

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032422\
 Data File : BF127510.D
 Acq On : 24 Mar 2022 18:49
 Operator : CG\JU
 Sample : N2090-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-46

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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127510.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	471	474	488	rBV	32515	48280	1.48%	0.280%
2	5.475	538	542	564	rBV	1165703	1365742	42.00%	7.933%
3	6.481	711	713	732	rBV	857453	932588	28.68%	5.417%
4	6.845	772	775	783	rBV	643895	512119	15.75%	2.975%
5	7.416	868	872	875	rBV	2050096	1943617	59.78%	11.289%
6	8.028	974	976	990	rBV	179537	265103	8.15%	1.540%
7	8.128	990	993	1002	rVB	783597	657103	20.21%	3.817%
8	9.204	1172	1176	1179	rBV	3697911	3251383	100.00%	18.885%
9	9.310	1191	1194	1203	rVB	320415	286558	8.81%	1.664%
10	9.686	1254	1258	1269	rBV4	14548	35376	1.09%	0.205%
11	9.886	1288	1292	1295	rBV	839038	751373	23.11%	4.364%
12	10.680	1423	1427	1438	rBV	2125695	1978131	60.84%	11.490%
13	11.374	1542	1545	1550	rBV	870942	717944	22.08%	4.170%
14	11.751	1606	1609	1612	rBV	98480	71307	2.19%	0.414%
15	11.927	1636	1639	1643	rVB	39403	35413	1.09%	0.206%
16	12.439	1720	1726	1727	rBV4	27343	40984	1.26%	0.238%
17	12.457	1727	1729	1739	rVB	255959	227162	6.99%	1.319%
18	12.545	1741	1744	1747	rVB	133347	106140	3.26%	0.616%
19	12.963	1810	1815	1818	rBV	2710094	2563239	78.84%	14.888%
20	13.174	1846	1851	1857	rBV3	40397	89702	2.76%	0.521%
21	13.392	1882	1888	1892	rBV2	109102	112375	3.46%	0.653%
22	13.804	1954	1958	1961	rBV	33846	43092	1.33%	0.250%
23	13.845	1961	1965	1967	rVV	48591	61658	1.90%	0.358%
24	13.880	1968	1971	1979	rVB	86961	111891	3.44%	0.650%
25	14.021	1992	1995	2005	rBV	522199	501429	15.42%	2.912%
26	15.504	2243	2247	2256	rVB	408582	506911	15.59%	2.944%

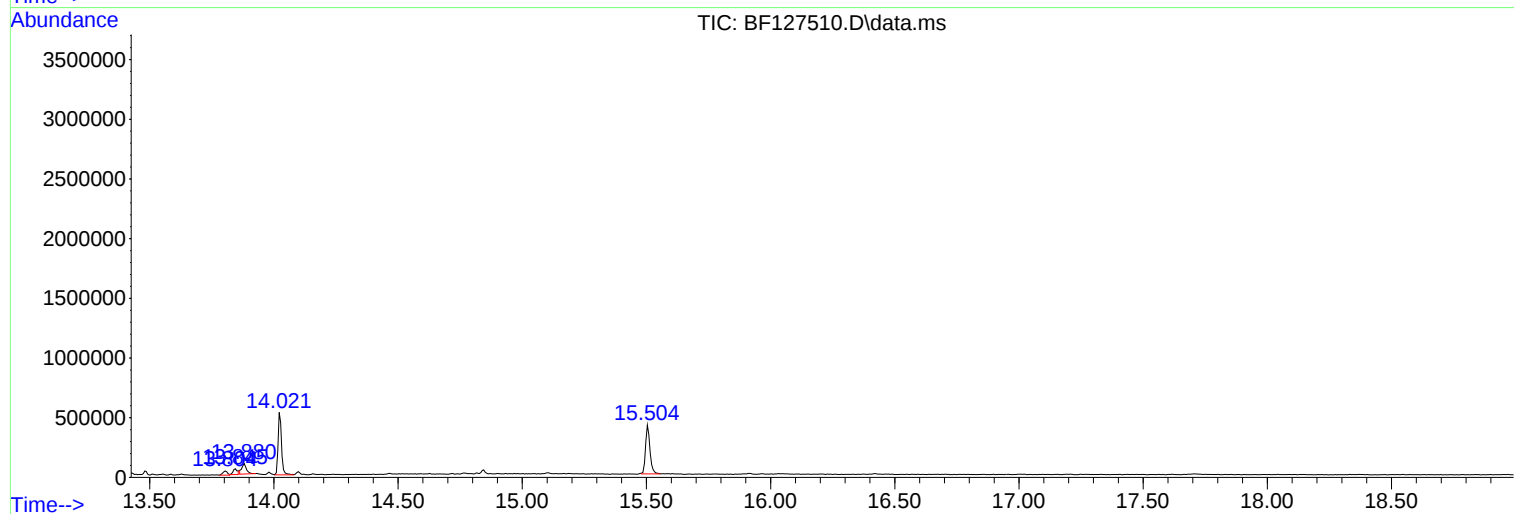
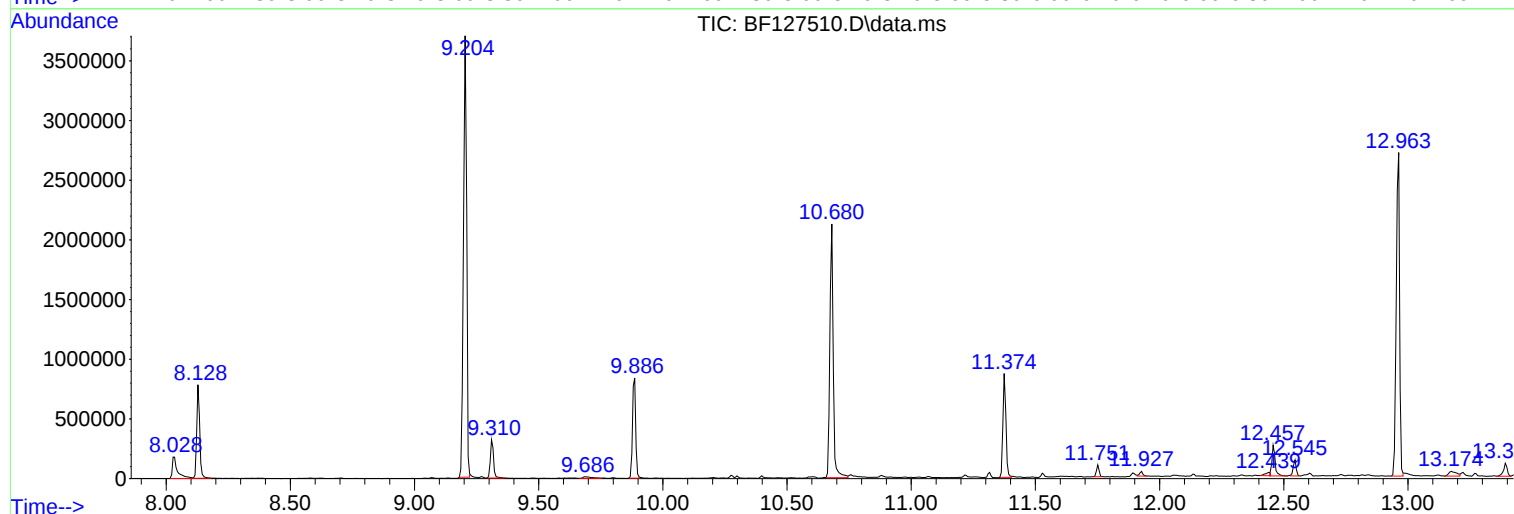
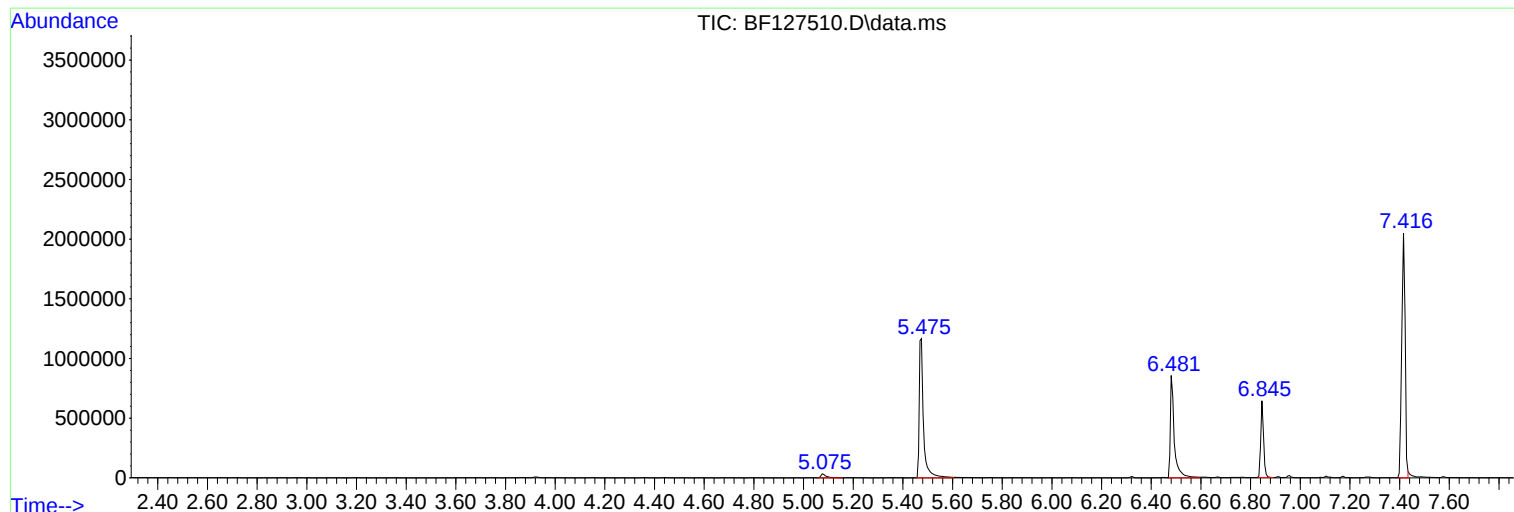
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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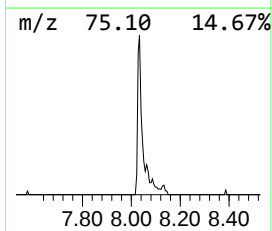
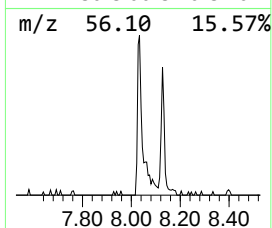
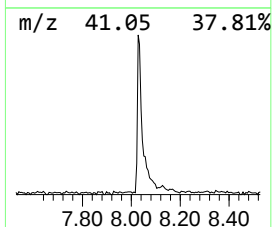
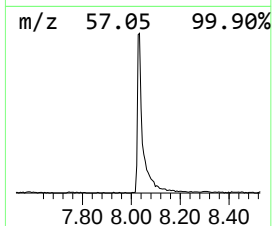
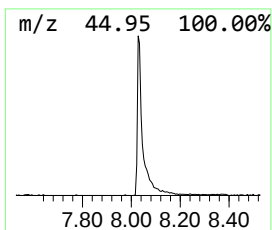
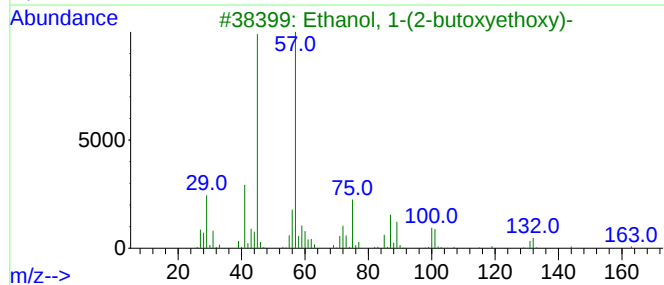
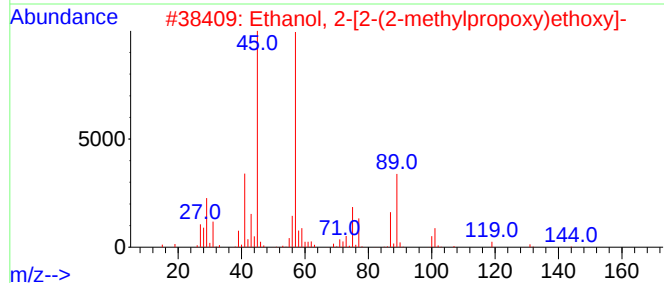
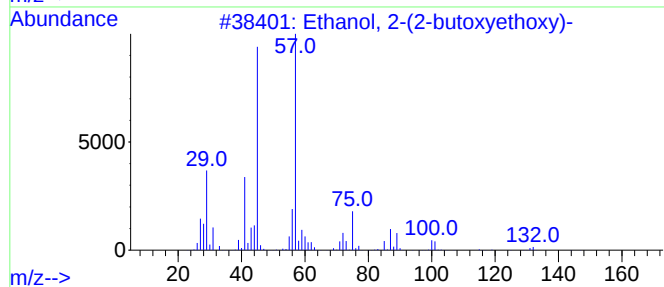
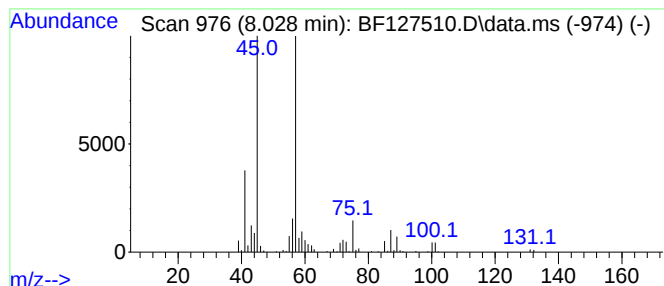
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	8.07 ng	265103	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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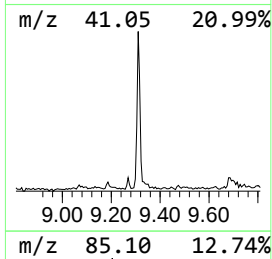
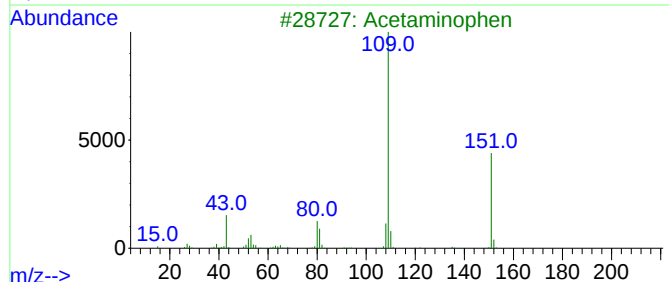
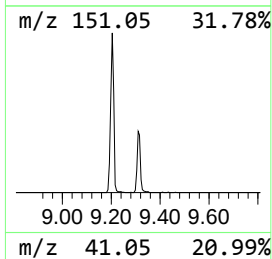
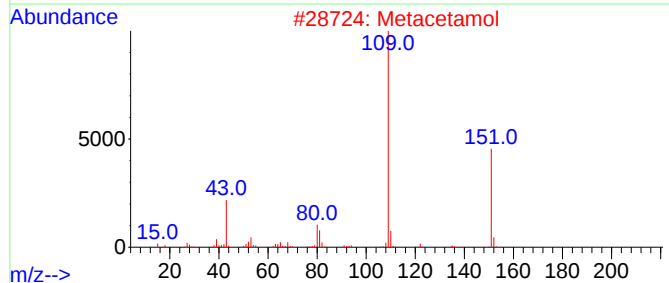
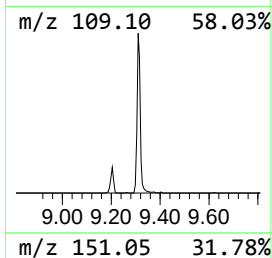
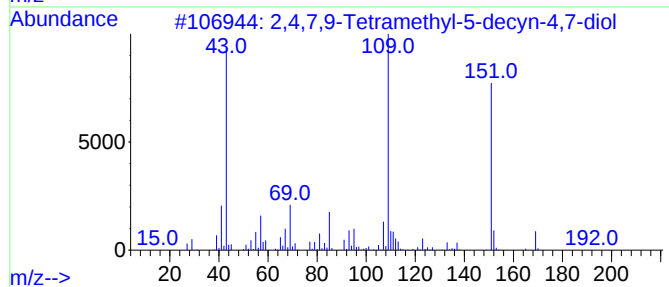
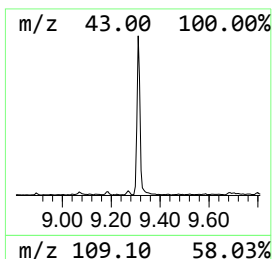
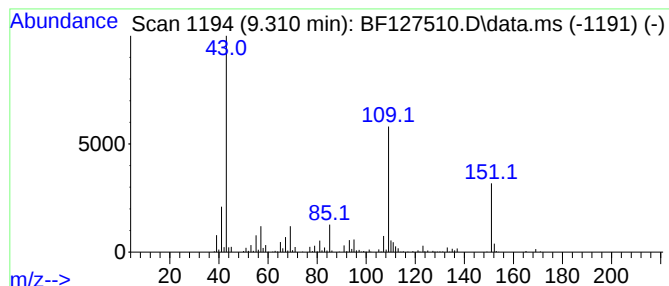
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.310	7.63 ng	286558	Acenaphthene-d10	9.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Metacetamol	151	C8H9NO2	000621-42-1	49	
3	Acetaminophen	151	C8H9NO2	000103-90-2	47	
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	42	
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	38	



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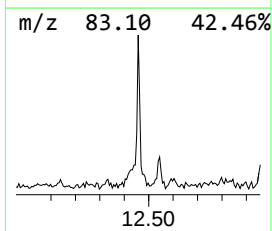
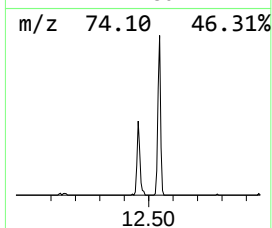
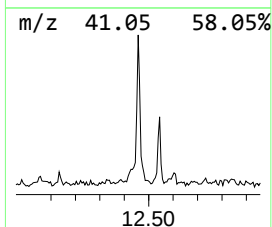
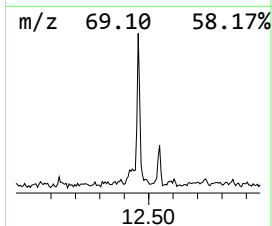
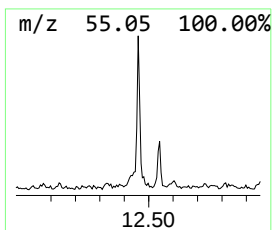
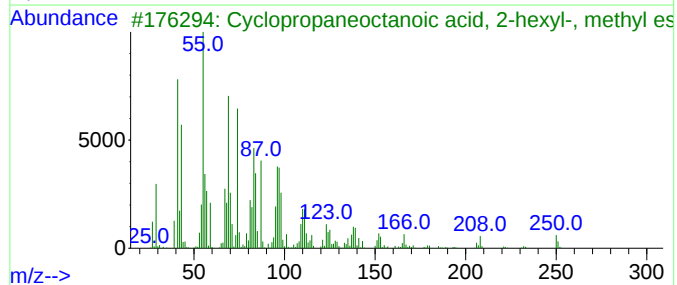
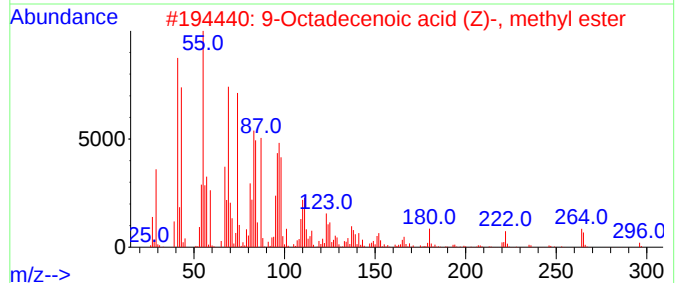
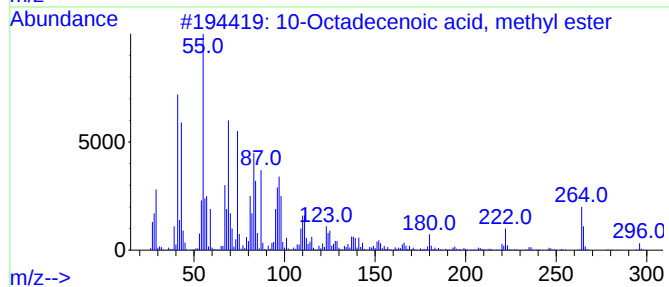
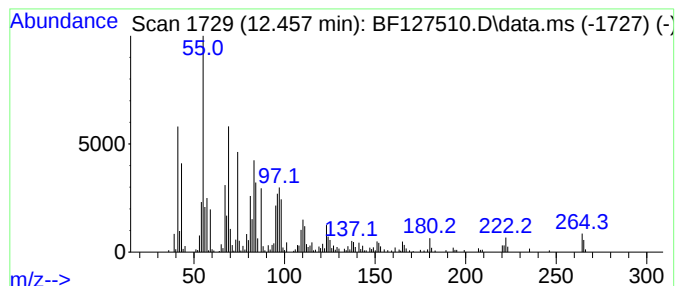
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Peak Number 3 10-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	6.33 ng	227162	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
3			Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
4			7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	87
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	86



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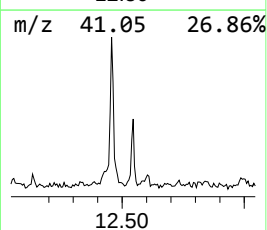
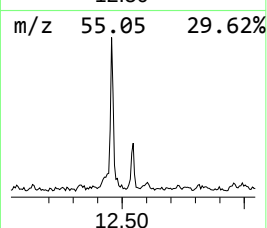
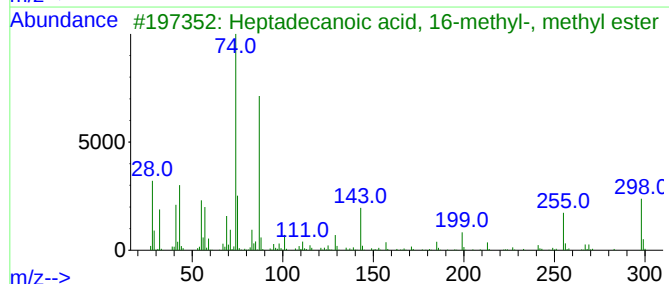
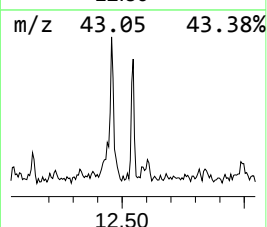
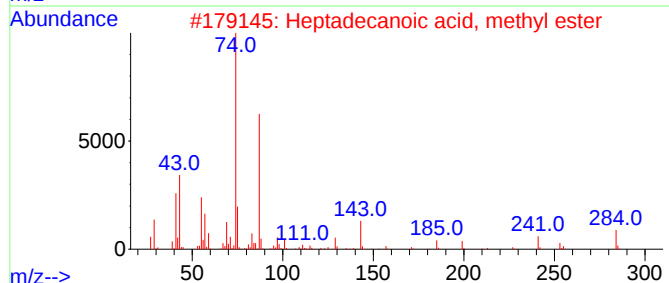
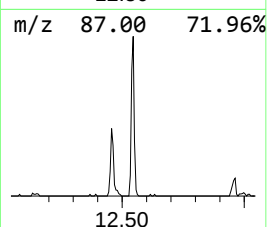
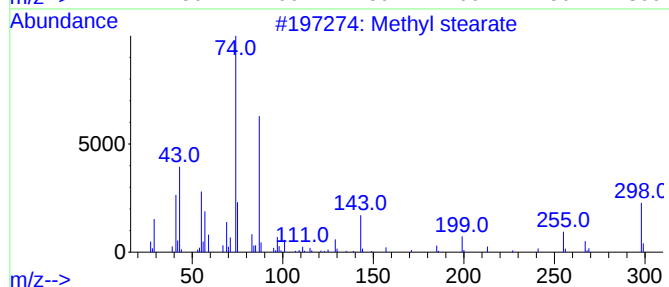
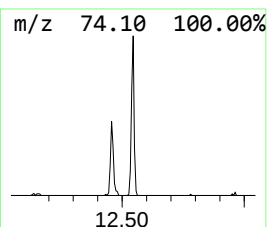
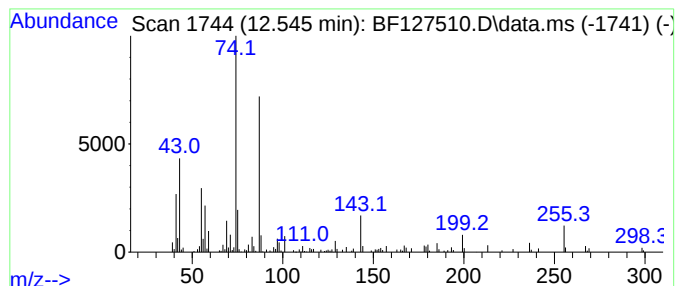
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	2.96 ng	106140	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	91
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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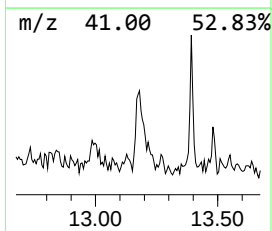
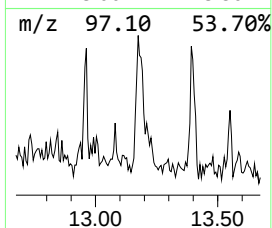
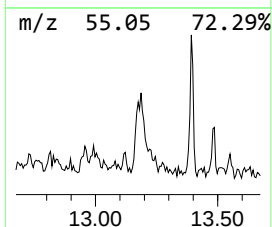
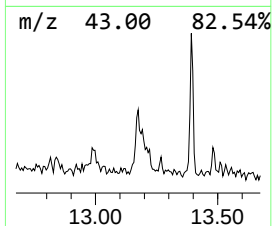
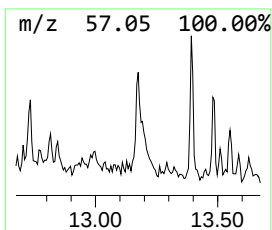
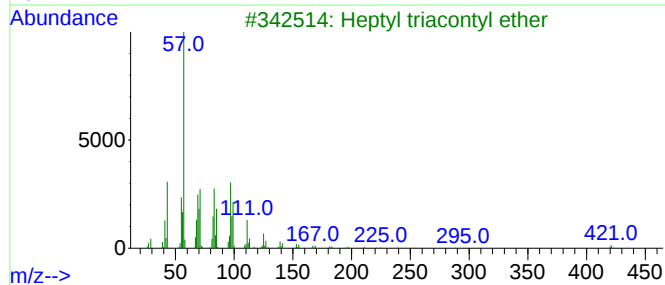
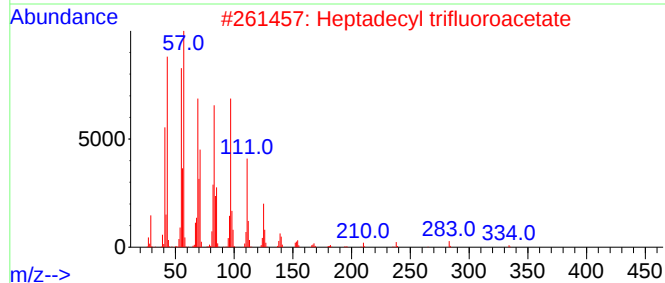
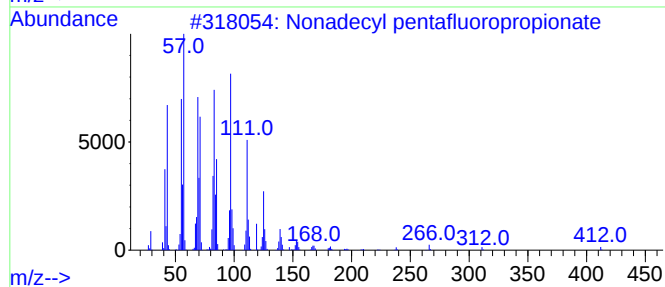
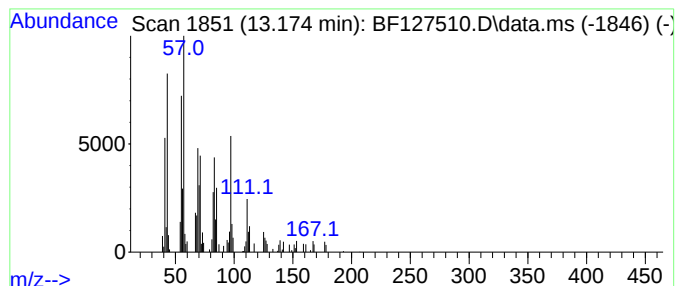
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Peak Number 5 Nonadecyl pentafluoropropio... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	3.58 ng	89702	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
3			Heptyl triacontyl ether	537	C37H76O	1000406-40-1	87
4			1-Hexacosene	364	C26H52	018835-33-1	86
5			Octacosyl propyl ether	452	C31H64O	1000406-28-5	81



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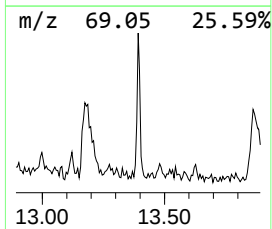
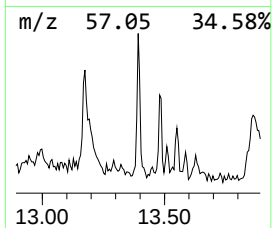
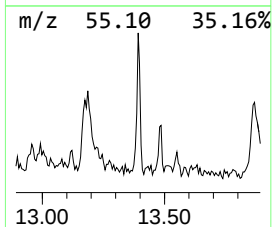
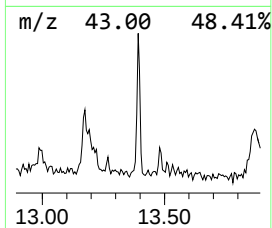
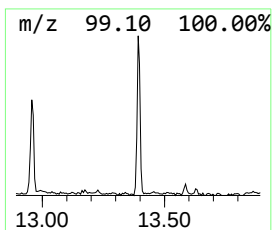
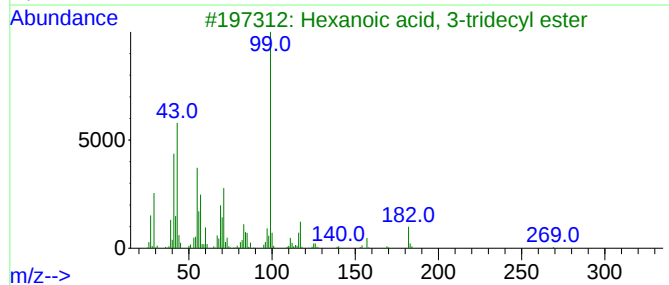
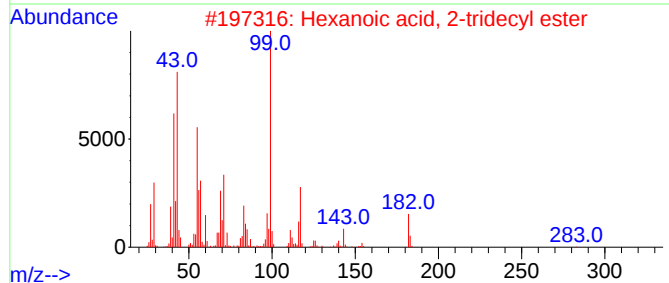
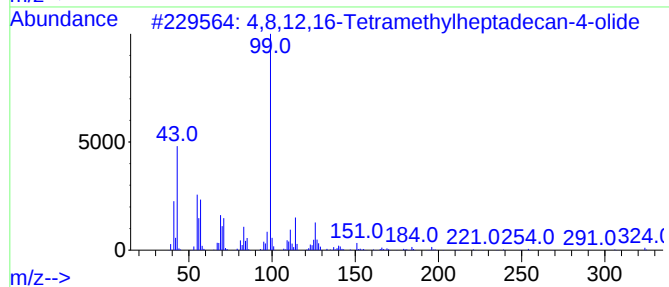
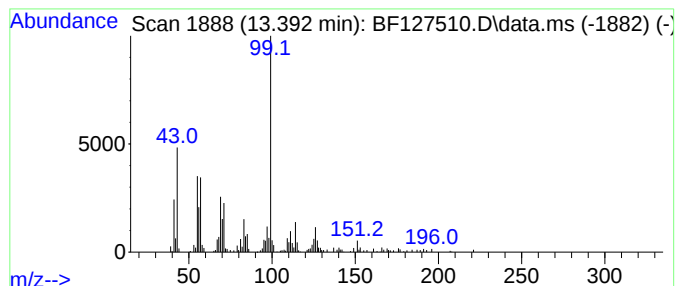
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4,8,12,16-Tetramethylheptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.392	4.48 ng	112375	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	83		
2	Hexanoic acid, 2-tridecyl ester	298	C19H38O2	055193-20-9	64		
3	Hexanoic acid, 3-tridecyl ester	298	C19H38O2	1000279-29-2	59		
4	trans-4-Hydroxy-3-methylundecano...	198	C12H22O2	148806-10-4	53		
5	.delta.-Dodecalactone	198	C12H22O2	000713-95-1	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032422\
Data File : BF127510.D
Acq On : 24 Mar 2022 18:49
Operator : CG\JU
Sample : N2090-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-46

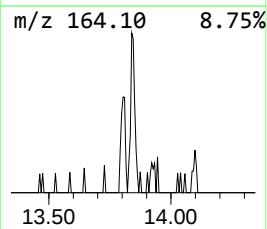
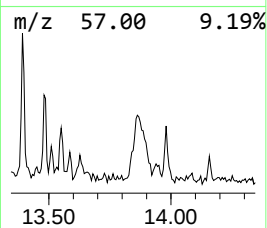
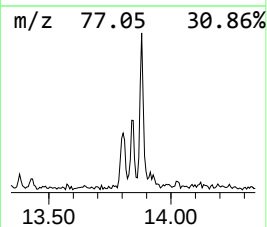
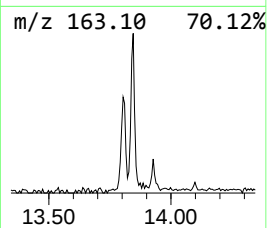
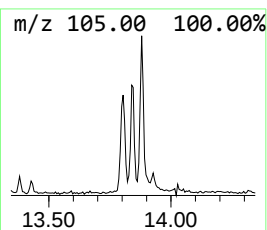
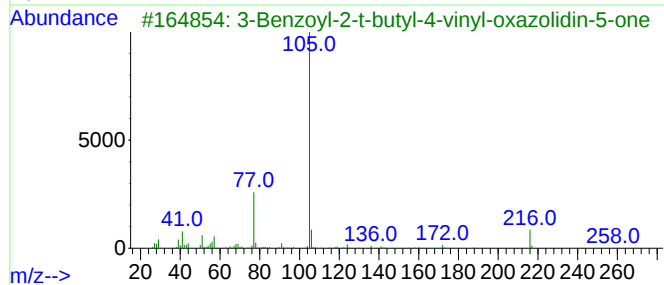
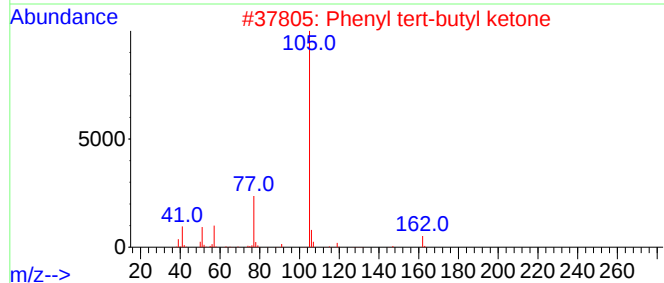
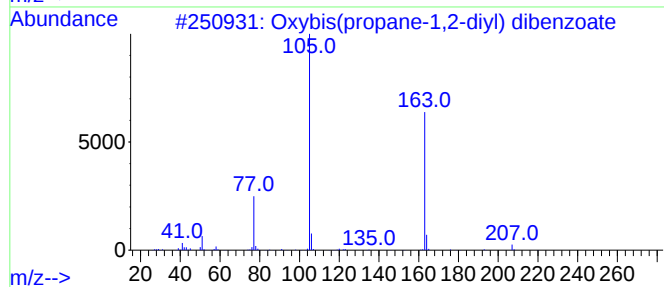
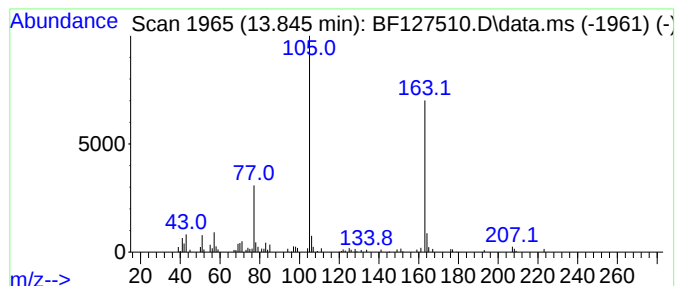
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxybis(propene-1,2-diyl) di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	2.46 ng	61658	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
2			Phenyl tert-butyl ketone	162	C11H14O	000938-16-9	35
3			3-Benzoyl-2-t-butyl-4-vinyl-oxaz...	273	C16H19NO3	109918-60-7	35
4			Benzoic acid, 2-methylphenyl ester	212	C14H12O2	000617-02-7	27
5			Ethanone, 2-bromo-1,2-diphenyl-	274	C14H11BrO	001484-50-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032422\
Data File : BF127510.D
Acq On : 24 Mar 2022 18:49
Operator : CG\JU
Sample : N2090-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-46

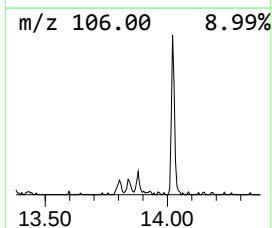
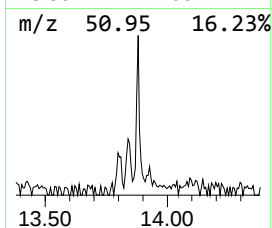
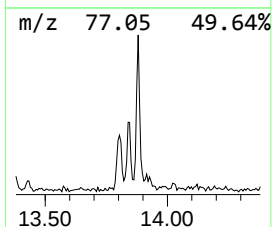
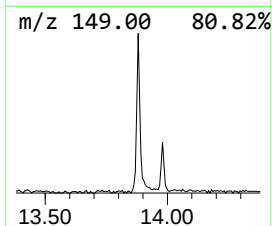
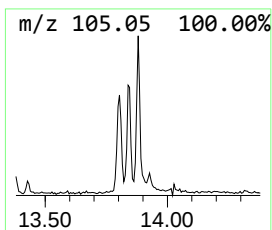
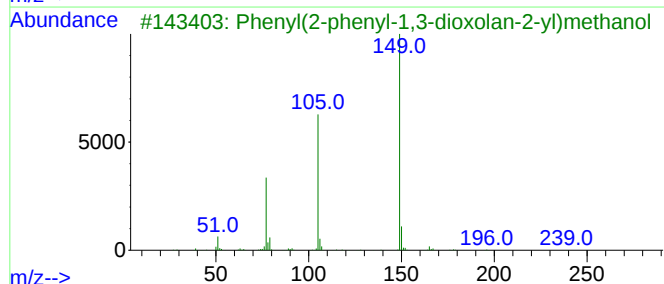
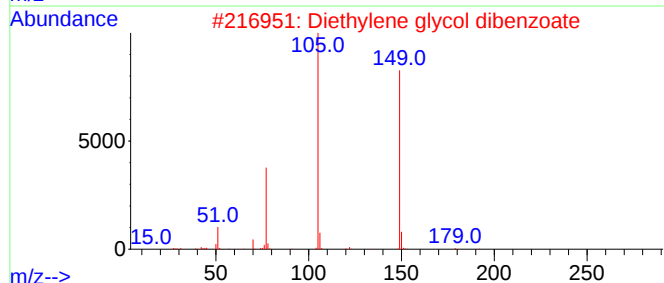
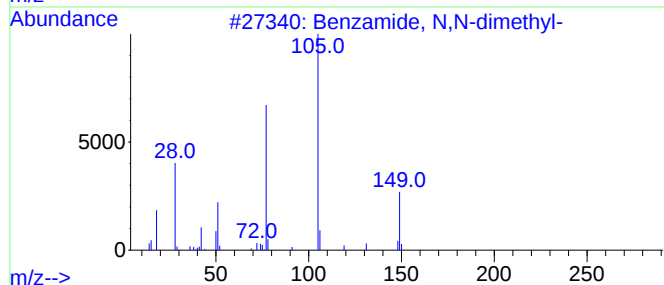
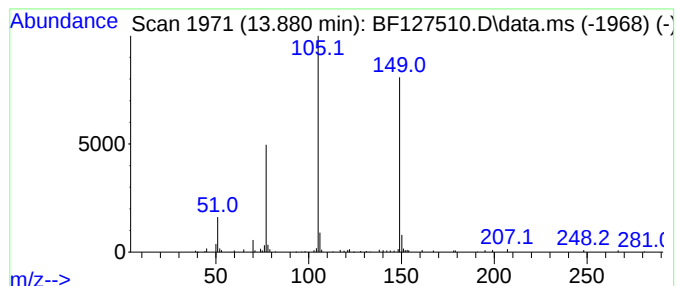
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzamide, N,N-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.46 ng	111891	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	83
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
3			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	256	C16H16O3	005694-69-9	78
4			N-(5-Pyrimidinyl)benzamide	199	C11H9N3O	103854-65-5	38
5			N-Benzoyl-dl-alanine	193	C10H11NO3	001205-02-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032422\
Data File : BF127510.D
Acq On : 24 Mar 2022 18:49
Operator : CG\JU
Sample : N2090-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-46

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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-(2-b...	8.028	8.1	ng	265103	2	8.128	657103	20.0
2,4,7,9-Tetrame...	9.310	7.6	ng	286558	3	9.886	751373	20.0
10-Octadecenoic...	12.457	6.3	ng	227162	4	11.374	717944	20.0
Methyl stearate	12.545	3.0	ng	106140	4	11.374	717944	20.0
Nonadecyl penta...	13.174	3.6	ng	89702	5	14.021	501429	20.0
4,8,12,16-Tetra...	13.392	4.5	ng	112375	5	14.021	501429	20.0
Oxybis(propane-...	13.845	2.5	ng	61658	5	14.021	501429	20.0
Benzamide, N,N-...	13.880	4.5	ng	111891	5	14.021	501429	20.0