

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
 Data File : BF123966.D
 Acq On : 17 May 2021 16:40
 Operator : JU/CG
 Sample : M2420-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONCESSION-CP-1

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	15	21	rBV	565566	736287	45.49%	6.794%
2	2.281	29	33	38	rVB	46089	56629	3.50%	0.523%
3	5.122	513	516	521	rVB2	17043	19225	1.19%	0.177%
4	5.516	578	583	586	rBV	1257757	1088941	67.28%	10.048%
5	6.522	749	754	757	rBV	1147714	1101732	68.07%	10.166%
6	6.722	785	788	794	rBV	45381	36906	2.28%	0.341%
7	6.904	815	819	822	rBV	340369	276543	17.09%	2.552%
8	7.463	909	914	917	rBV	837289	727630	44.96%	6.714%
9	8.186	1033	1037	1040	rBV	450183	346412	21.40%	3.197%
10	9.263	1216	1220	1223	rBV	1667572	1295597	80.05%	11.955%
11	9.651	1283	1286	1289	rBV	182185	125798	7.77%	1.161%
12	9.939	1331	1335	1339	rBV	510444	409299	25.29%	3.777%
13	10.728	1465	1469	1472	rBV	1127434	913976	56.47%	8.434%
14	11.427	1584	1588	1591	rBV	569329	445493	27.52%	4.111%
15	11.951	1674	1677	1680	rBV	91468	78022	4.82%	0.720%
16	13.016	1853	1858	1861	rBV	1913674	1618524	100.00%	14.935%
17	13.910	2007	2010	2020	rBV2	232260	265678	16.41%	2.452%
18	14.068	2033	2037	2040	rVB	486675	398767	24.64%	3.680%
19	14.233	2061	2065	2068	rBV3	19436	20952	1.29%	0.193%
20	14.545	2110	2118	2125	rBV4	42419	66034	4.08%	0.609%
21	14.704	2142	2145	2149	rVB	219325	193679	11.97%	1.787%
22	14.798	2158	2161	2165	rBV5	17385	27719	1.71%	0.256%
23	14.939	2181	2185	2189	rBV	149674	142649	8.81%	1.316%
24	15.204	2227	2230	2234	rBV2	19695	26070	1.61%	0.241%
25	15.562	2285	2291	2295	rBV	286188	361069	22.31%	3.332%
26	16.051	2369	2374	2378	rBV2	16468	21628	1.34%	0.200%
27	16.104	2378	2383	2390	rVV7	17020	35708	2.21%	0.330%

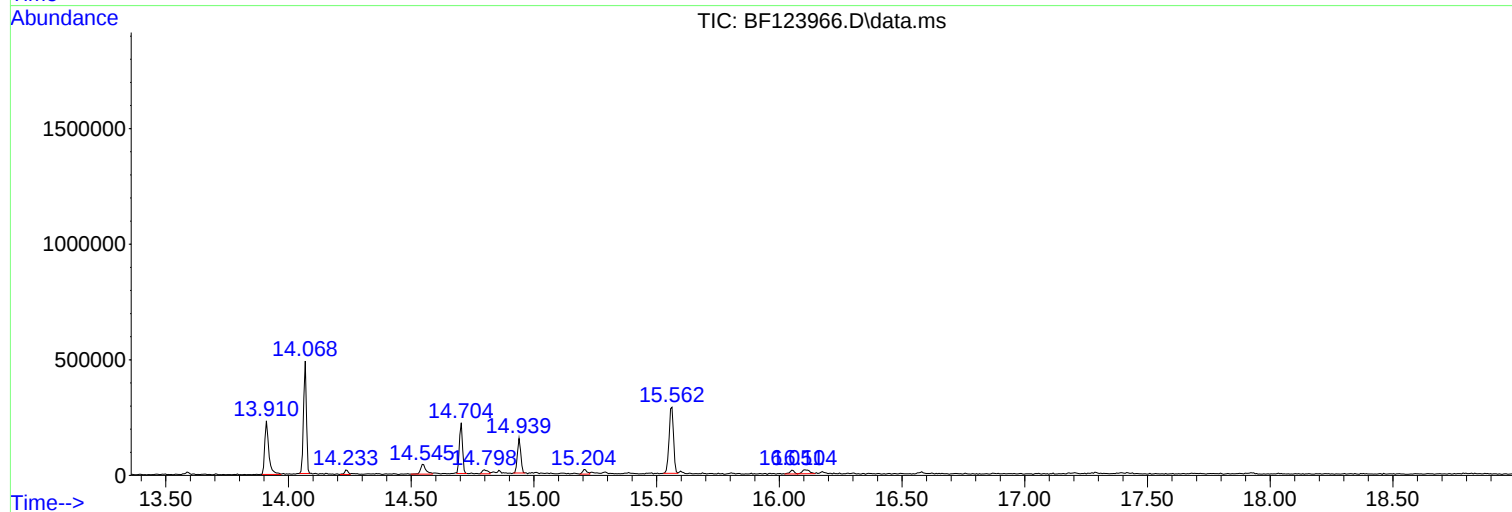
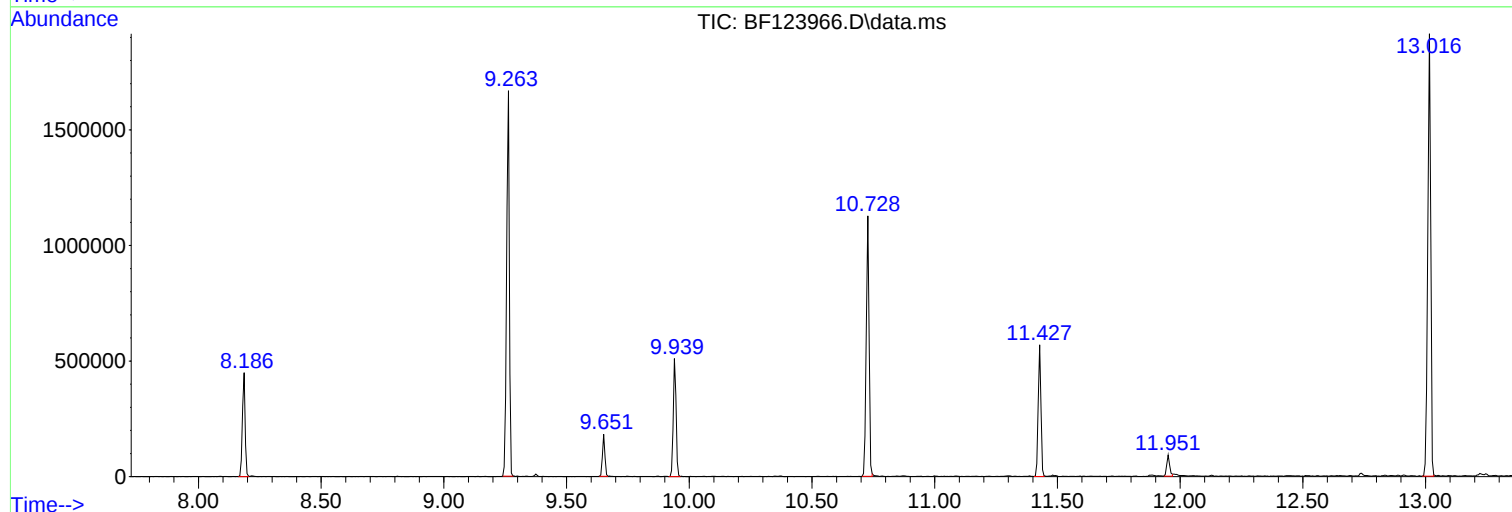
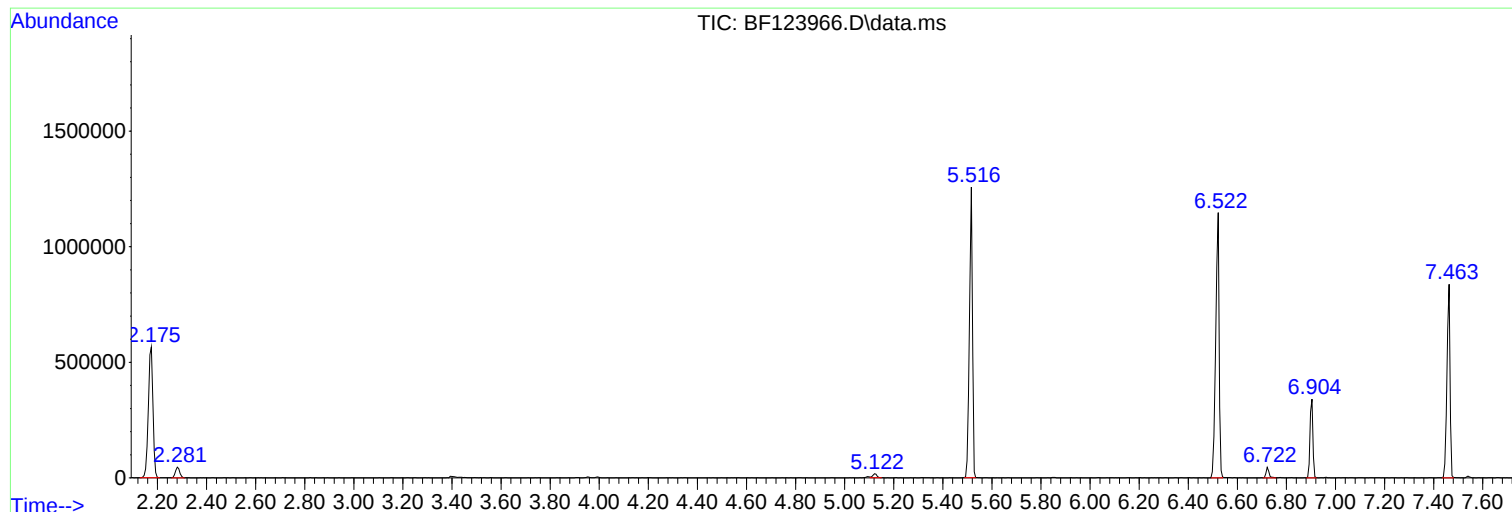
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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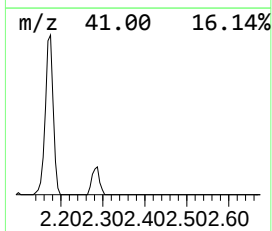
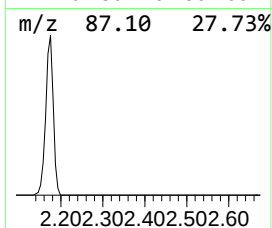
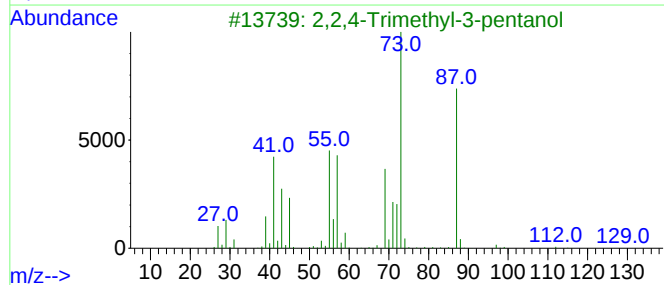
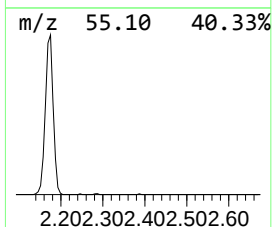
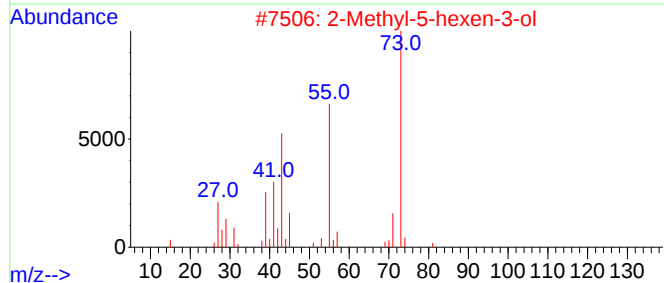
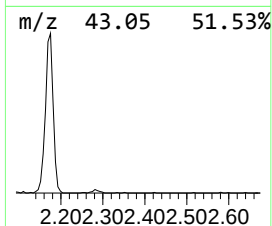
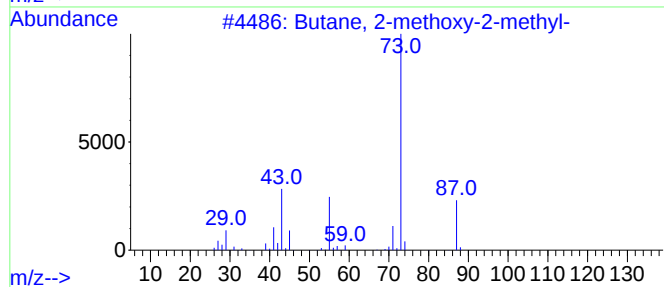
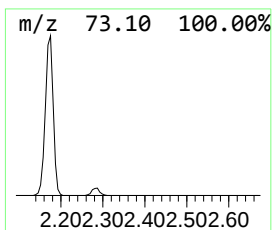
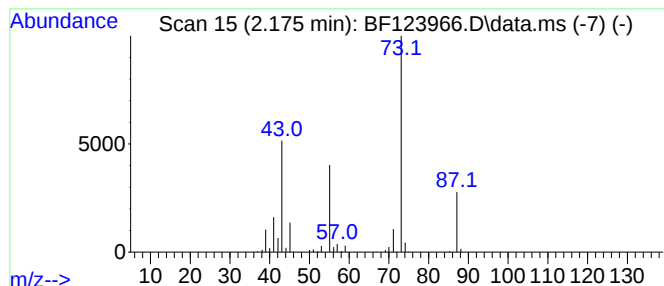
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.175	53.25 ng	736287	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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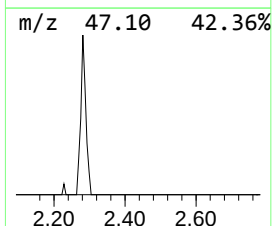
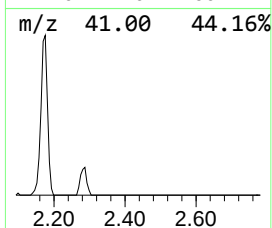
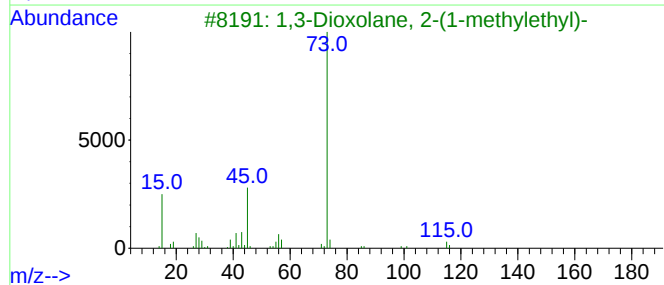
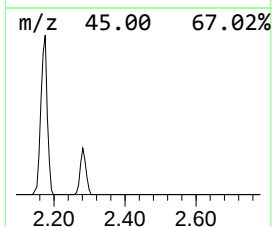
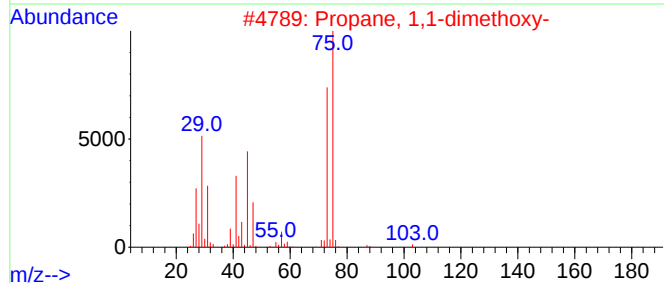
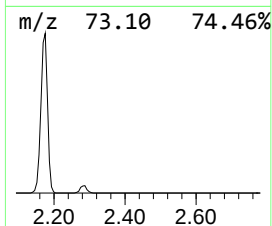
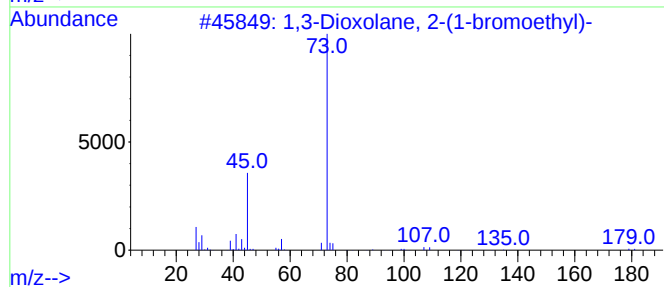
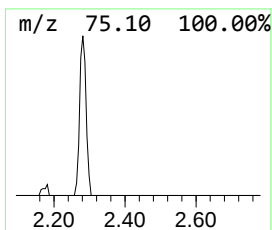
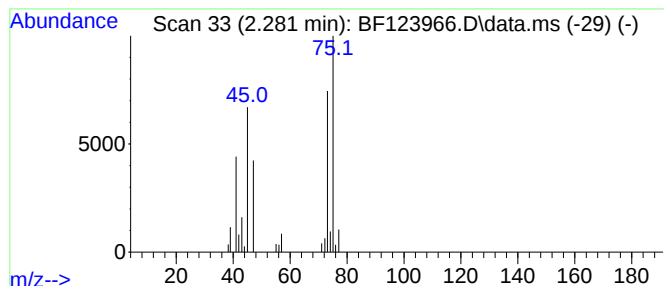
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown2.28 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	4.10 ng	56629	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	7
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	7



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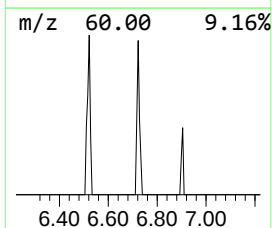
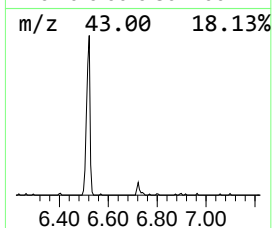
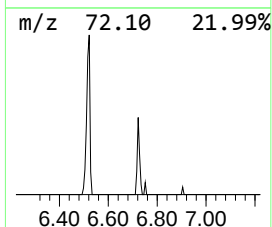
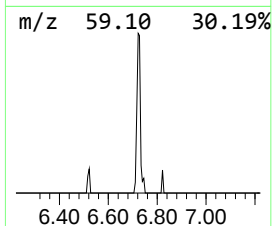
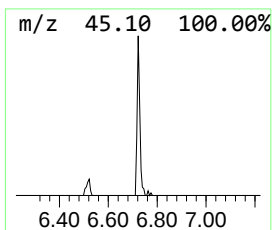
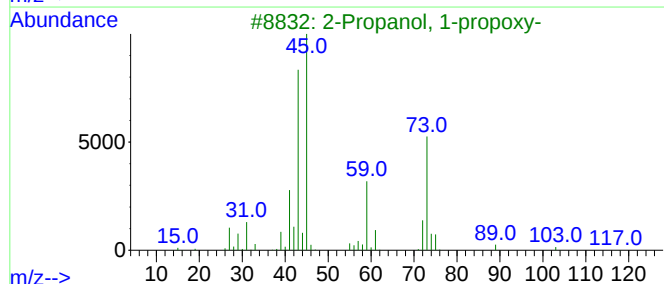
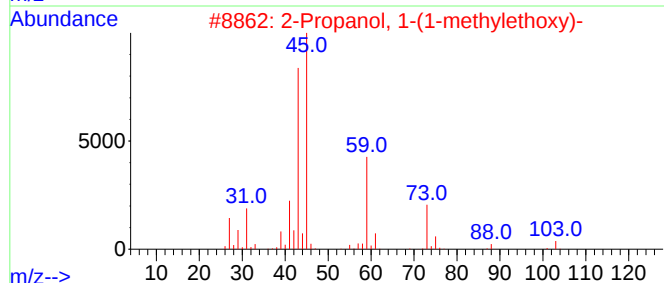
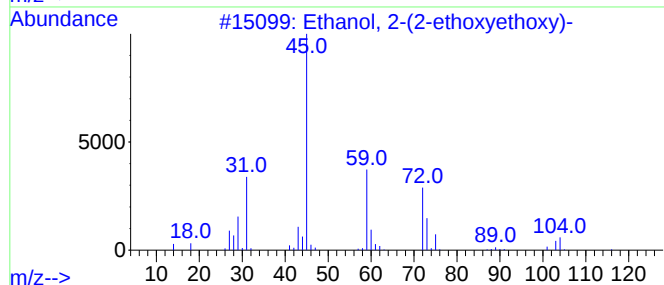
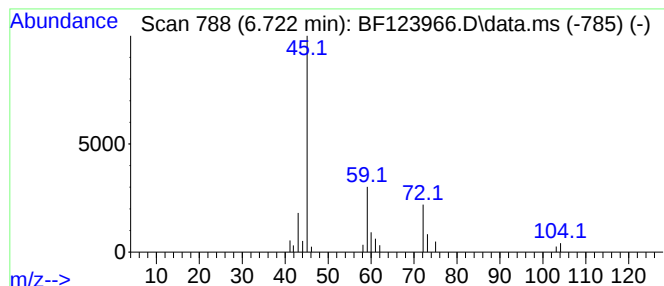
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	2.67 ng	36906	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
5			Ethyl ether	74	C4H10O	000060-29-7	28



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CONCESSION-CP-1

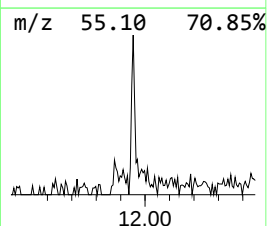
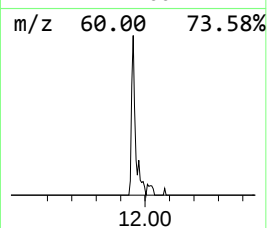
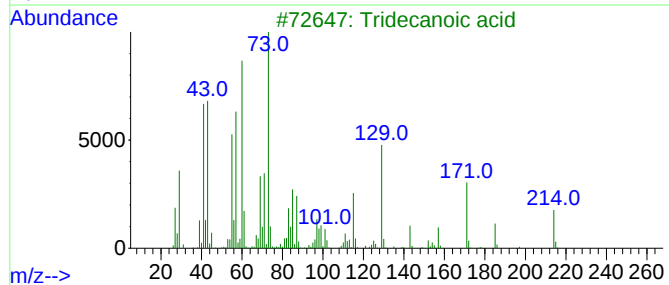
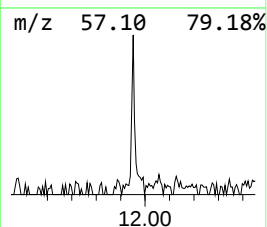
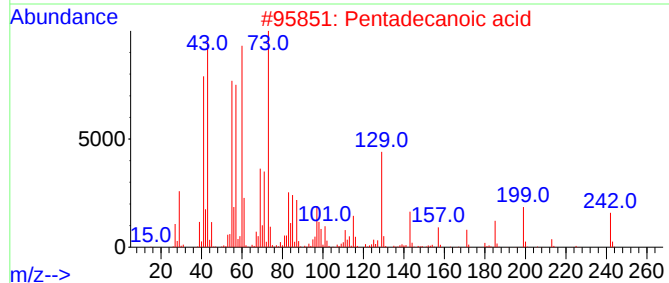
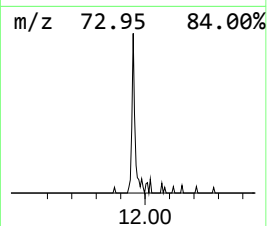
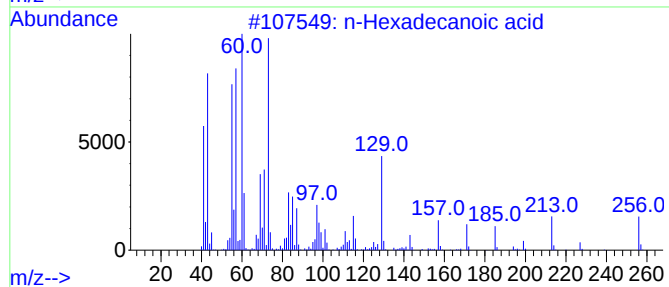
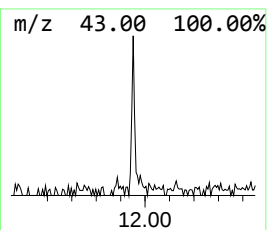
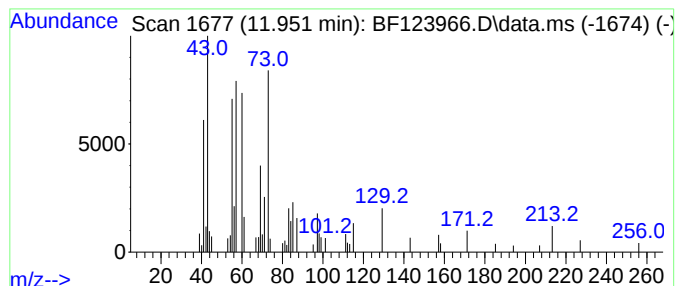
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.50 ng	78022	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



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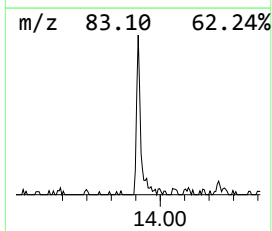
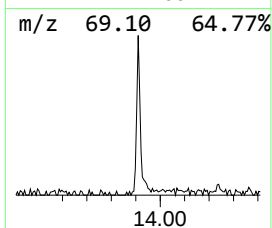
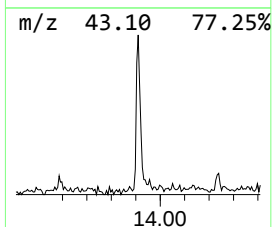
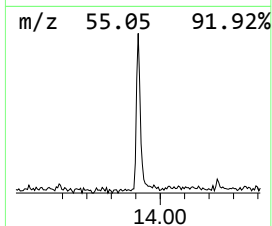
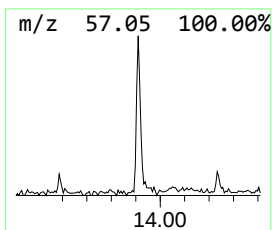
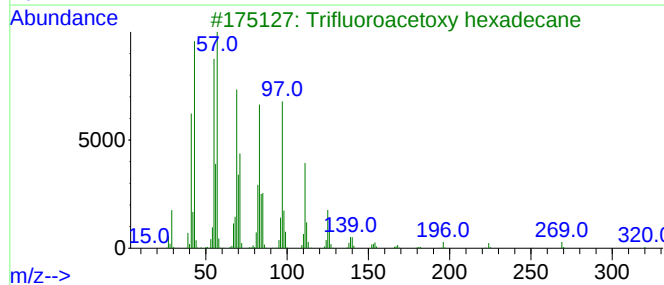
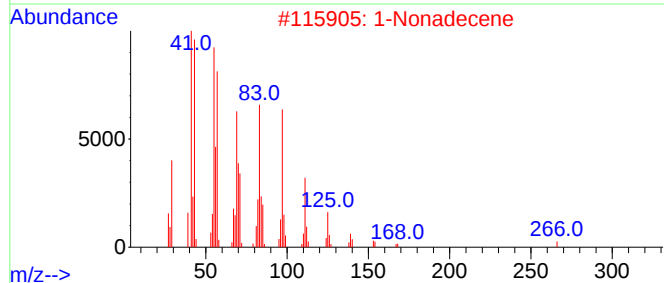
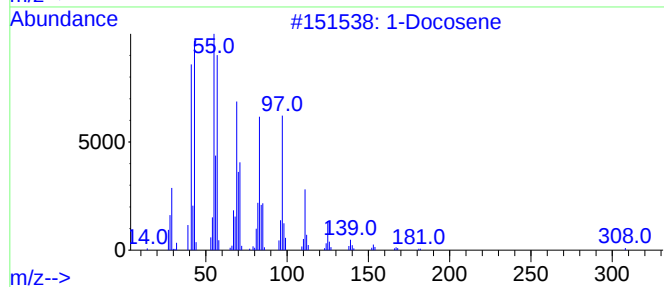
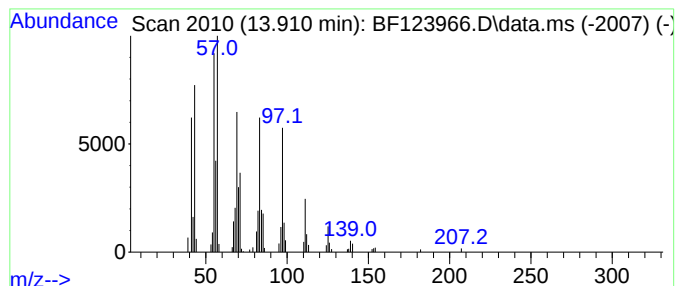
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Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.910	13.32 ng	265678	Chrysene-d12	14.069	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90



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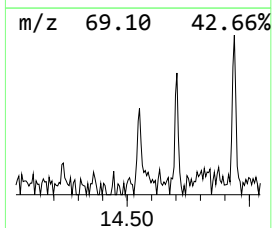
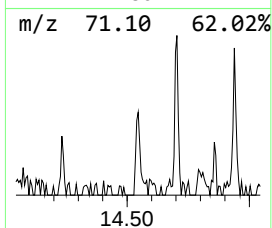
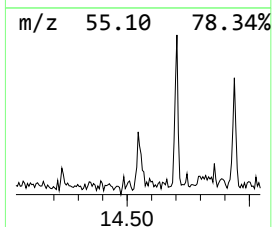
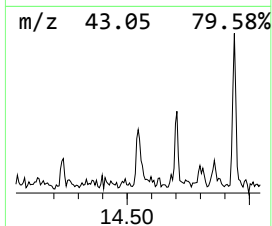
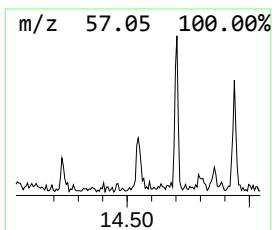
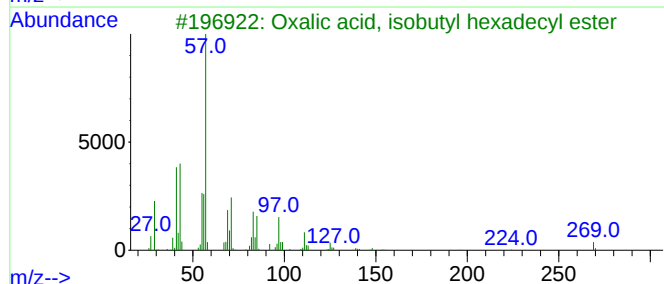
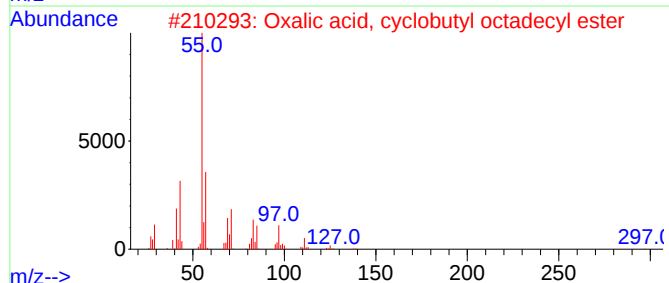
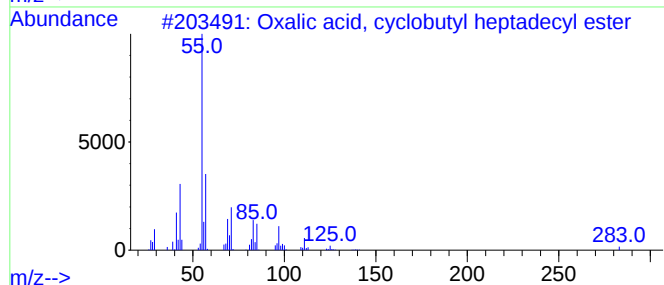
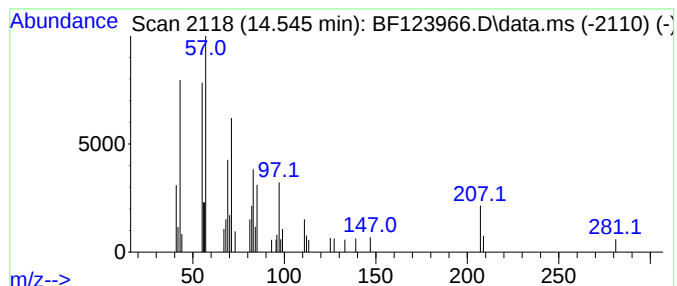
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, cyclobutyl hep... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	3.31 ng	66034	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	83
2			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	83
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	80
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	80
5			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123966.D
Acq On : 17 May 2021 16:40
Operator : JU/CG
Sample : M2420-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-1

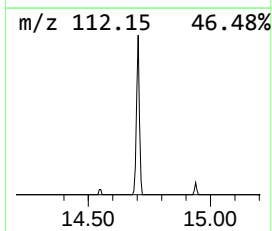
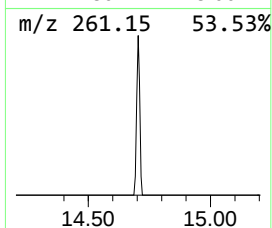
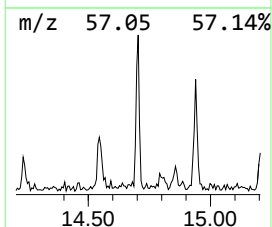
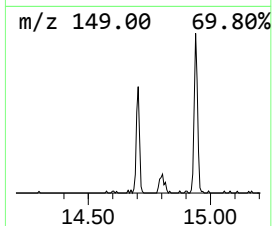
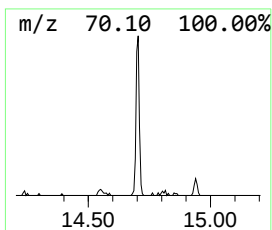
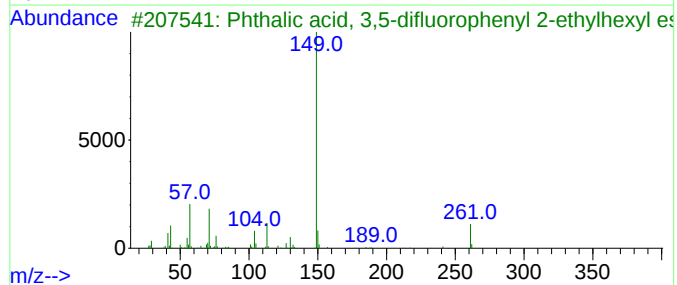
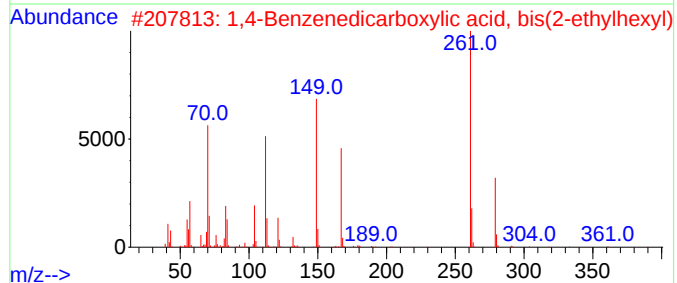
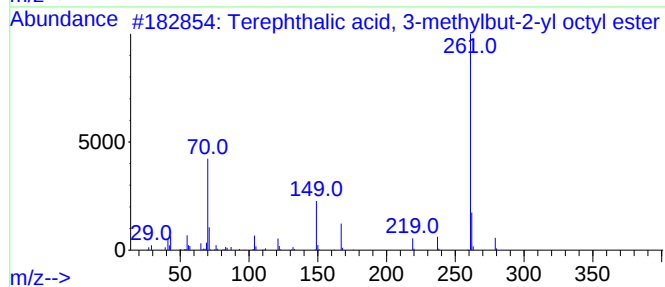
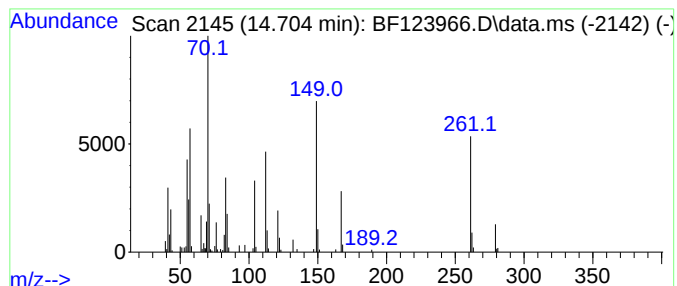
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Terephthalic acid, 3-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	9.71 ng	193679	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
3			Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	27
4			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	27
5			Terephthalic acid, 4-bromophenyl...	432	C22H25BrO4	1000323-68-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123966.D
Acq On : 17 May 2021 16:40
Operator : JU/CG
Sample : M2420-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-1

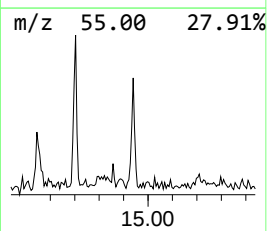
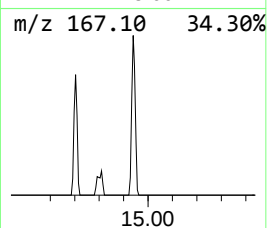
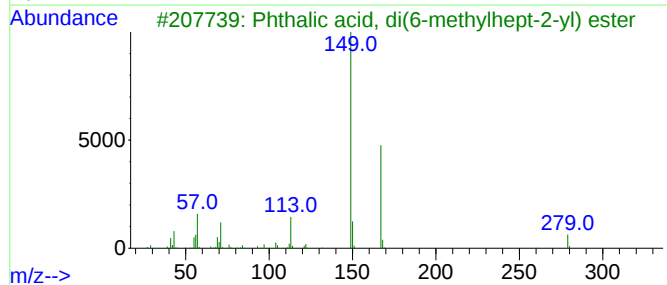
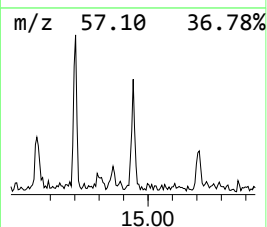
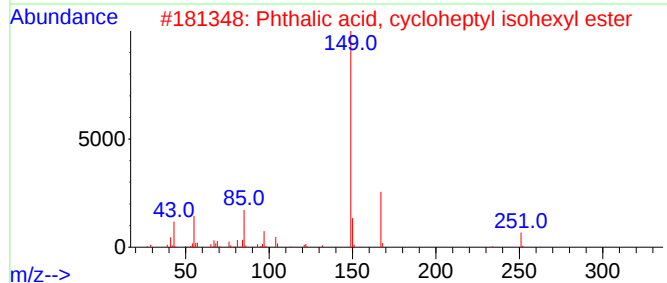
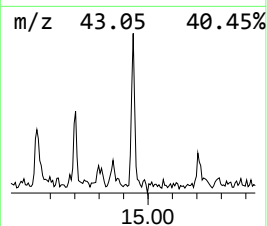
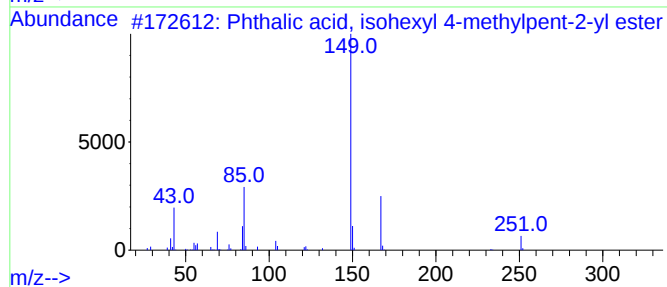
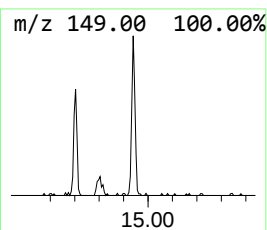
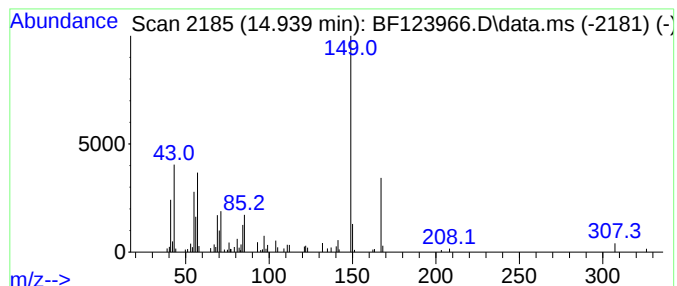
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Phthalic acid, isohexyl 4-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	7.90 ng	142649	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, isohexyl 4-methyl...	334	C20H30O4	1000356-87-5	64
2			Phthalic acid, cycloheptyl isohexyl...	346	C21H30O4	1000322-83-1	64
3			Phthalic acid, di(6-methylhept-2-yl)	390	C24H38O4	1000377-97-3	59
4			Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	59
5			2-(Nonyloxycarbonyl)benzoic acid	292	C17H24O4	1000373-89-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123966.D
Acq On : 17 May 2021 16:40
Operator : JU/CG
Sample : M2420-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	53.3	ng	736287	1	6.904	276543	20.0
unknown2.28	2.281	4.1	ng	56629	1	6.904	276543	20.0
Ethanol, 2-(2-e...	6.722	2.7	ng	36906	1	6.904	276543	20.0
n-Hexadecanoic ...	11.951	3.5	ng	78022	4	11.428	445493	20.0
1-Docosene	13.910	13.3	ng	265678	5	14.069	398767	20.0
Oxalic acid, cy...	14.545	3.3	ng	66034	5	14.069	398767	20.0
Terephthalic ac...	14.704	9.7	ng	193679	5	14.069	398767	20.0
Phthalic acid, ...	14.939	7.9	ng	142649	6	15.563	361069	20.0