

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
 Data File : BF140071.D
 Acq On : 26 Oct 2024 20:33
 Operator : RC/JU
 Sample : P4545-01 2X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-215

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	20	rVB	563801	888306	62.96%	5.799%
2	5.498	573	579	589	rBV	801472	1071610	75.95%	6.995%
3	6.498	744	749	763	rBV	811377	1055719	74.82%	6.892%
4	6.886	810	815	820	rBV	784690	953872	67.60%	6.227%
5	7.445	901	910	914	rBV	545637	691437	49.00%	4.514%
6	7.698	948	953	959	rVB	27976	34188	2.42%	0.223%
7	8.169	1026	1033	1038	rBV	982283	1197616	84.88%	7.818%
8	8.822	1136	1144	1146	rBV8	8226	19354	1.37%	0.126%
9	9.051	1179	1183	1185	rBV4	13042	20734	1.47%	0.135%
10	9.163	1199	1202	1204	rBV3	26032	32079	2.27%	0.209%
11	9.239	1210	1215	1225	rBV	889915	1182999	83.84%	7.723%
12	9.322	1225	1229	1233	rBV	75974	104980	7.44%	0.685%
13	9.633	1278	1282	1287	rBV3	168140	257306	18.24%	1.680%
14	9.792	1305	1309	1312	rBV3	163330	246924	17.50%	1.612%
15	9.839	1313	1317	1320	rVB2	224306	315939	22.39%	2.062%
16	9.922	1326	1331	1335	rVB	865851	1136717	80.56%	7.420%
17	10.180	1372	1375	1378	rBV2	131321	174442	12.36%	1.139%
18	10.333	1398	1401	1406	rBV4	310138	438837	31.10%	2.865%
19	10.839	1484	1487	1494	rVB	362018	551864	39.11%	3.603%
20	11.416	1582	1585	1595	rVB	641422	918627	65.10%	5.997%
21	12.998	1850	1854	1862	rVB	613156	873167	61.88%	5.700%
22	14.051	2026	2033	2046	rVB3	627596	1411017	100.00%	9.211%
23	14.733	2146	2149	2152	rBV	56978	76611	5.43%	0.500%
24	14.827	2161	2165	2168	rBV	116152	168475	11.94%	1.100%
25	14.915	2176	2180	2184	rBV	119927	181882	12.89%	1.187%
26	14.957	2184	2187	2191	rVB	112509	145326	10.30%	0.949%
27	15.009	2192	2196	2200	rVB	136946	199529	14.14%	1.303%
28	15.051	2201	2203	2207	rVV	67085	77345	5.48%	0.505%
29	15.104	2207	2212	2218	rVB2	138121	278504	19.74%	1.818%
30	15.527	2279	2284	2295	rVB	353734	613453	43.48%	4.005%

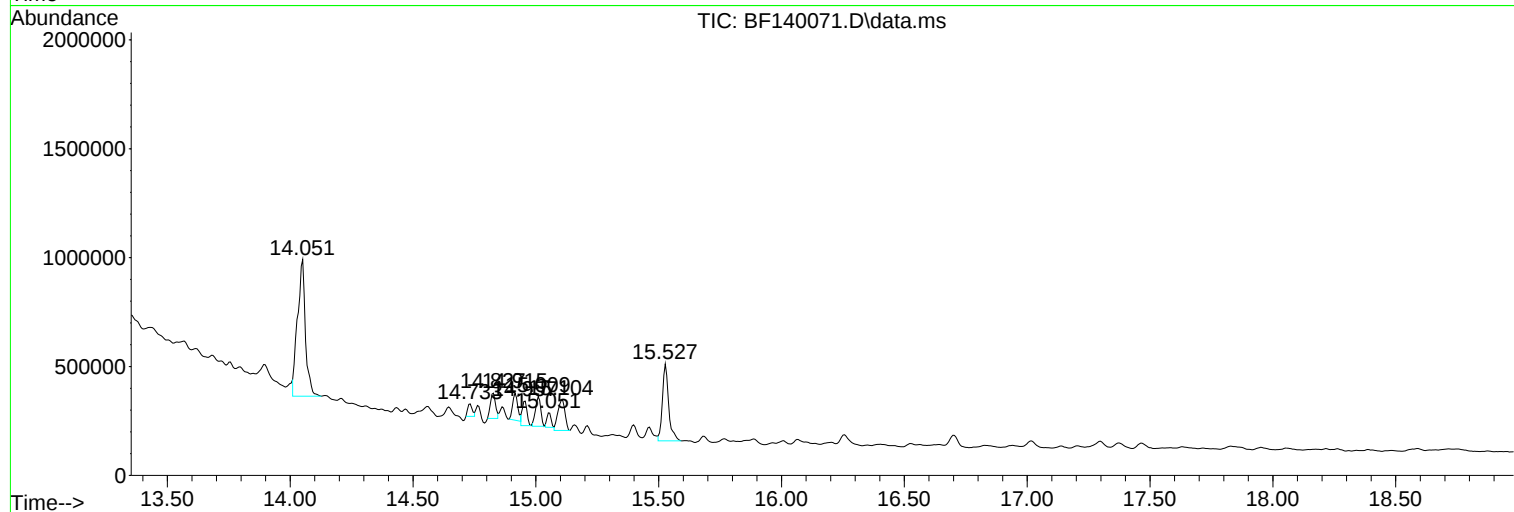
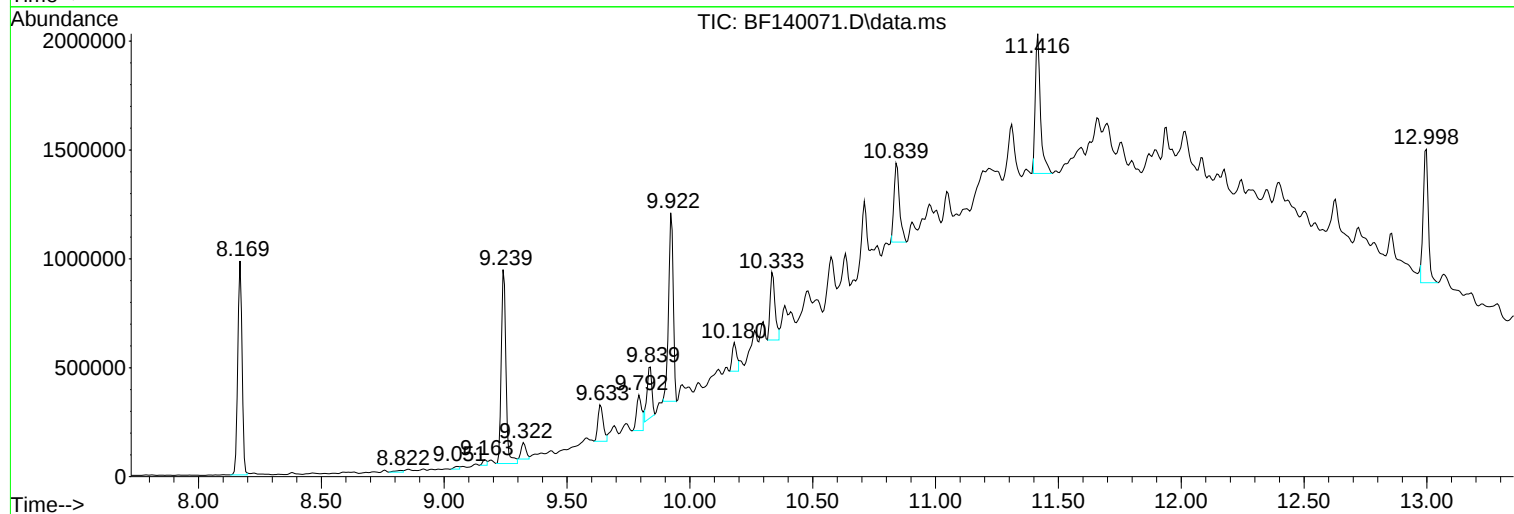
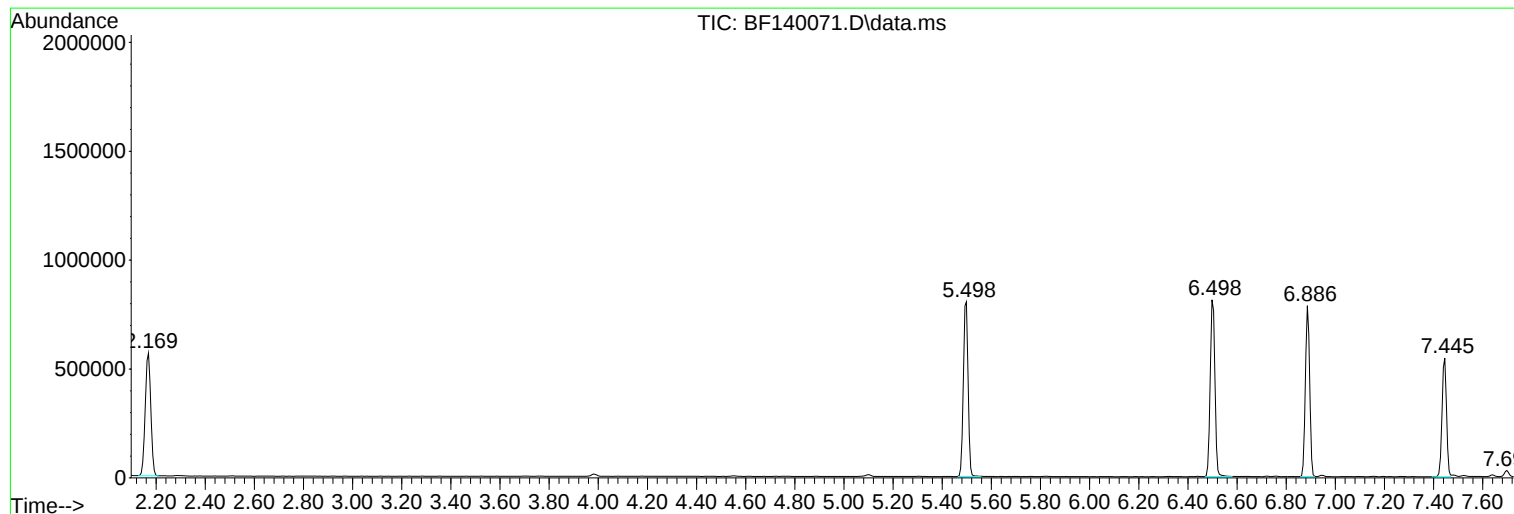
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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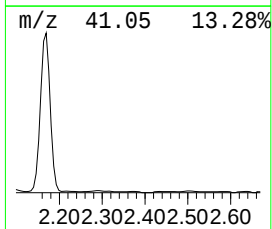
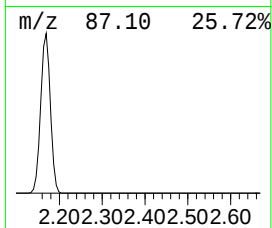
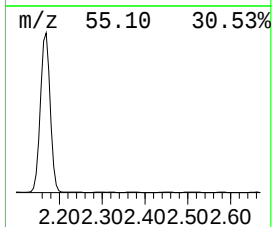
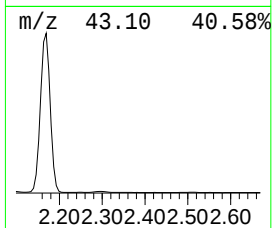
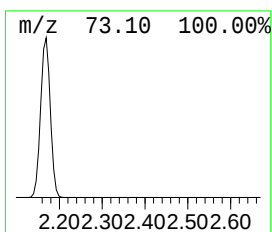
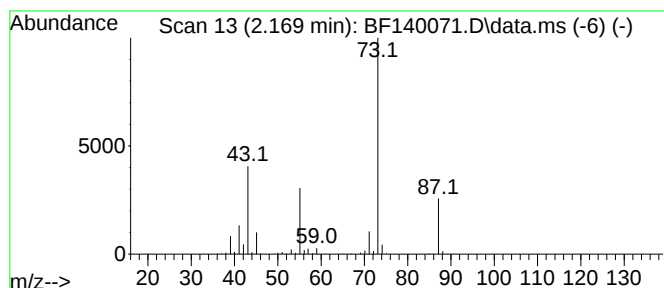
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	18.63 ng	888306	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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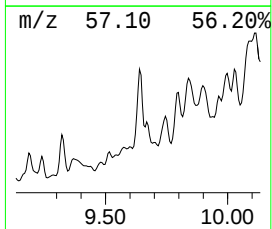
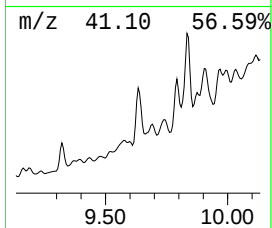
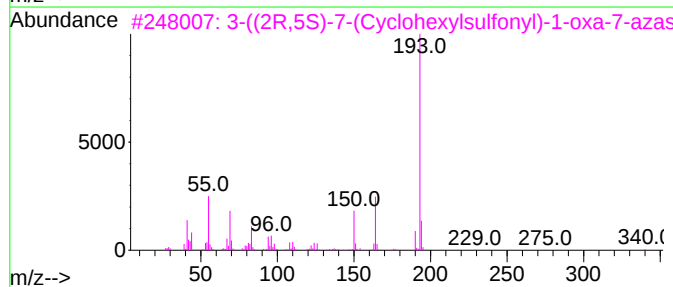
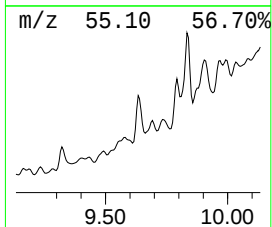
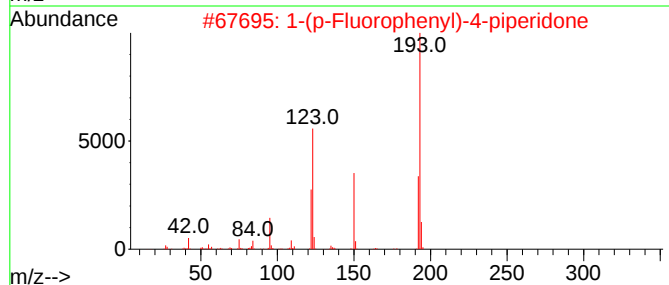
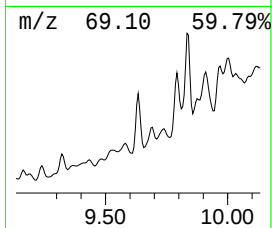
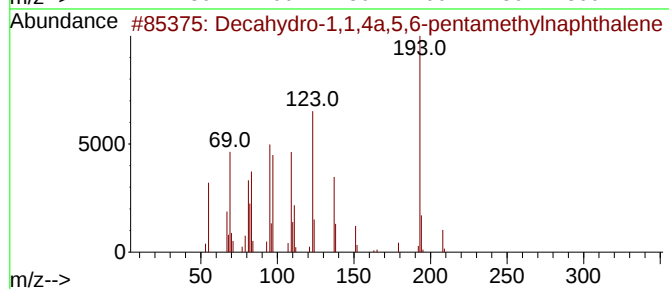
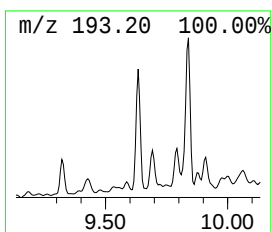
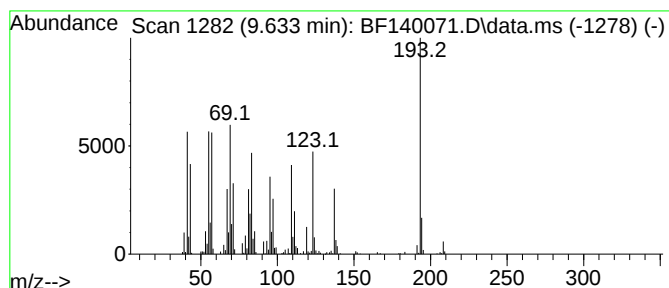
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.633	4.53 ng	257306	Acenaphthene-d10	9.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	53
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3	3-((2R,5S)-7-(Cyclohexylsulfonyl)...	340	C17H28N2O3S	1000483-82-6	22
4	2,6-Dodecadiene, 2,6-dimethyl-	194	C14H26	1000164-67-6	22
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22



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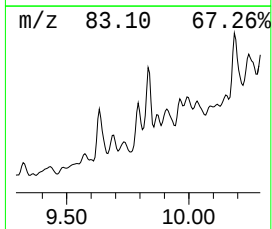
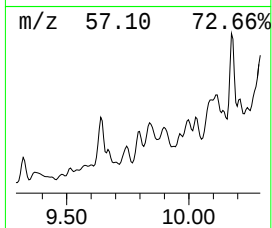
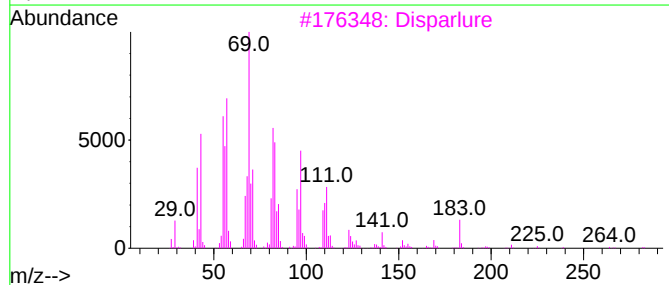
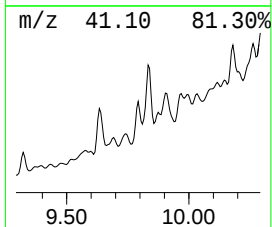
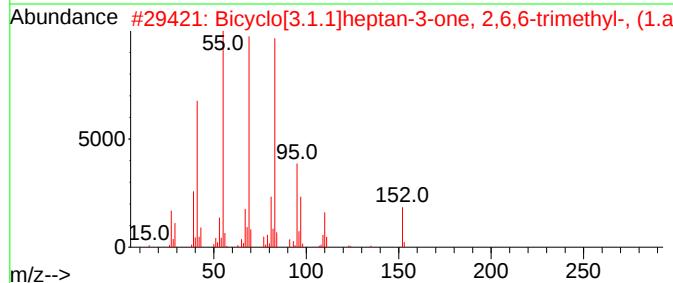
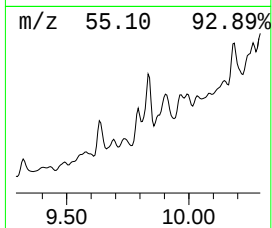
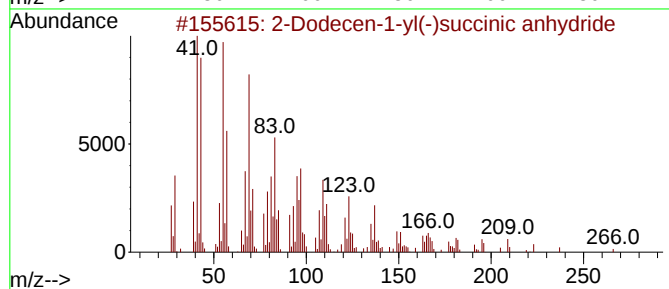
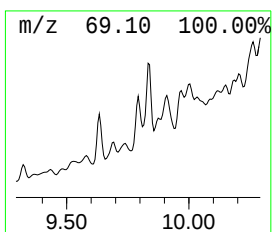
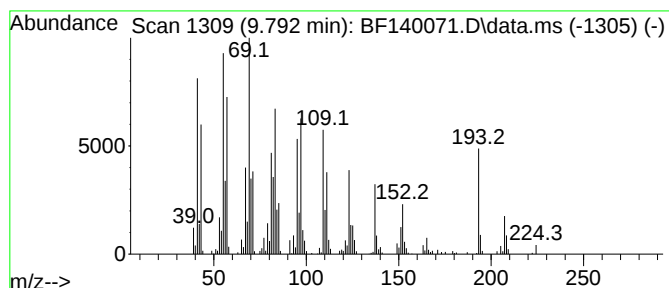
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Dodecen-1-yl(-)succinic a... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	4.34 ng	246924	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	64
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	43
3		Disparlure	282	C19H38O	029804-22-6	43
4		1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	43
5		Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	30



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

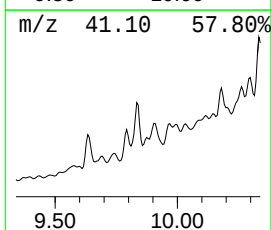
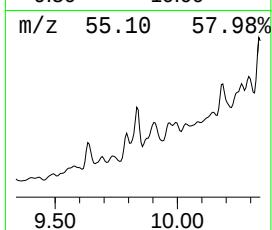
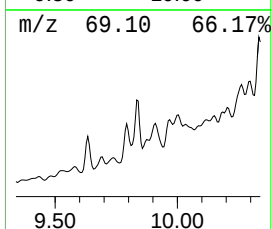
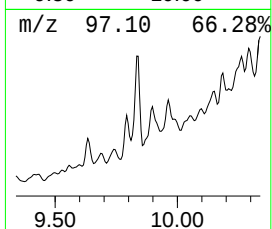
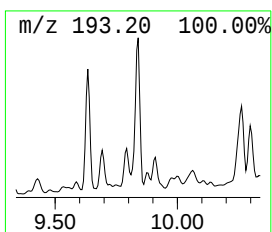
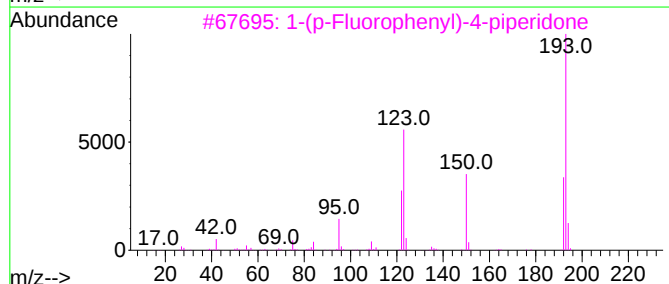
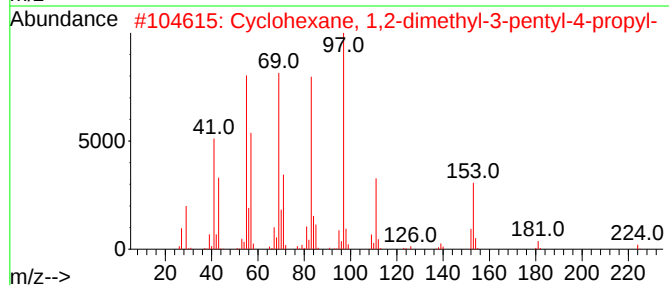
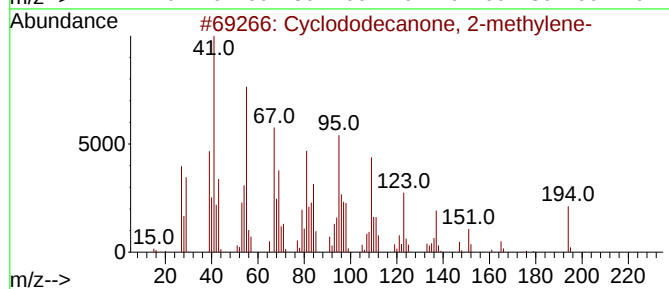
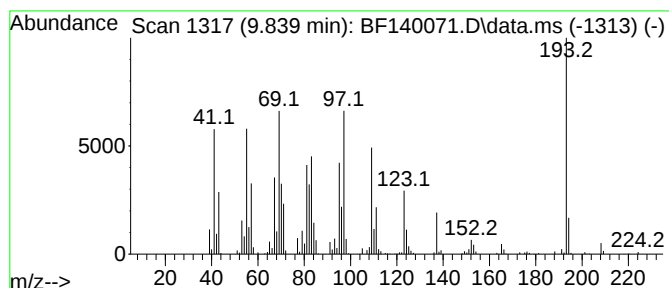
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.839 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.839	5.56 ng	315939	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
2			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	35
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
4			Spiro[5.6]dodecane-1,7-dione	194	C12H18O2	050803-80-0	25
5			9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	14



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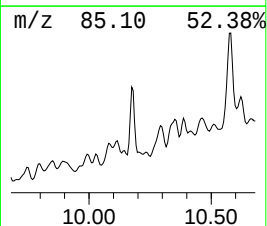
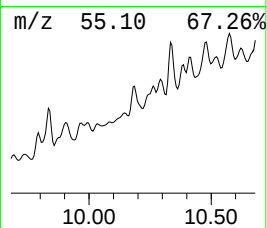
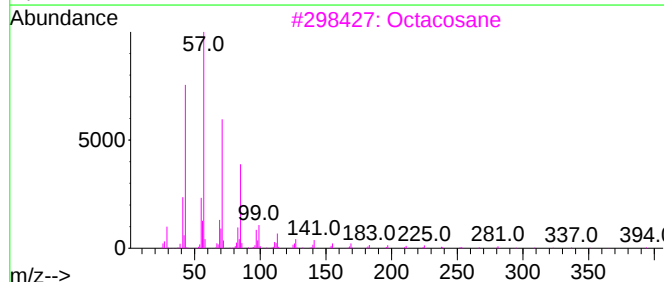
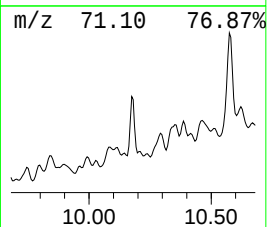
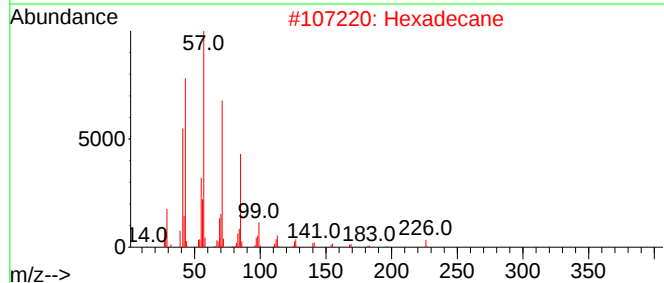
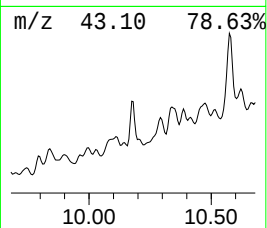
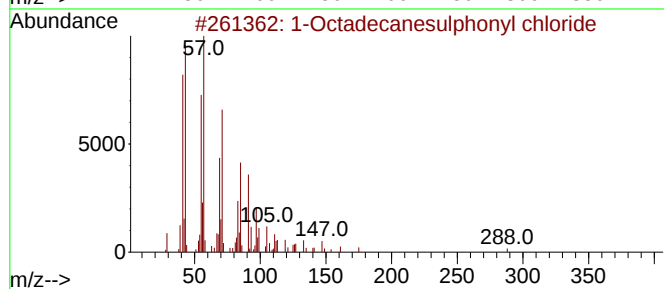
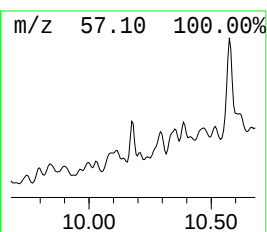
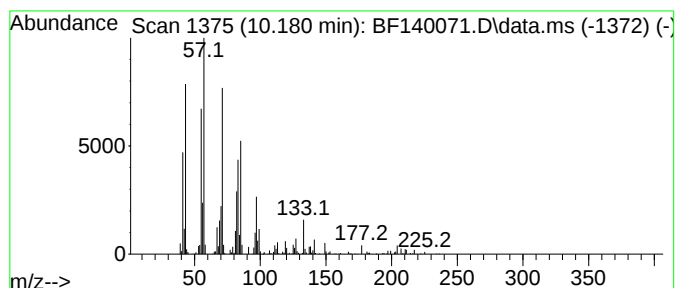
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Peak Number 5 1-Octadecanesulphonyl chloride Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.180	3.07 ng	174442	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	72
2			Hexadecane	226	C16H34	000544-76-3	52
3			Octacosane	394	C28H58	000630-02-4	52
4			Pentadecane	212	C15H32	000629-62-9	49
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	49



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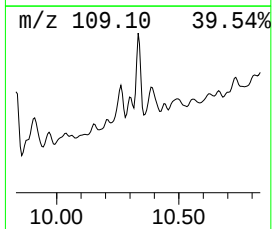
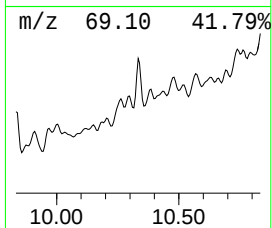
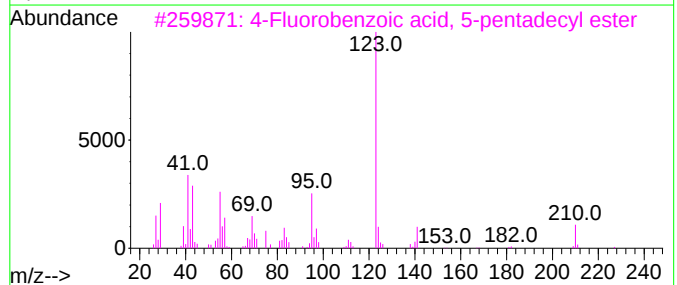
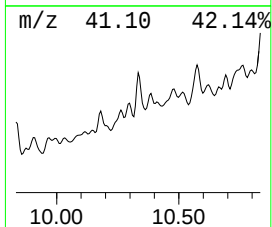
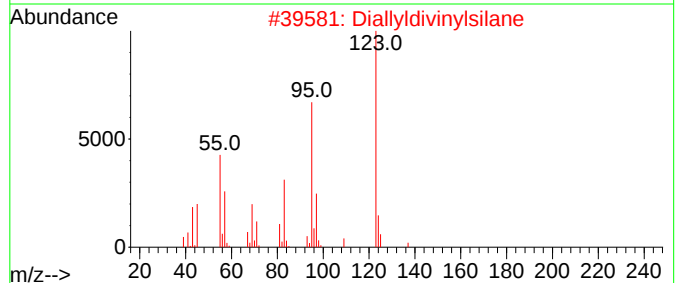
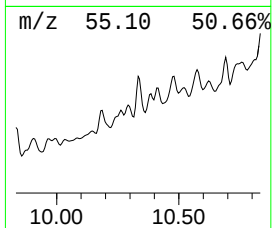
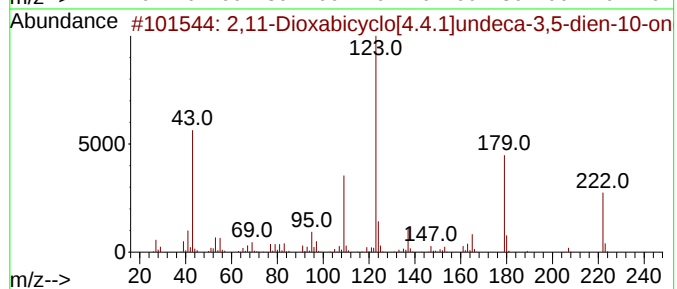
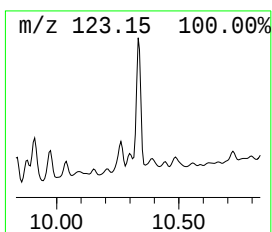
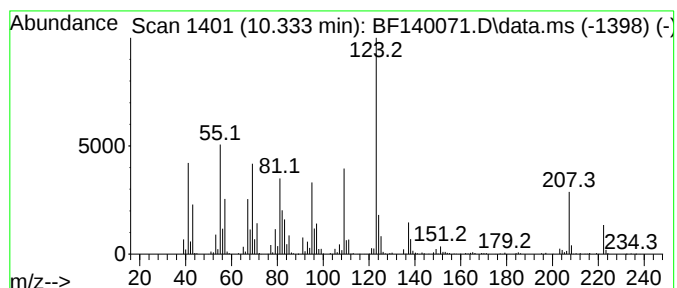
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.333	7.72 ng	438837	Acenaphthene-d10		9.922	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...		222	C13H18O3	070412-52-1	59
2	Diallyldivinylsilane		164	C10H16Si	119901-88-1	47
3	4-Fluorobenzoic acid, 5-pentadec...		350	C22H35FO2	1000280-68-6	43
4	3-Fluorobenzoic acid, 3-methylbu...		208	C12H13FO2	154559-38-3	43
5	1,3-Benzenediamine, 4-methoxy-		138	C7H10N2O	000615-05-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-215

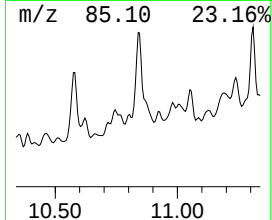
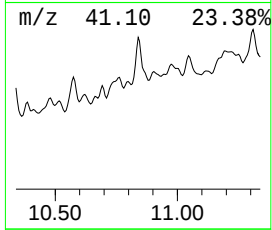
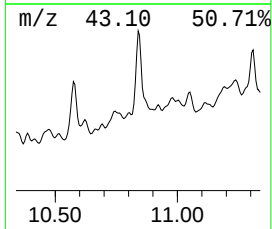
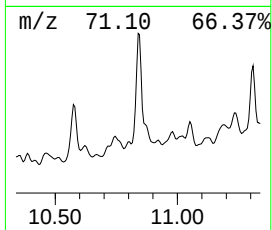
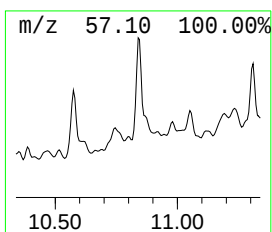
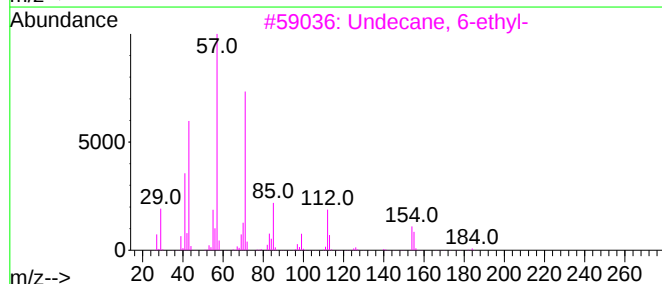
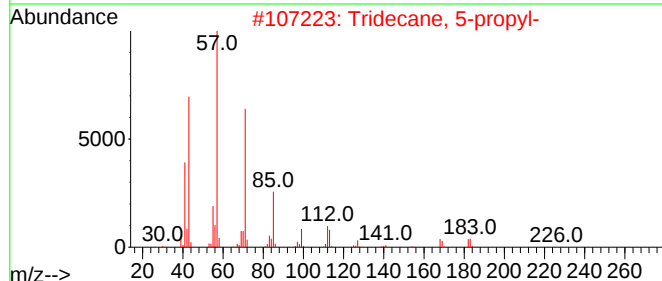
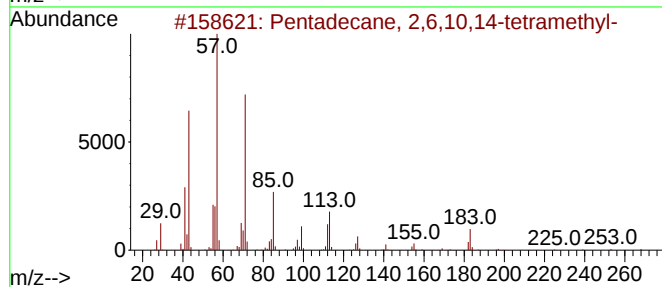
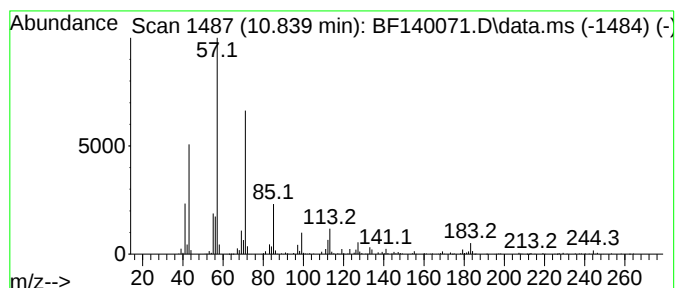
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane, 2,6,10,14-tetr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.839	12.02 ng	551864	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2			Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
3			Undecane, 6-ethyl-	184	C13H28	017312-60-6	87
4			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
5			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-215

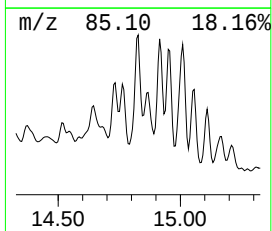
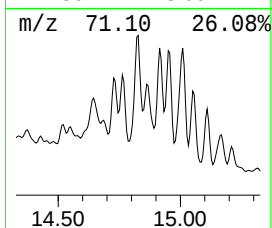
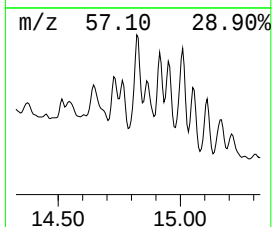
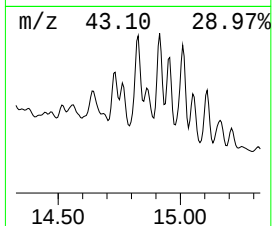
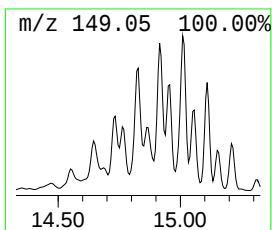
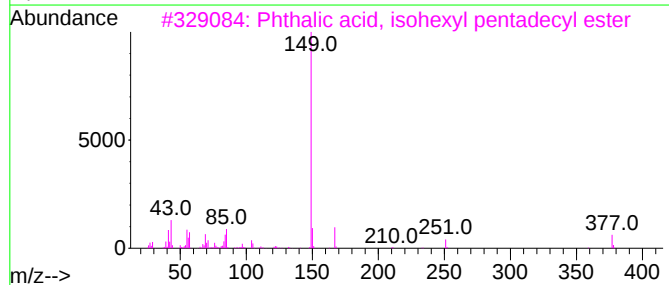
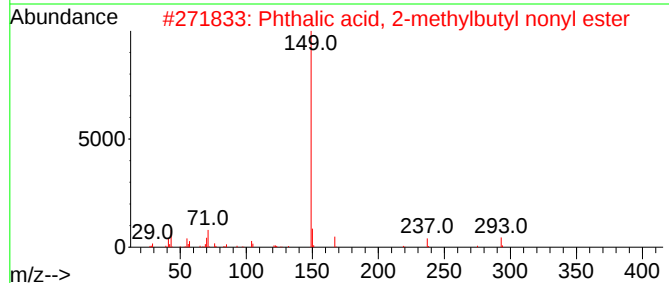
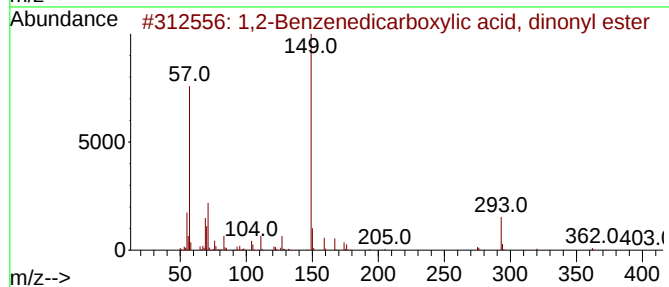
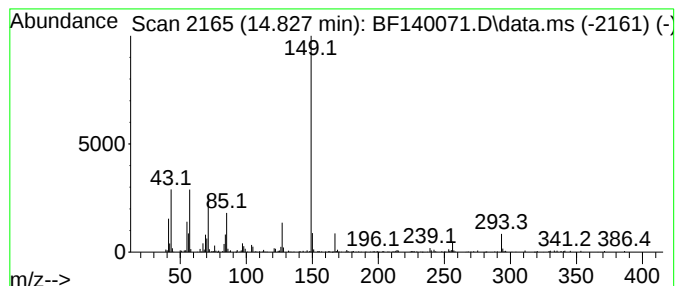
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.827	5.49 ng	168475	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	59
2	Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	53
3	Phthalic acid, isohexyl pentadec...	460	C29H48O4	1000308-98-3	53
4	Phthalic acid, 3-fluorophenyl oc...	372	C22H25FO4	1010356-72-8	53
5	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

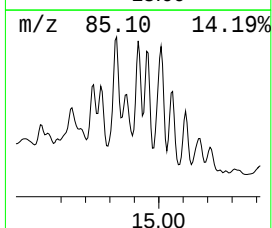
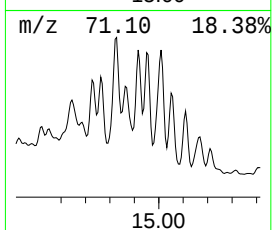
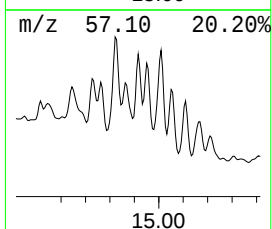
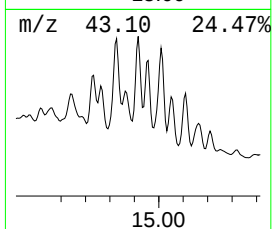
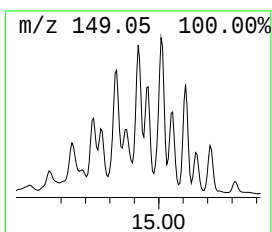
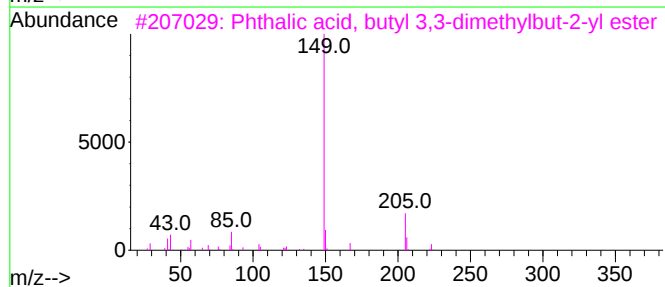
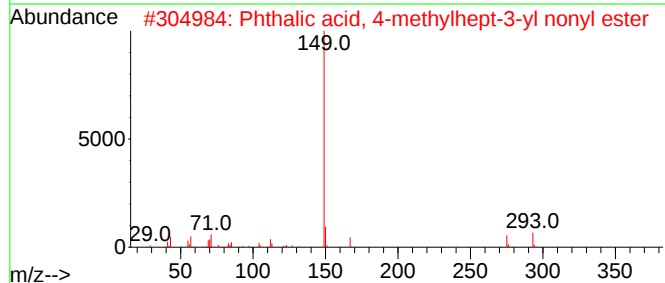
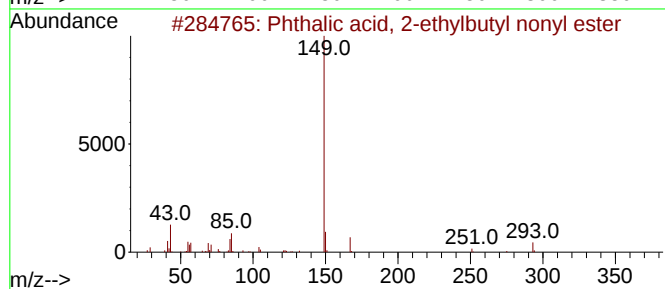
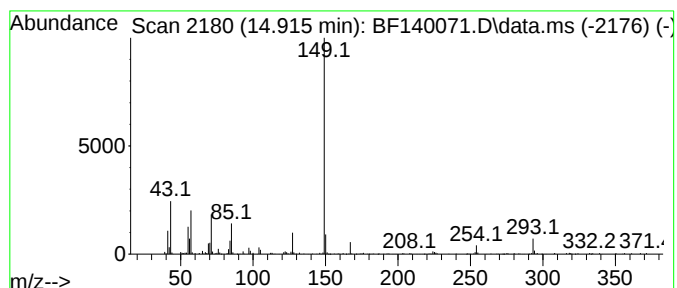
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, 2-ethylbutyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.915	5.93 ng	181882	Perylene-d12		15.527	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phthalic acid, 2-ethylbutyl nonyl...		376	C23H36O4	1000356-89-4	72
2	Phthalic acid, 4-methylhept-3-yl...		404	C25H40O4	1000377-94-4	64
3	Phthalic acid, butyl 3,3-dimethy...		306	C18H26O4	1000357-00-2	64
4	Phthalic acid, 3,3-dimethylbut-2...		320	C19H28O4	1000357-00-3	64
5	Phthalic acid, isohexyl tridecyl...		432	C27H44O4	1000309-02-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-215

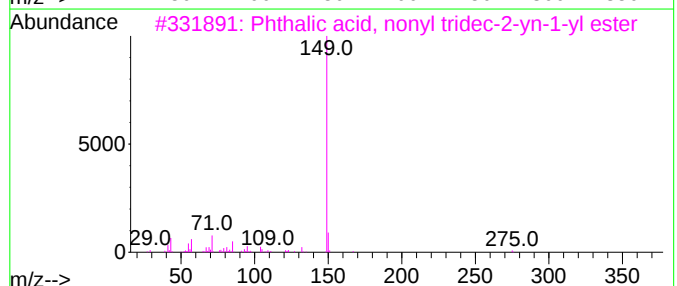
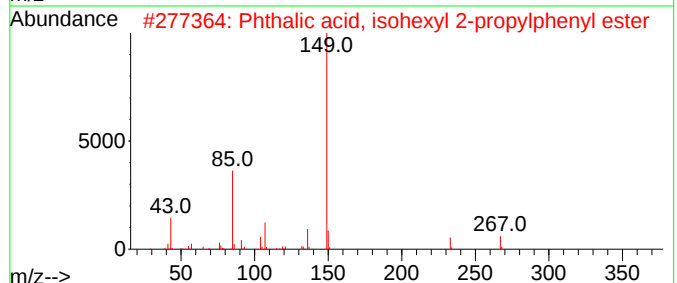
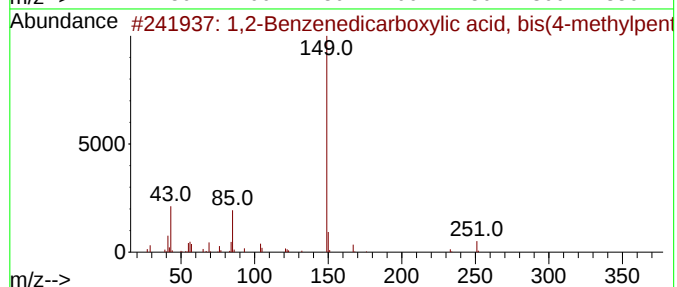
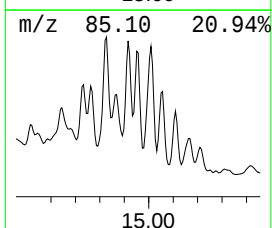
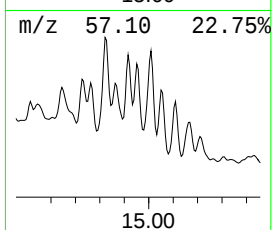
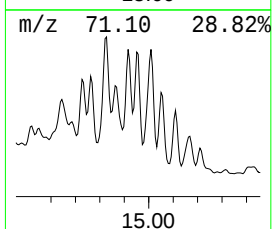
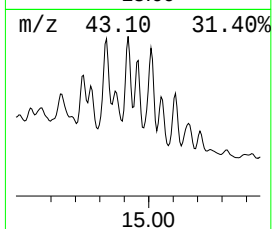
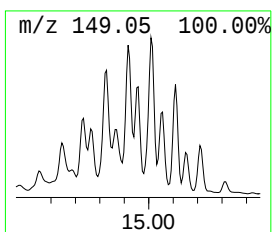
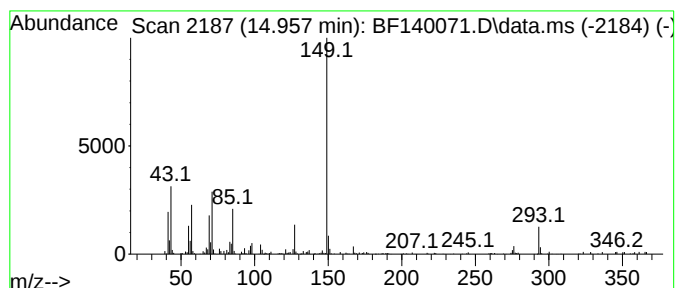
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	4.74 ng	145326	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	52
2			Phthalic acid, isohexyl 2-propyl...	368	C23H28O4	1000357-02-1	50
3			Phthalic acid, nonyl tridec-2-yn...	470	C30H46O4	1000315-44-2	50
4			Phthalic acid, isohexyl tetradec...	446	C28H46O4	1000309-05-1	50
5			Phthalic acid, cycloheptyl isoe...	346	C21H30O4	1000322-83-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

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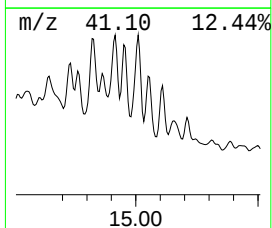
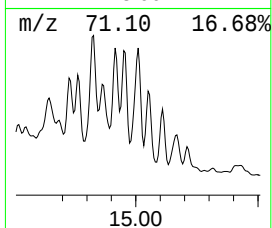
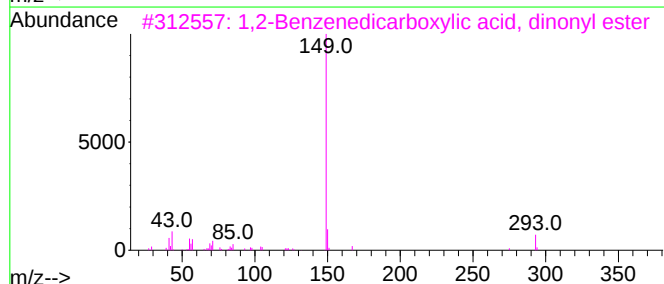
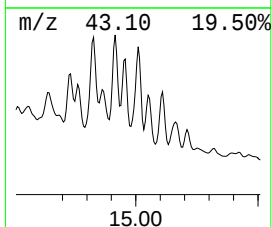
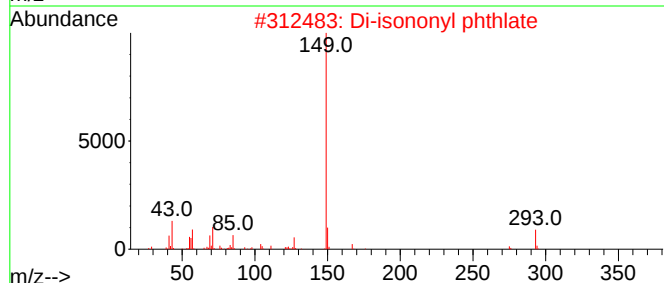
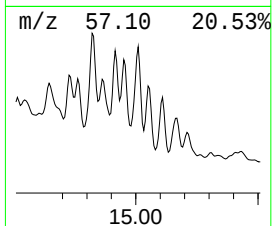
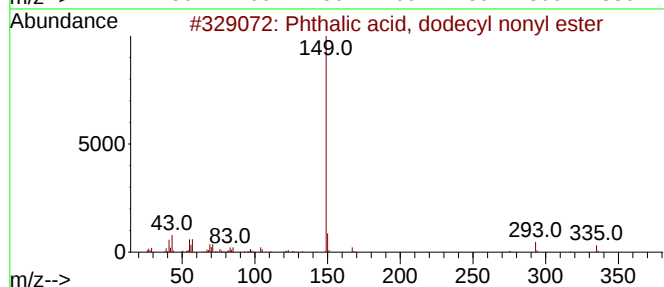
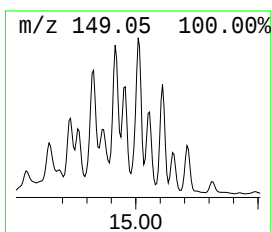
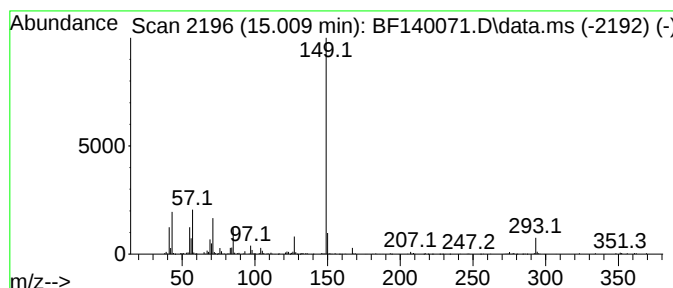
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phthalic acid, dodecyl nony... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.009	6.51 ng	199529	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phthalic acid, dodecyl nonyl ester	460	C29H48O4	1000308-92-6	72
2		Di-isononyl phthlate	418	C26H42O4	020548-62-3	72
3		1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	64
4		Phthalic acid, decyl nonyl ester	432	C27H44O4	1000308-89-8	64
5		Diisodecyl phthalate	446	C28H46O4	000089-16-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140071.D
Acq On : 26 Oct 2024 20:33
Operator : RC/JU
Sample : P4545-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	18.6	ng	888306	1	6.886	953872	20.0
Decahydro-1,1,4...	9.633	4.5	ng	257306	3	9.922	1136720	20.0
2-Dodecen-1-yl(...	9.792	4.3	ng	246924	3	9.922	1136720	20.0
unknown9.839	9.839	5.6	ng	315939	3	9.922	1136720	20.0
1-Octadecanesul...	10.180	3.1	ng	174442	3	9.922	1136720	20.0
2,11-Dioxabicyc...	10.333	7.7	ng	438837	3	9.922	1136720	20.0
Pentadecane, 2,...	10.839	12.0	ng	551864	4	11.416	918627	20.0
1,2-Benzenedica...	14.827	5.5	ng	168475	6	15.527	613453	20.0
Phthalic acid, ...	14.915	5.9	ng	181882	6	15.527	613453	20.0
1,2-Benzenedica...	14.957	4.7	ng	145326	6	15.527	613453	20.0
Phthalic acid, ...	15.009	6.5	ng	199529	6	15.527	613453	20.0