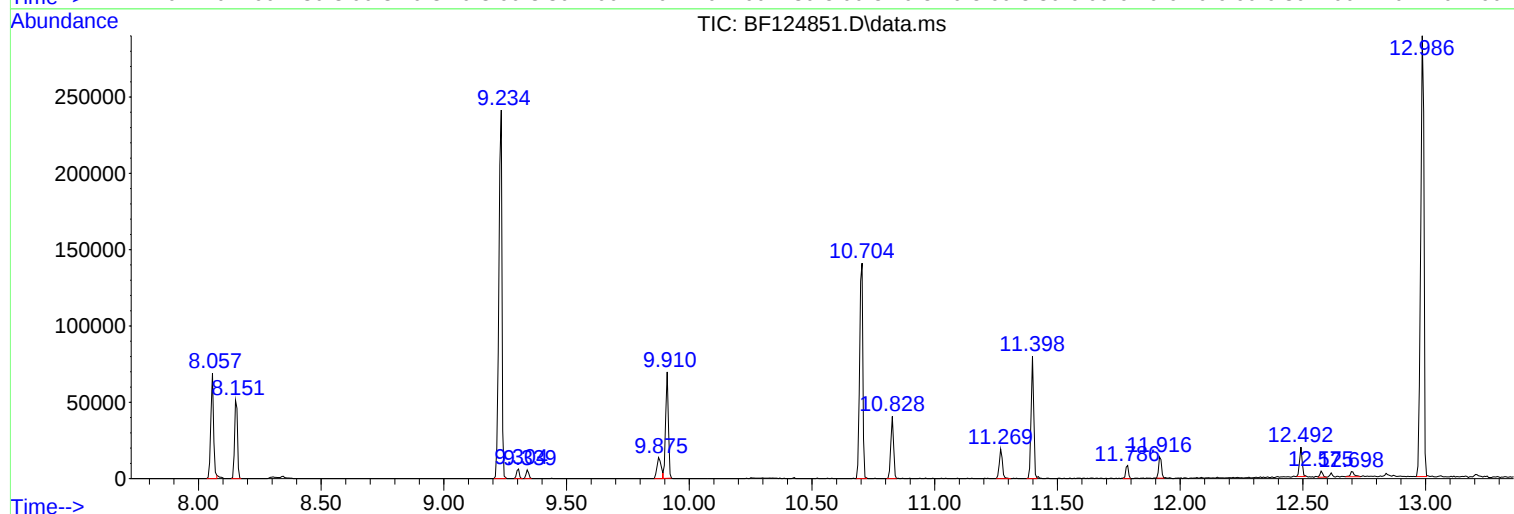
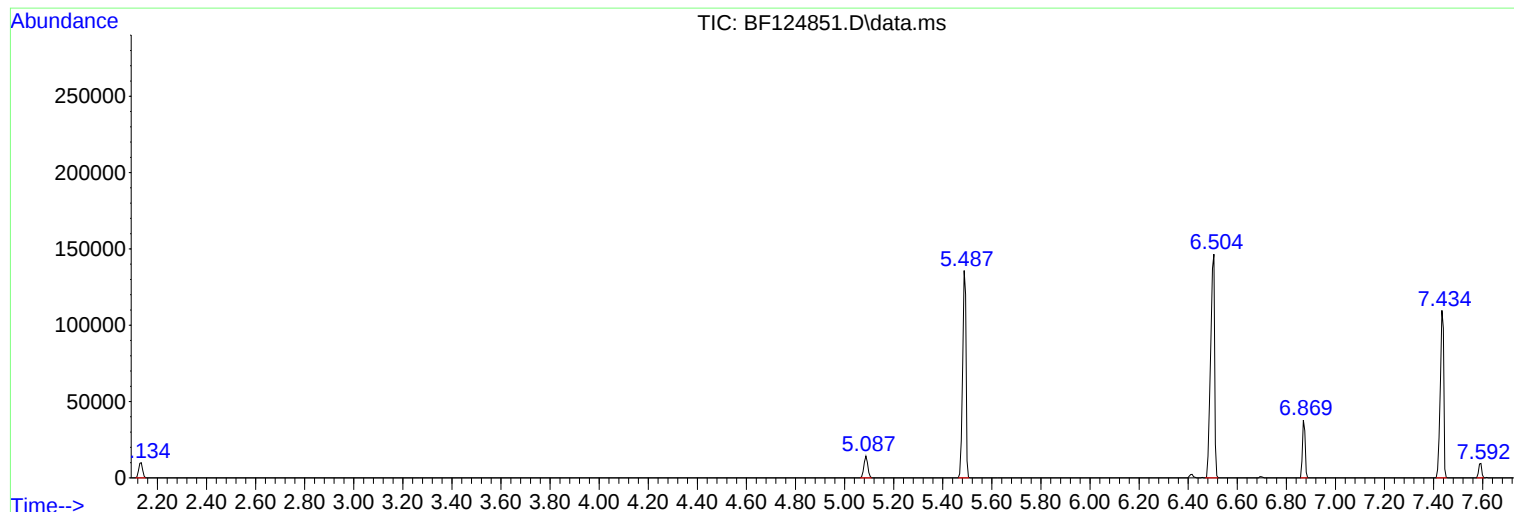
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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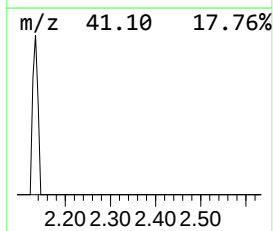
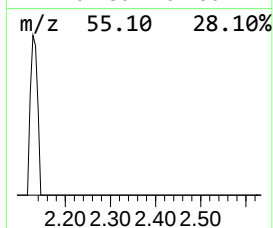
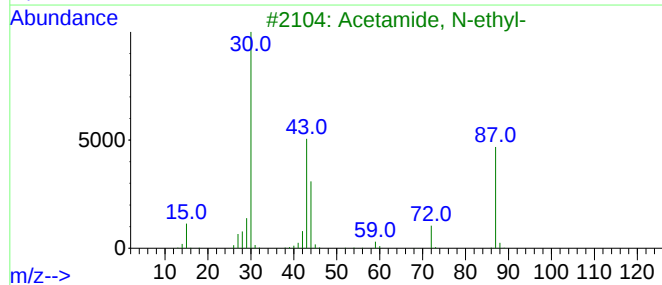
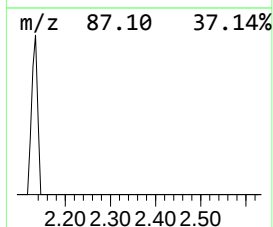
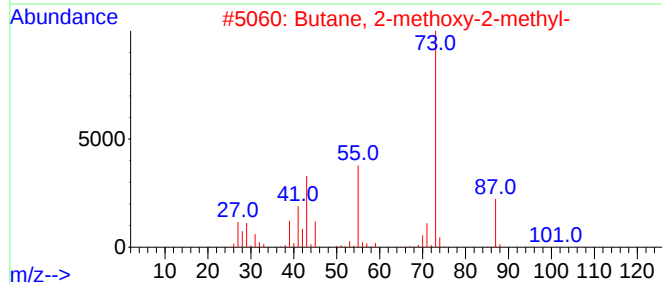
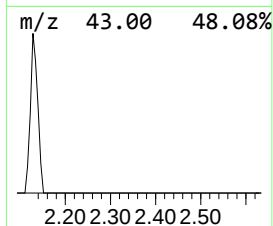
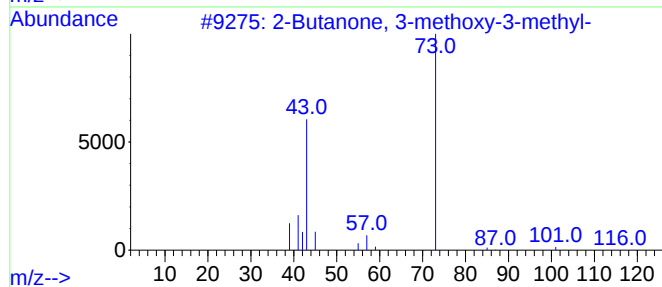
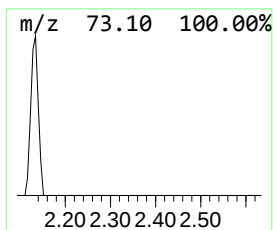
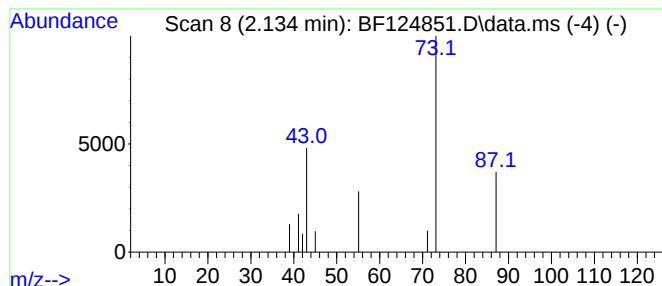
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.134 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	7.48 ng	11003	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9		
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9		
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5		
4	Isobutylamine	73	C4H11N	000078-81-9	5		
5	N-Ethylformamide	73	C3H7NO	000627-45-2	4		



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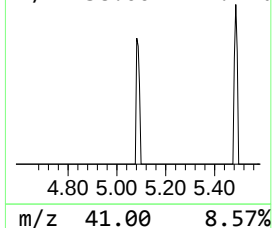
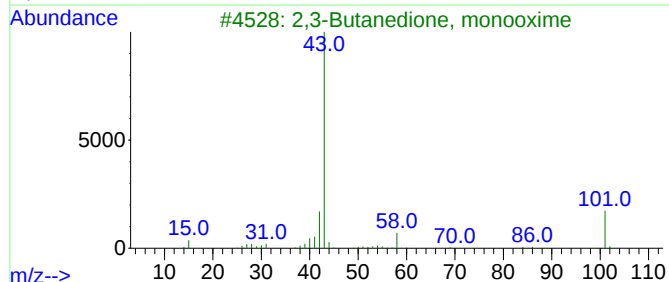
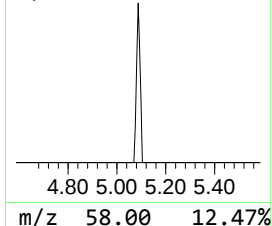
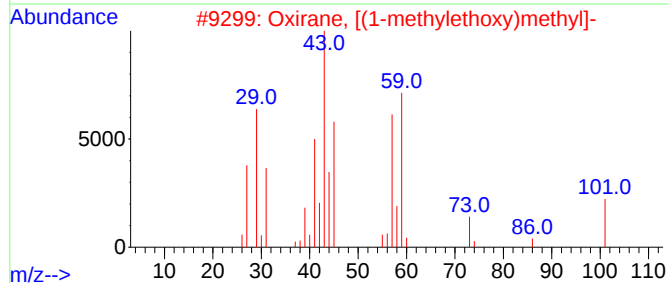
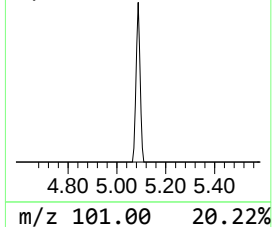
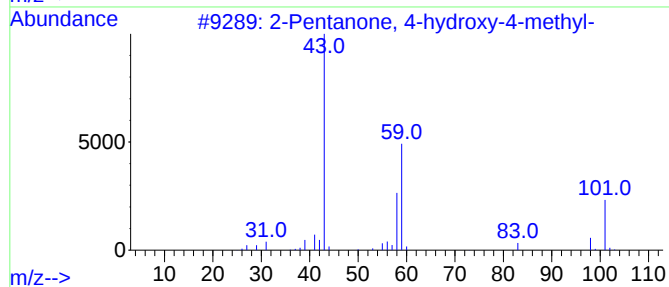
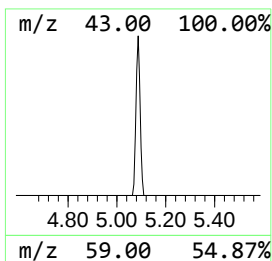
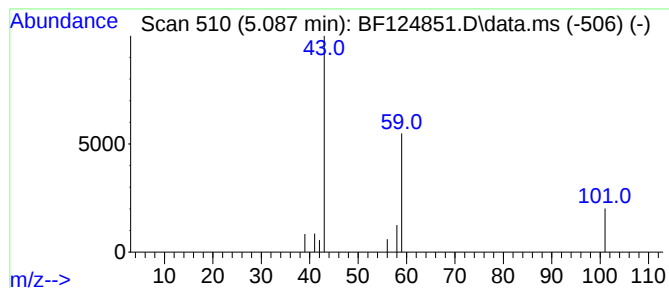
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.087	10.65 ng	15674	1,4-Dichlorobenzene-d4			6.869
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	43
2	Oxirane, [(1-methylethoxy)methyl]-		116	C6H12O2	004016-14-2	9
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	7
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	5
5	N-(n-Propyl)acetamide		101	C5H11NO	005331-48-6	4



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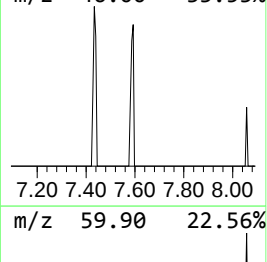
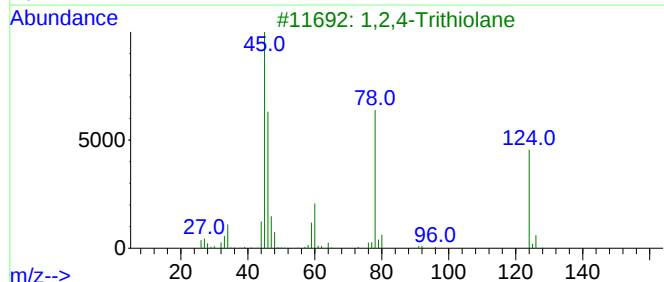
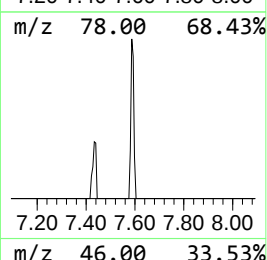
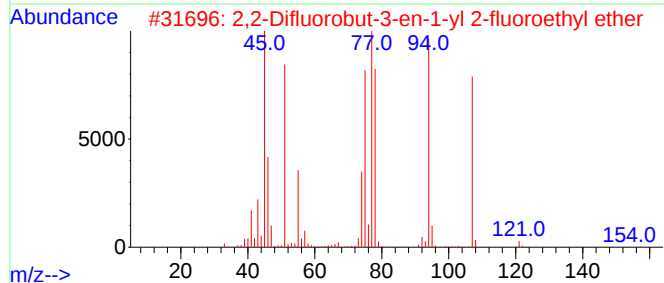
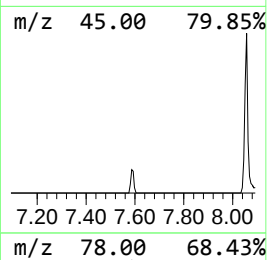
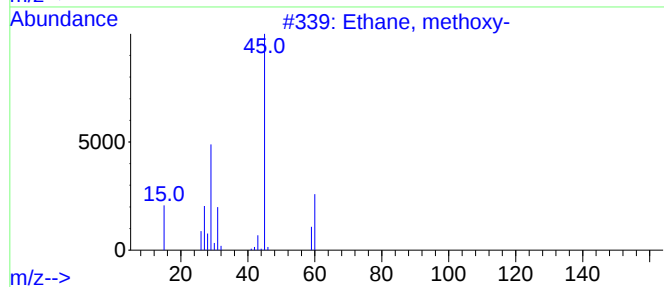
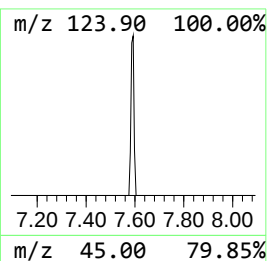
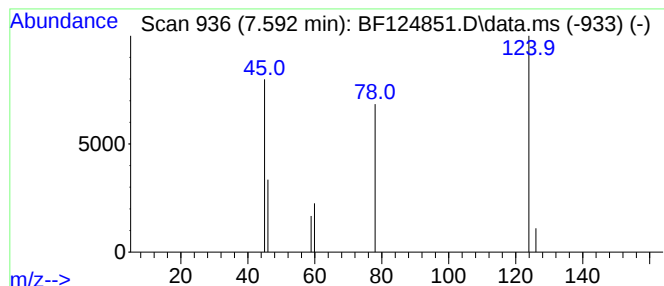
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.592 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.592	3.87 ng	8237	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, methoxy-	60	C3H8O	000540-67-0	9
2			2,2-Difluorobut-3-en-1-yl 2-fluo...	154	C6H9F3O	1000394-29-3	9
3			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	9
4			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	7
5			Carbonochloridothioic acid, S-et...	124	C3H5ClOS	002941-64-2	7



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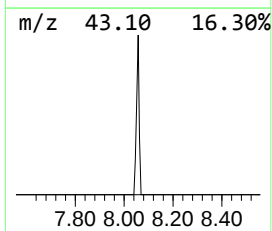
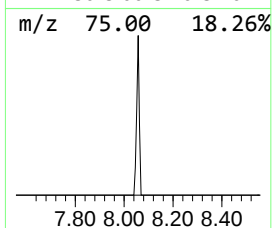
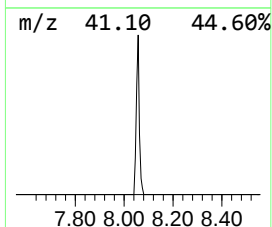
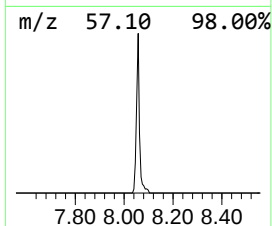
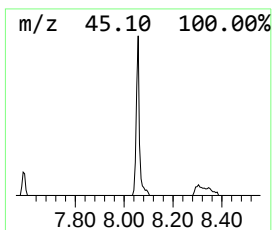
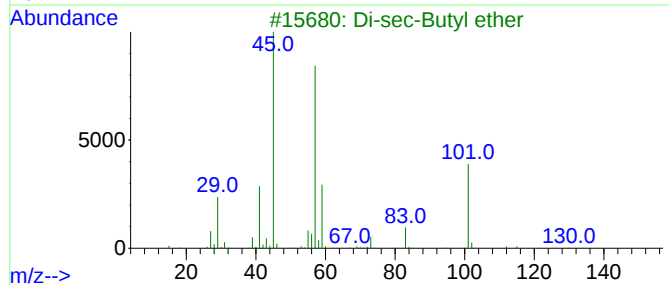
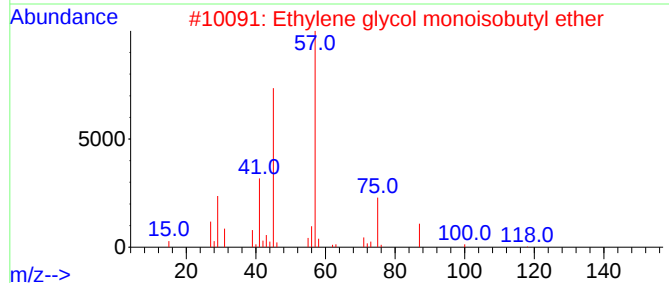
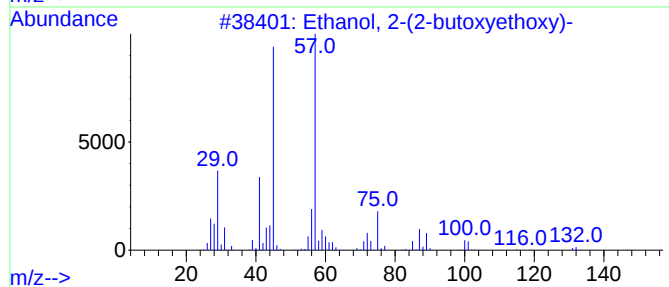
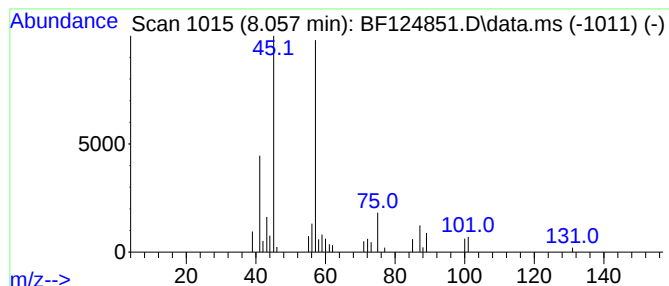
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	25.44 ng	54199	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	45



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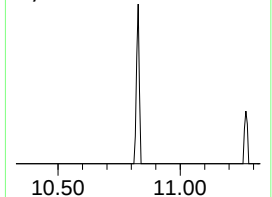
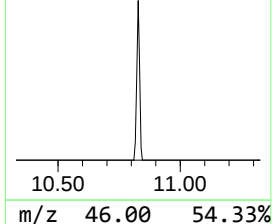
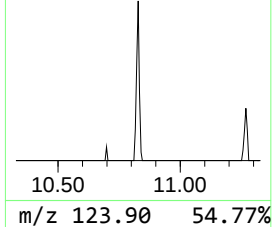
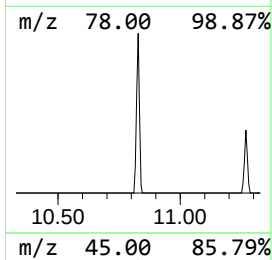
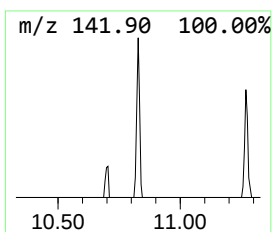
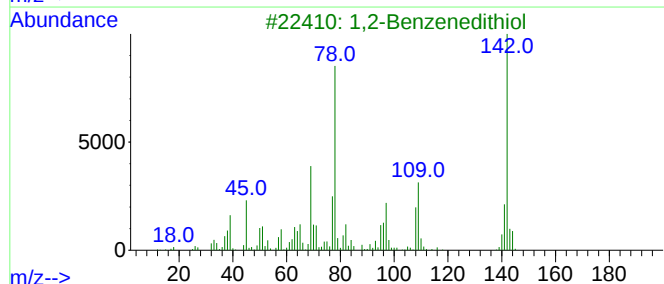
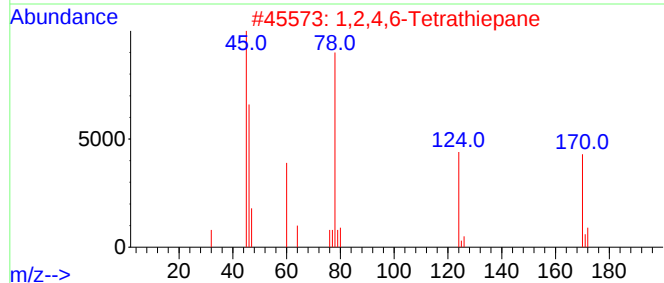
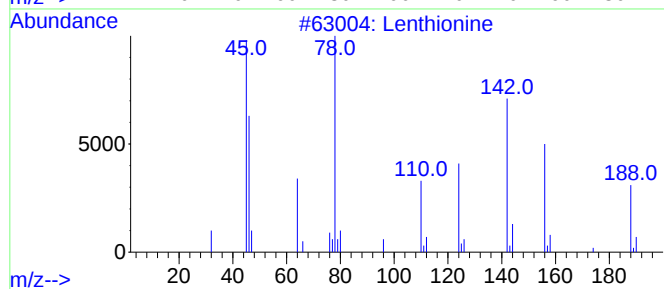
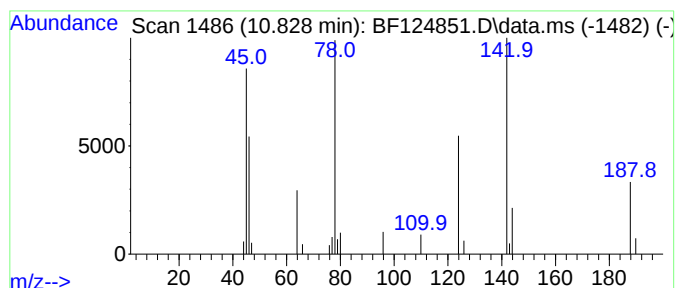
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Lenthionine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	10.74 ng	32545	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	87
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	59
3			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	59
4			Thiophene-2-carboxaldehyde, 3-me...	142	C6H6O2S	035134-07-7	10
5			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	10



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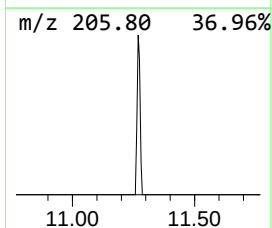
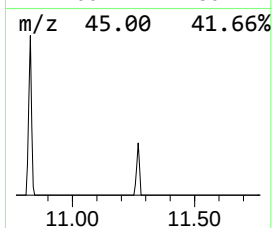
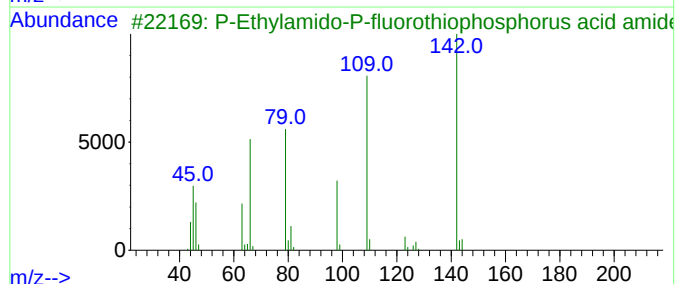
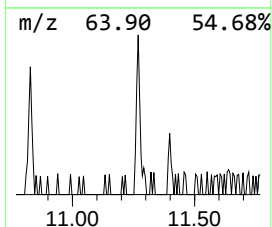
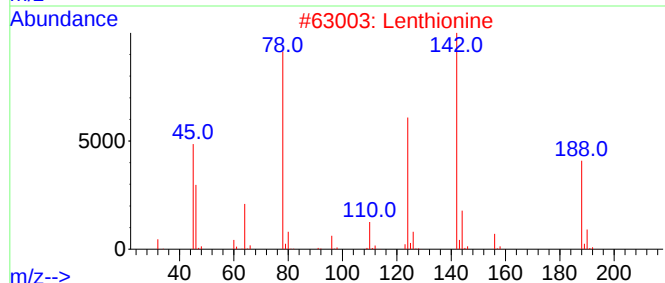
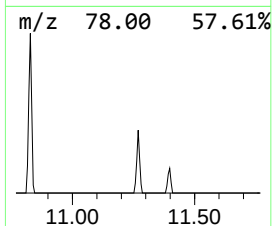
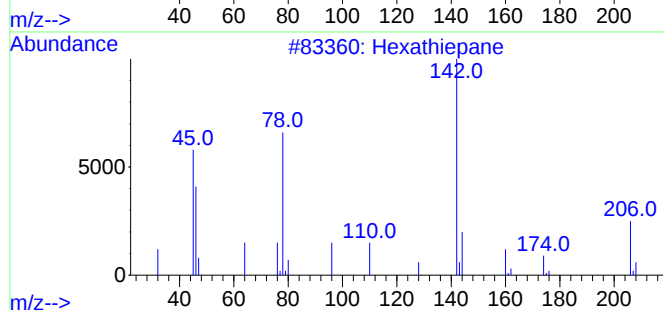
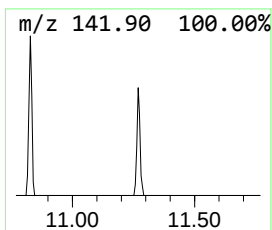
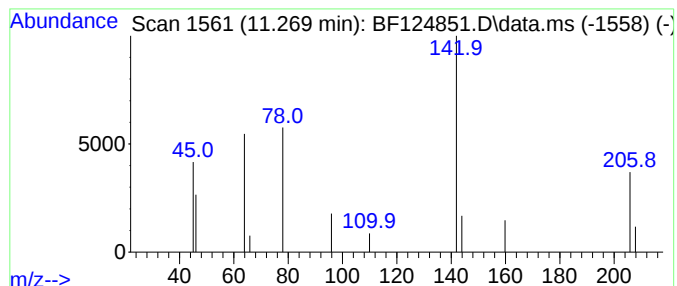
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.269 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	5.66 ng	17135	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiepane	206	CH2S6	017233-71-5	35
2			Lenthionine	188	C2H4S5	000292-46-6	27
3			P-Ethylamido-P-fluorothiophospho...	142	C2H8FN2PS	1000311-29-7	10
4			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9
5			1,3-Benzenedithiol	142	C6H6S2	000626-04-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124851.D
Acq On : 29 Jul 2021 15:03
Operator : JU/CG
Sample : M3206-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210590-AMENDED-COM-4

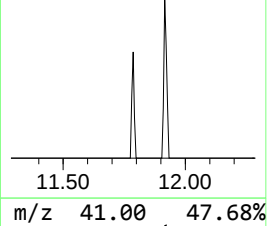
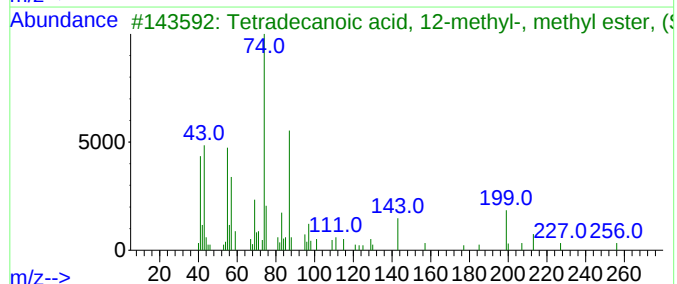
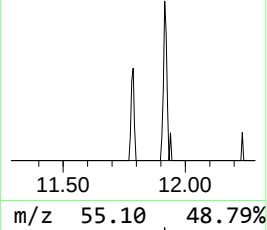
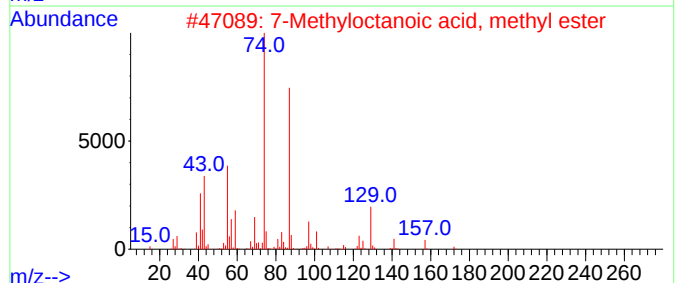
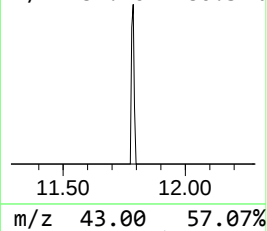
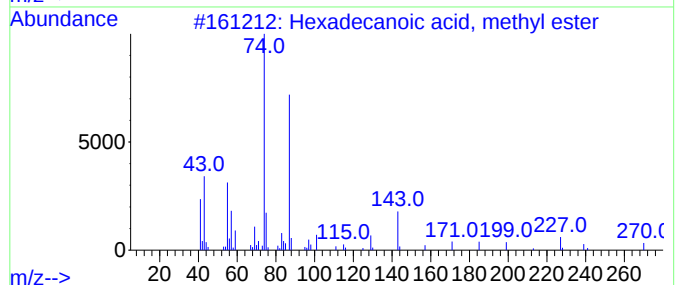
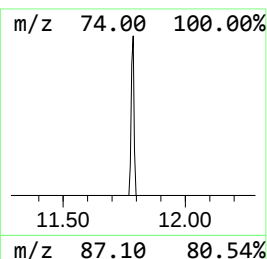
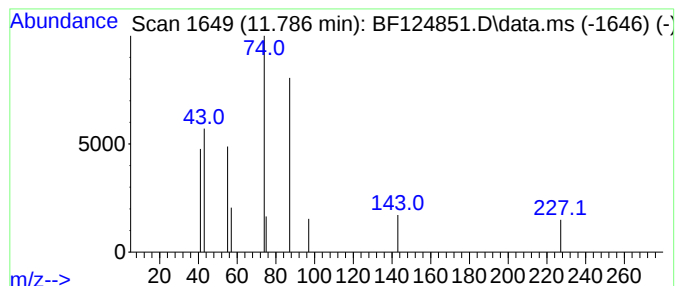
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	2.26 ng	6841	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	74
2			7-Methyloctanoic acid, methyl ester	172	C10H20O2	005129-53-3	56
3			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	062691-05-8	43
4			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	9
5			Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124851.D
Acq On : 29 Jul 2021 15:03
Operator : JU/CG
Sample : M3206-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210590-AMENDED-COM-4

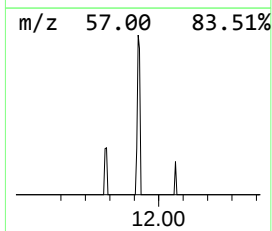
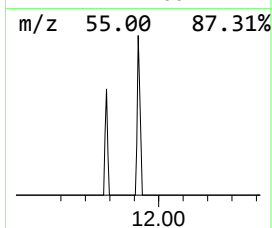
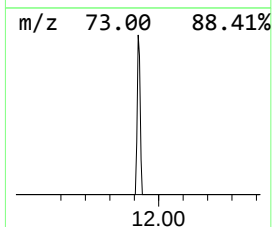
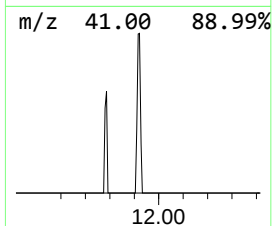
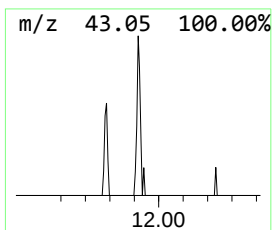
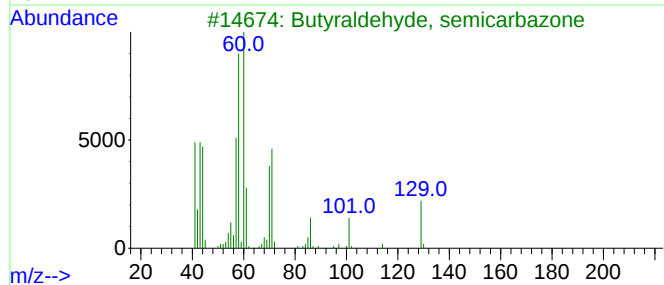
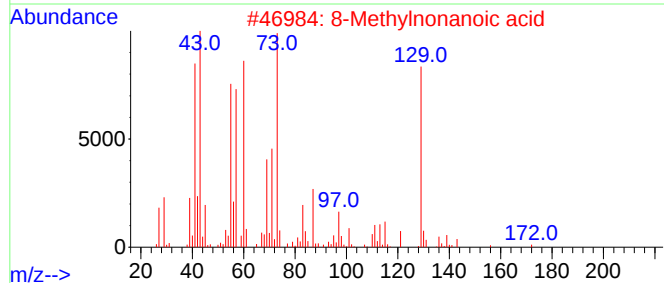
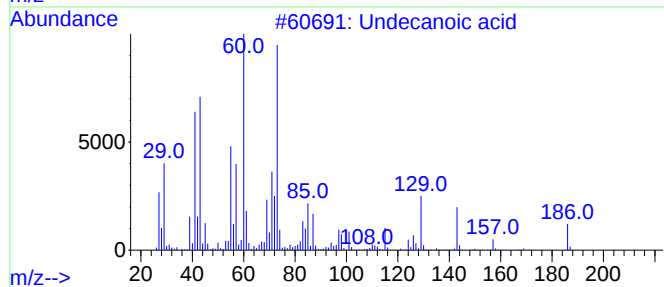
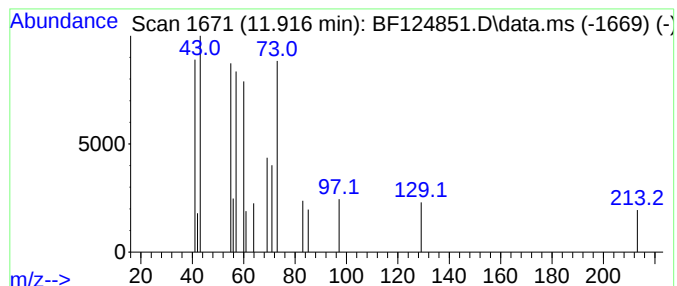
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.77 ng	11410	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	53
2			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50
3			Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	46
4			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	27
5			Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124851.D
Acq On : 29 Jul 2021 15:03
Operator : JU/CG
Sample : M3206-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210590-AMENDED-COM-4

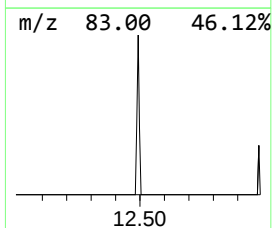
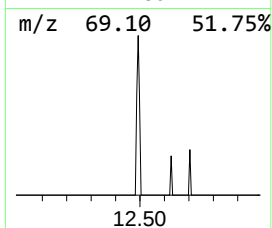
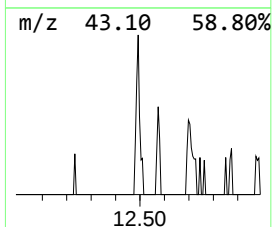
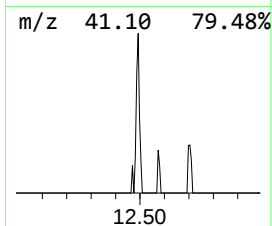
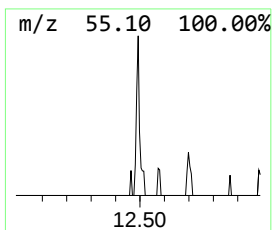
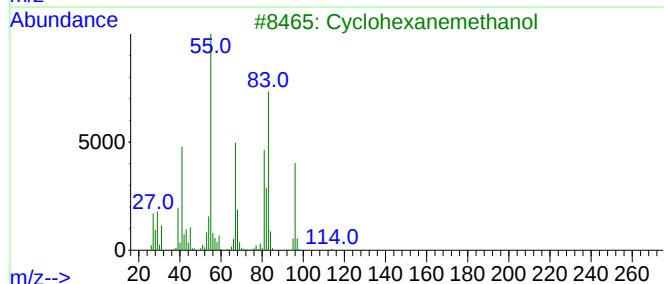
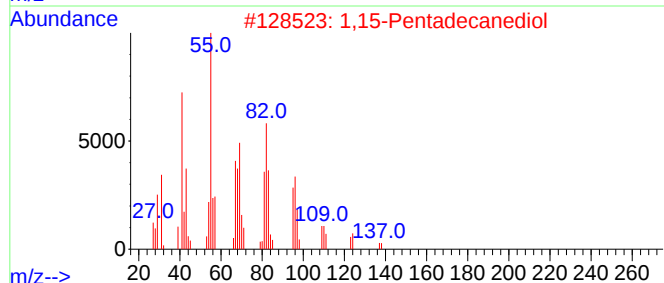
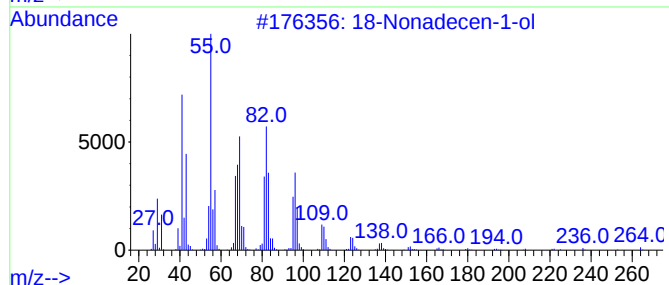
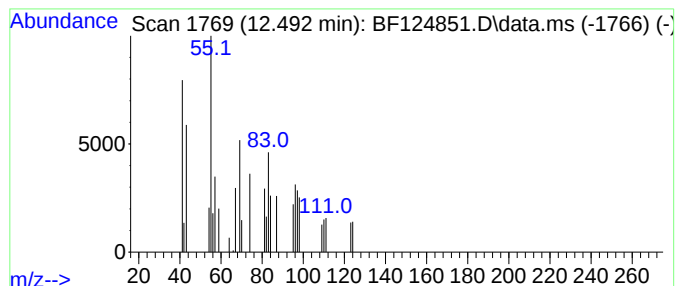
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.492 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	4.78 ng	14490	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Nonadecen-1-ol			282	C19H38O	1000142-89-2	38
2	1,15-Pentadecanediol			244	C15H32O2	014722-40-8	27
3	Cyclohexanemethanol			114	C7H14O	000100-49-2	27
4	Octanenitrile			125	C8H15N	000124-12-9	27
5	1-Decanol			158	C10H22O	000112-30-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124851.D
Acq On : 29 Jul 2021 15:03
Operator : JU/CG
Sample : M3206-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210590-AMENDED-COM-4

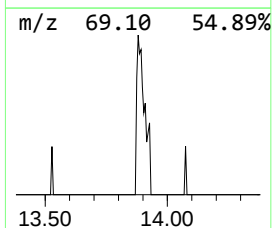
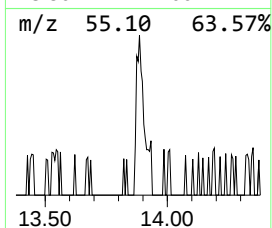
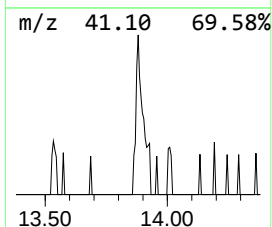
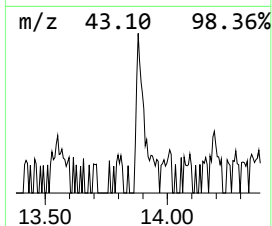
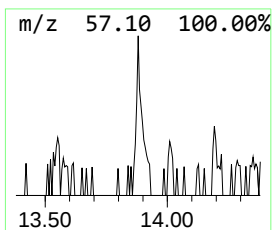
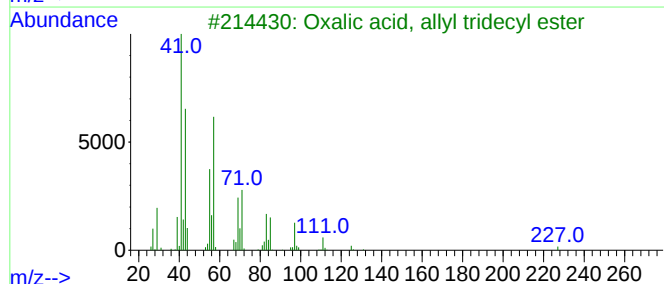
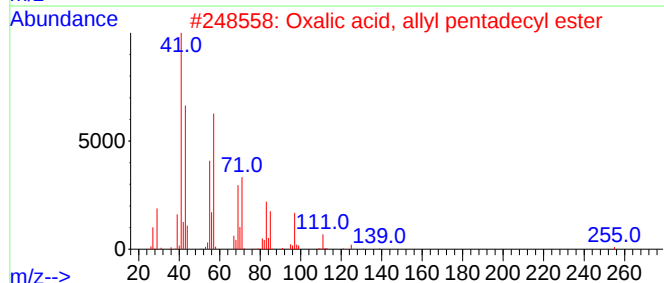
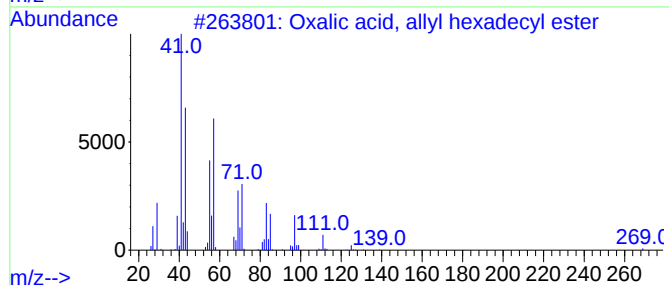
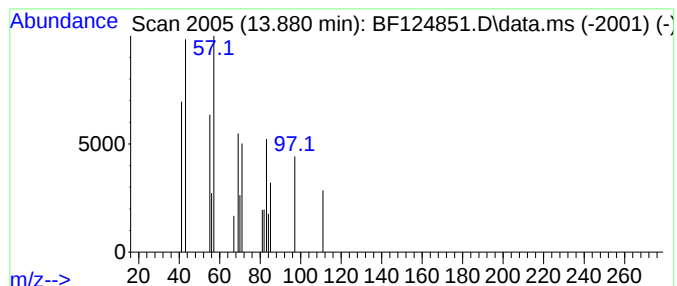
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, allyl hexadecy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.04 ng	24746	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	72
2			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	72
3			Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	59
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	53
5			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124851.D
Acq On : 29 Jul 2021 15:03
Operator : JU/CG
Sample : M3206-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210590-AMENDED-COM-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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
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unknown7.592	7.592	3.9	ng	8237	2	8.151	42602	20.0
Ethanol, 2-(2-b...	8.057	25.4	ng	54199	2	8.151	42602	20.0
Lenthionine	10.828	10.7	ng	32545	4	11.398	60580	20.0
unknown11.269	11.269	5.7	ng	17135	4	11.398	60580	20.0
Hexadecanoic ac...	11.786	2.3	ng	6841	4	11.398	60580	20.0
Undecanoic acid	11.916	3.8	ng	11410	4	11.398	60580	20.0
unknown12.492	12.492	4.8	ng	14490	4	11.398	60580	20.0
Oxalic acid, al...	13.880	10.0	ng	24746	5	14.039	49313	20.0