

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126935.D
 Acq On : 17 Feb 2022 19:16
 Operator : CG\JU
 Sample : N1573-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-12

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.457	365	369	376	rVB	337485	361719	8.38%	1.559%
2	5.157	484	488	494	rBV	112905	125974	2.92%	0.543%
3	5.546	549	554	557	rBV	1952239	1720610	39.88%	7.417%
4	6.540	719	723	727	rVB	1217674	1121480	25.99%	4.834%
5	6.722	751	754	756	rBV	197851	144425	3.35%	0.623%
6	6.751	756	759	762	rVB	196422	154510	3.58%	0.666%
7	6.840	771	774	783	rBV	265357	249575	5.78%	1.076%
8	6.928	786	789	792	rBV	812614	606586	14.06%	2.615%
9	6.981	795	798	803	rBV	97260	83704	1.94%	0.361%
10	7.492	880	885	888	rVB	2369724	2366530	54.85%	10.202%
11	7.563	893	897	902	rBV	68284	94721	2.20%	0.408%
12	7.922	954	958	963	rBV2	53739	63093	1.46%	0.272%
13	8.110	986	990	997	rBV2	61359	86257	2.00%	0.372%
14	8.210	1003	1007	1010	rBV	1054750	830495	19.25%	3.580%
15	8.357	1029	1032	1040	rBV	55276	57896	1.34%	0.250%
16	8.539	1056	1063	1069	rBV2	141466	187394	4.34%	0.808%
17	9.157	1164	1168	1173	rBV	195070	207612	4.81%	0.895%
18	9.286	1183	1190	1193	rBV	4539228	4314326	100.00%	18.598%
19	9.381	1202	1206	1212	rVB	798580	621359	14.40%	2.679%
20	9.969	1302	1306	1309	rVB	1116818	877115	20.33%	3.781%
21	10.381	1372	1376	1379	rVB	149575	123653	2.87%	0.533%
22	10.669	1422	1425	1427	rBV	164840	123657	2.87%	0.533%
23	10.757	1436	1440	1444	rBV	2699531	2705206	62.70%	11.661%
24	11.457	1555	1559	1562	rBV	1194999	906082	21.00%	3.906%
25	11.833	1620	1623	1626	rBV	146436	113347	2.63%	0.489%
26	13.051	1825	1830	1833	rBV	3915903	3885454	90.06%	16.749%
27	14.098	2005	2008	2012	rBV	623933	521652	12.09%	2.249%
28	15.604	2258	2264	2273	rBV	443011	543340	12.59%	2.342%

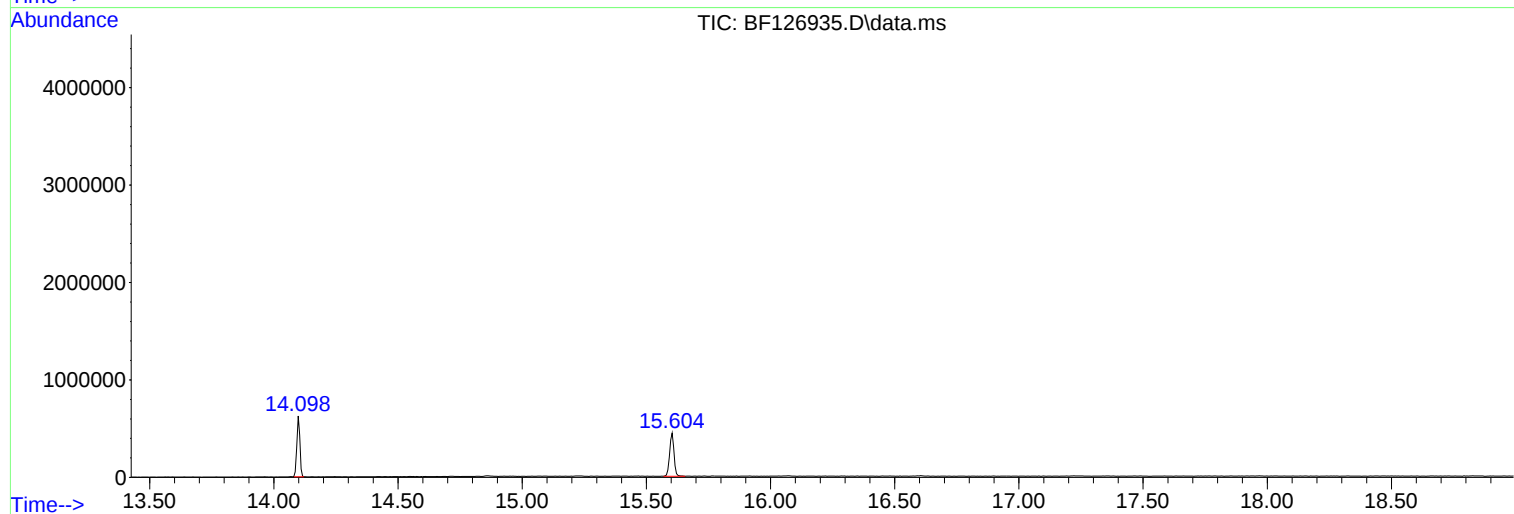
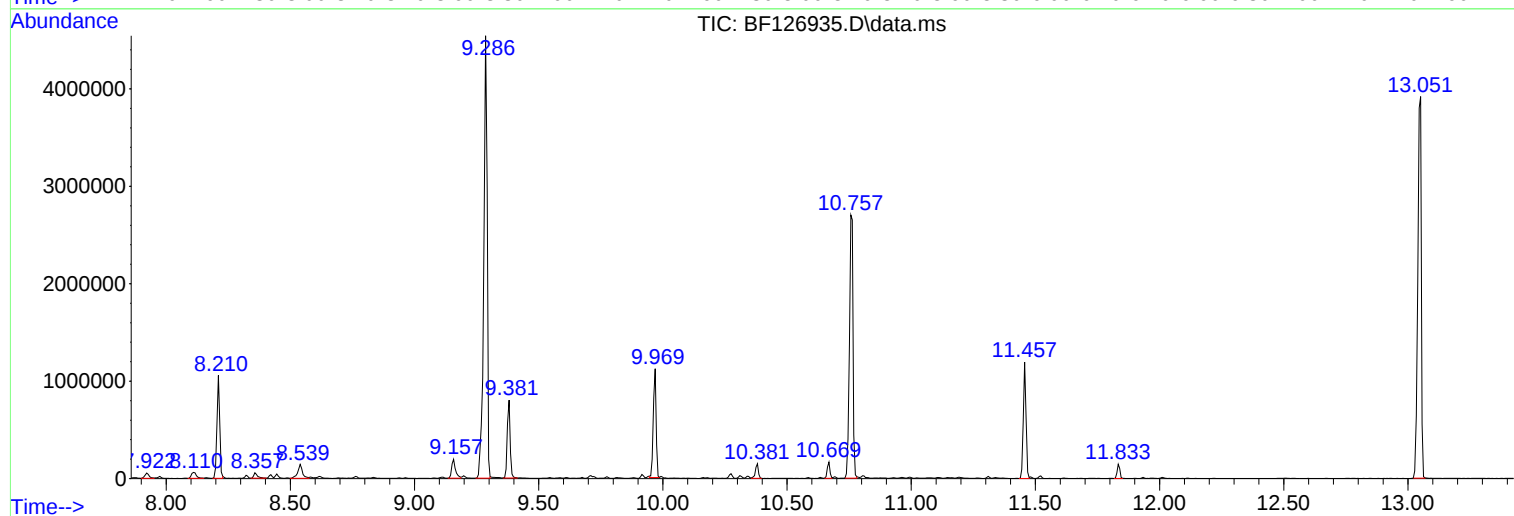
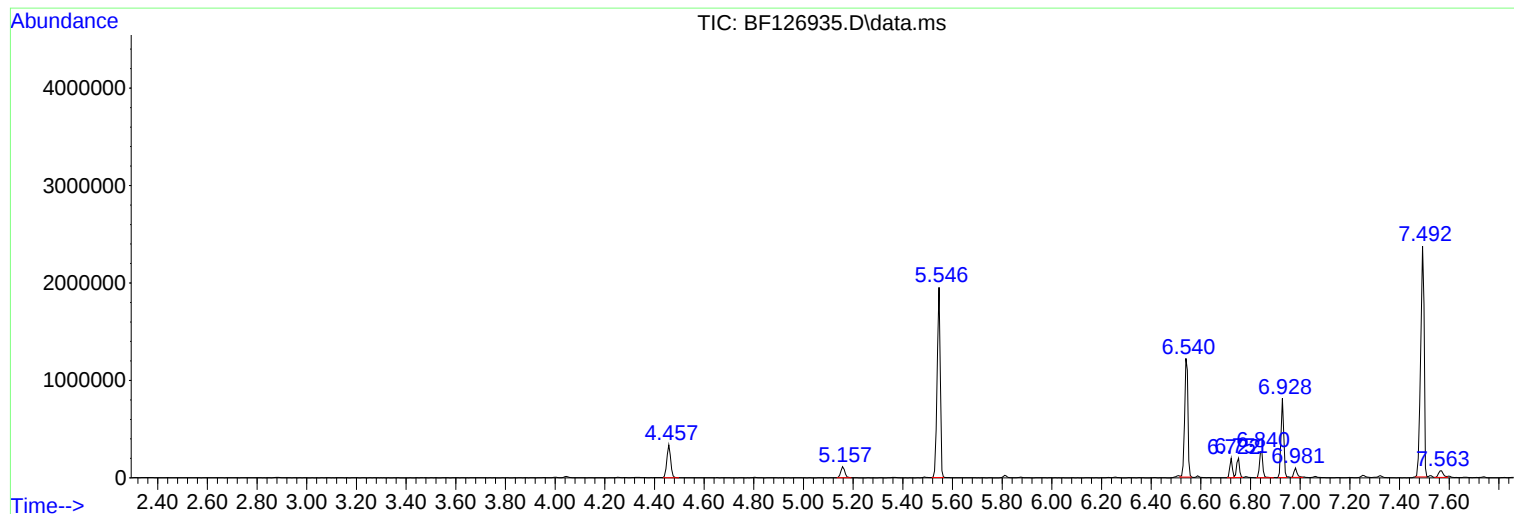
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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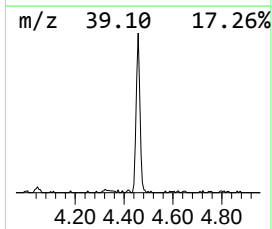
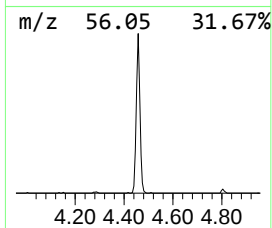
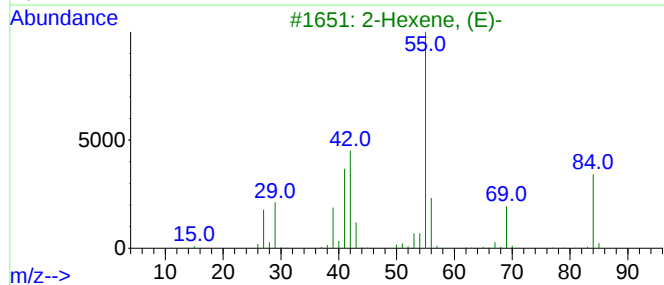
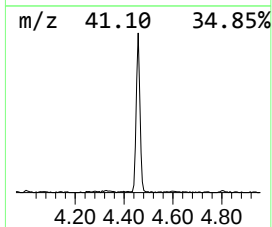
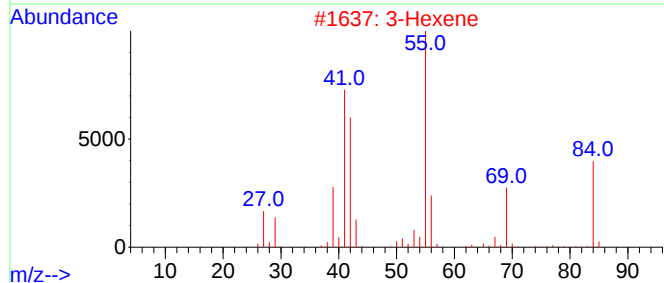
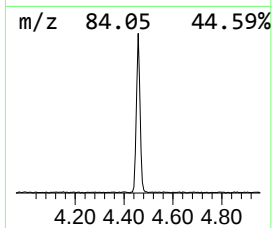
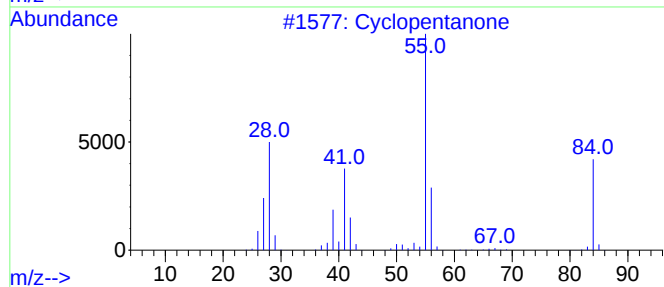
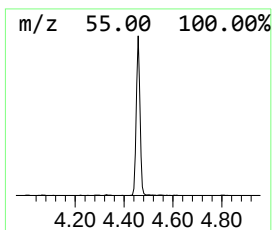
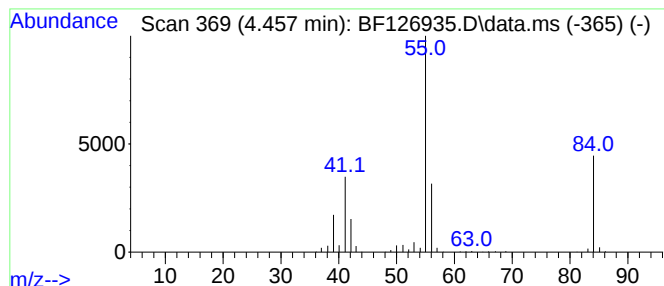
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	11.93 ng	361719	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			3-Hexene	84	C6H12	000592-47-2	64
3			2-Hexene, (E)-	84	C6H12	004050-45-7	64
4			2-Hexene	84	C6H12	000592-43-8	59
5			3-Hexene, (Z)-	84	C6H12	007642-09-3	59



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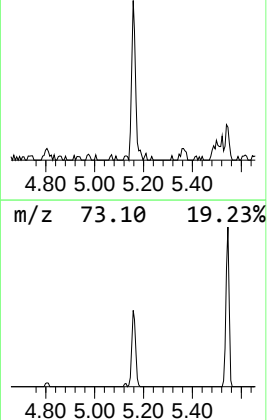
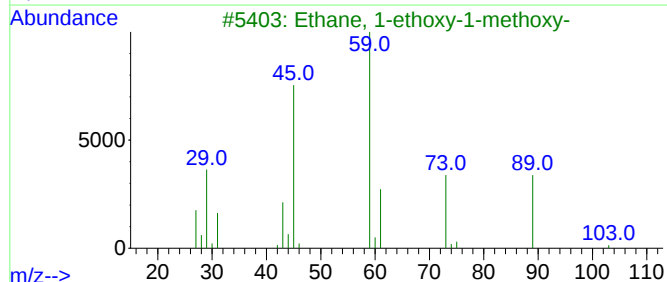
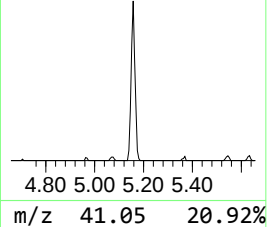
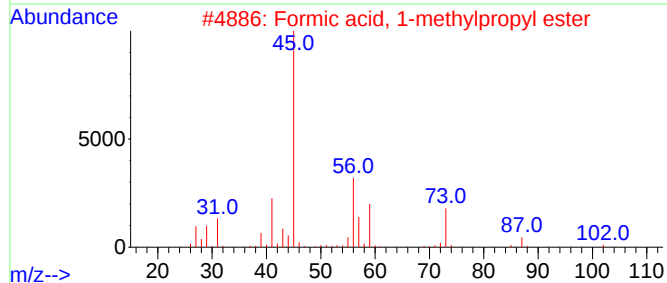
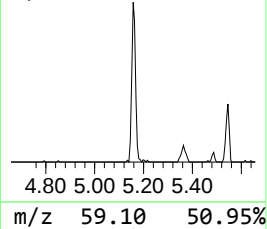
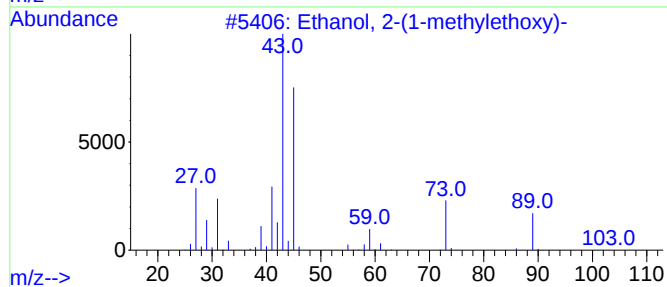
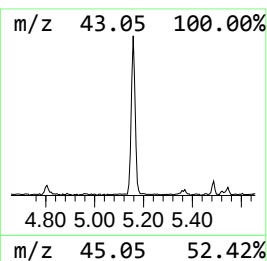
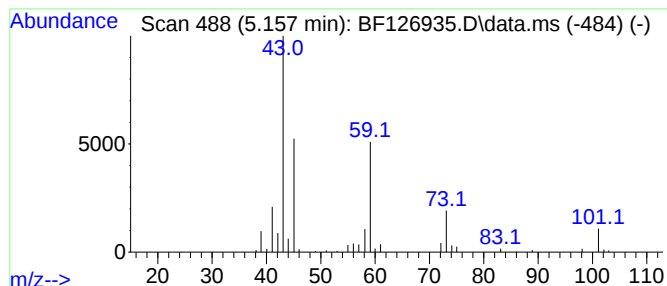
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.157 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	4.15 ng	125974	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	47
2			Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	43
3			Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	40
4			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	38
5			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33



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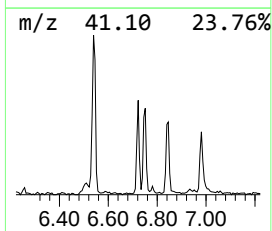
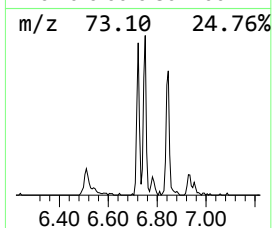
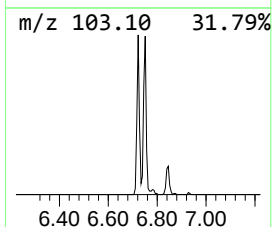
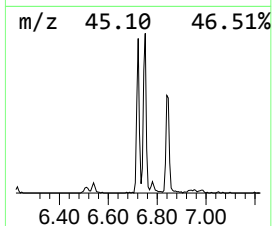
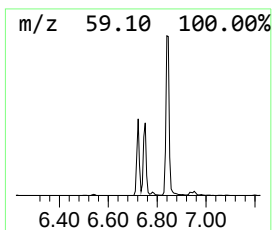
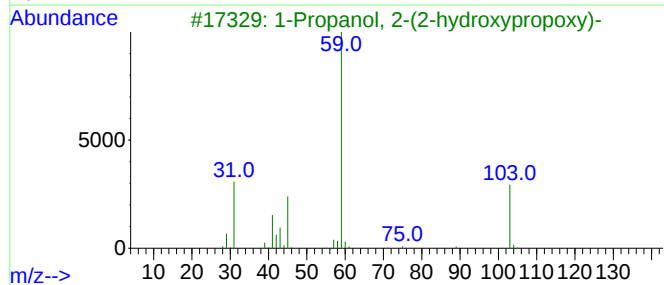
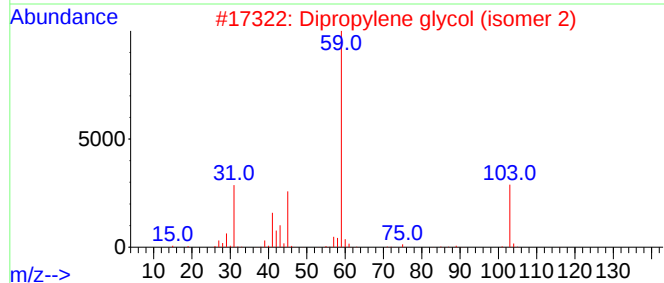
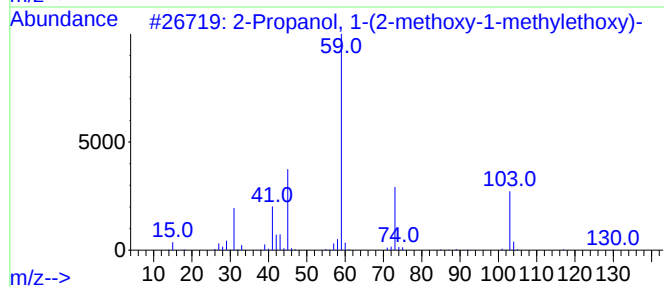
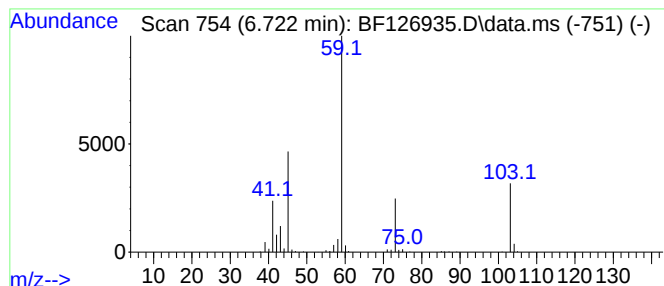
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	4.76 ng	144425	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	42
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	42
5			2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	42



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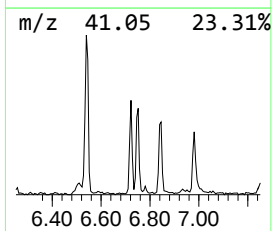
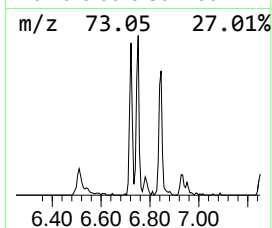
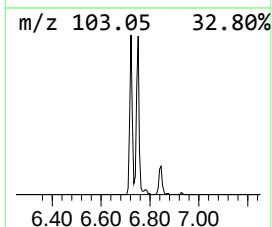
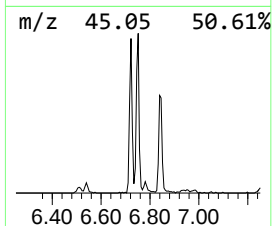
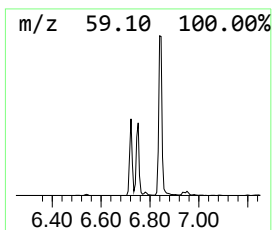
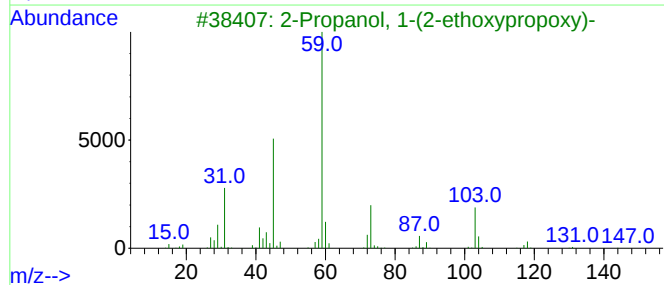
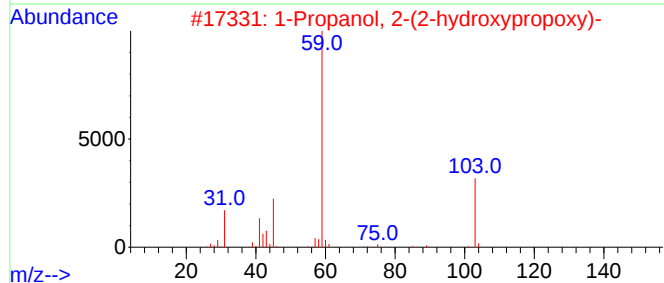
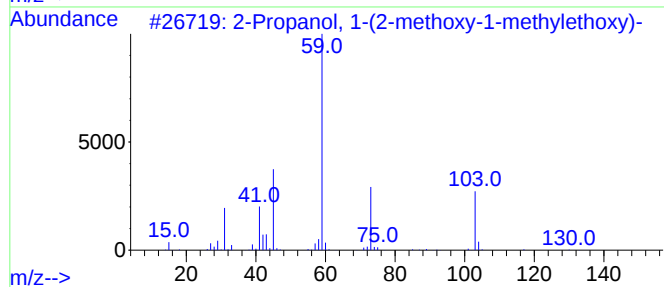
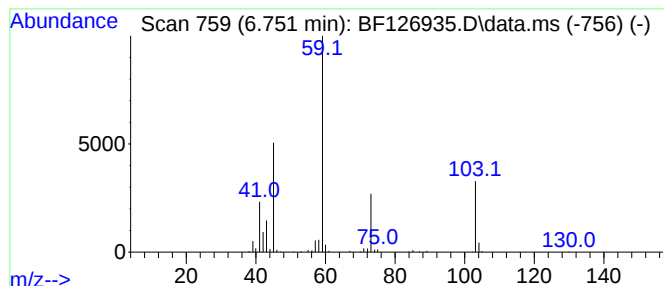
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	5.09 ng	154510	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
3	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53		



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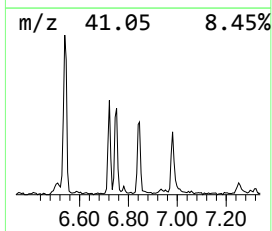
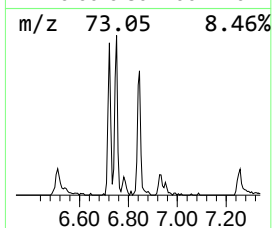
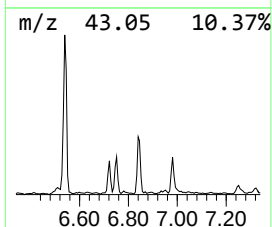
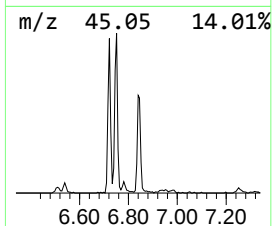
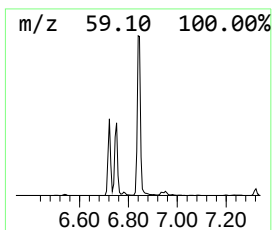
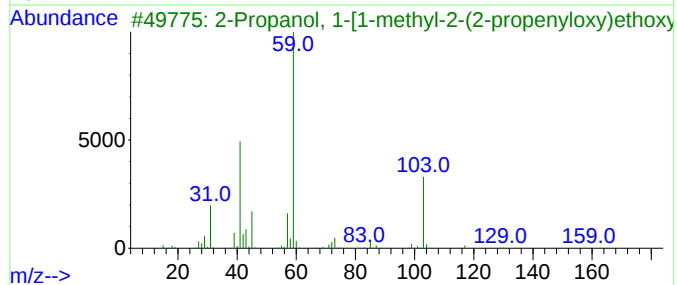
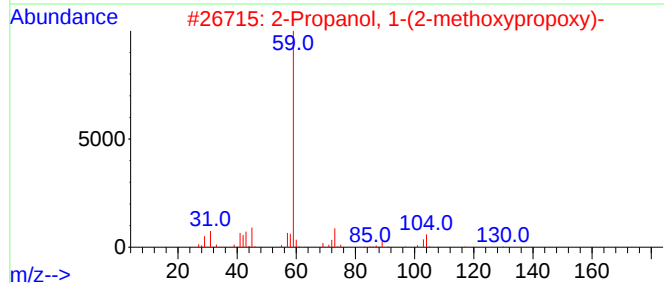
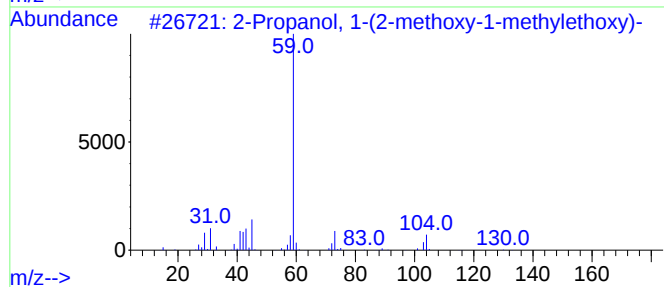
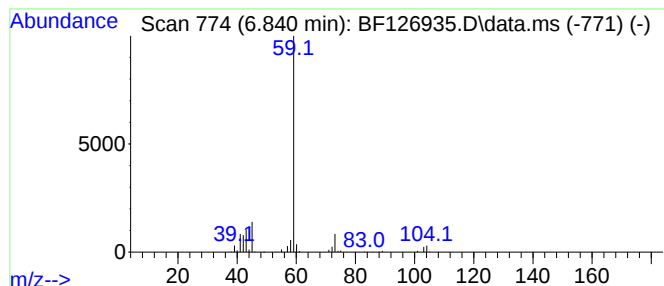
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TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.840	8.23 ng	249575	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83		
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74		
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	56		
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	43		



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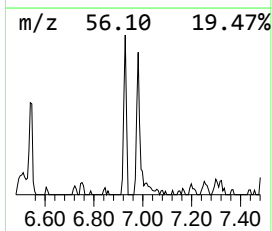
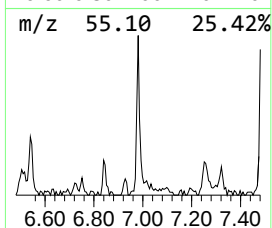
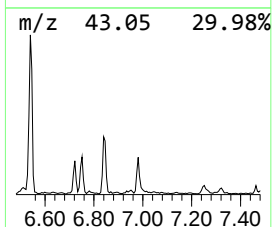
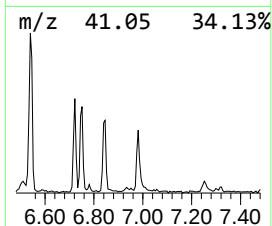
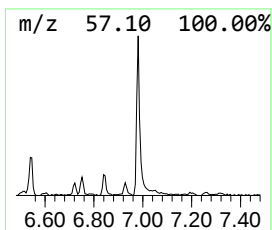
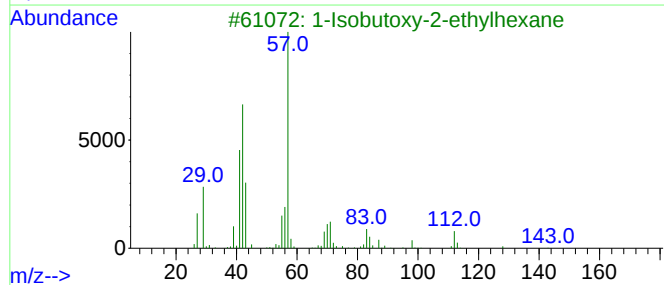
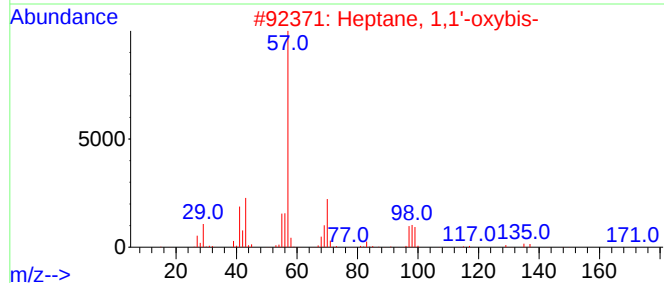
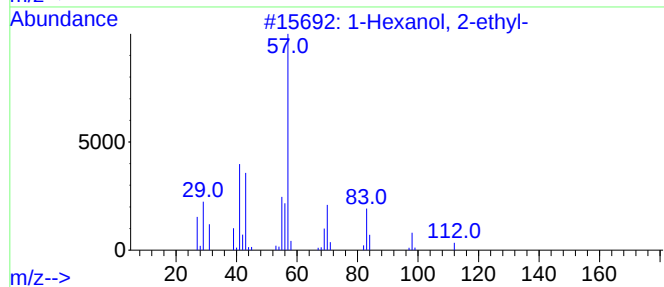
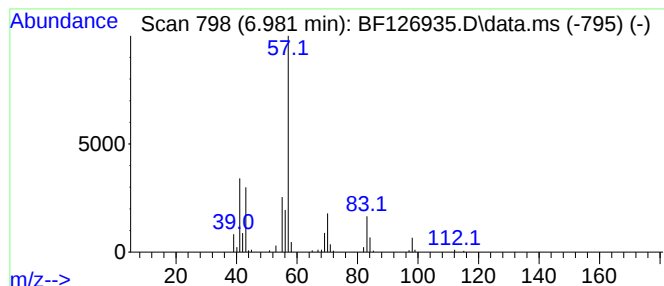
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	2.76 ng	83704	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	53
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
Operator : CG\JU
Sample : N1573-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

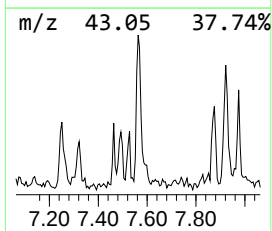
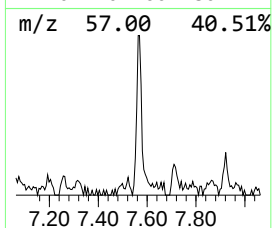
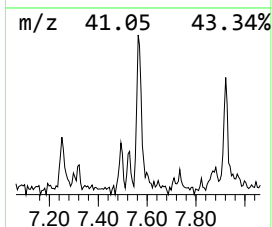
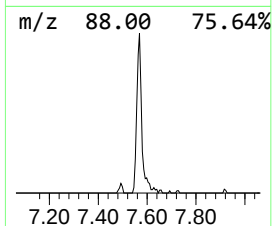
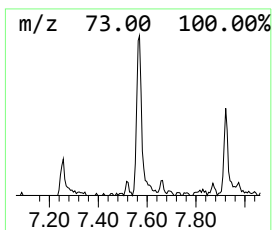
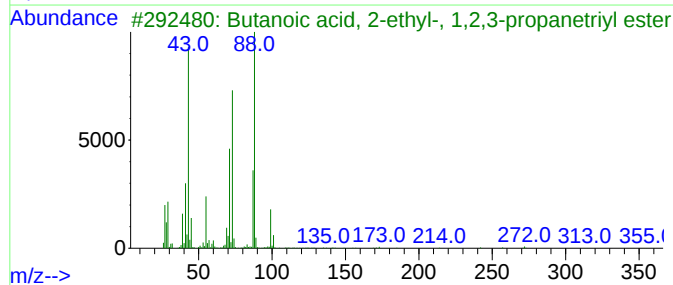
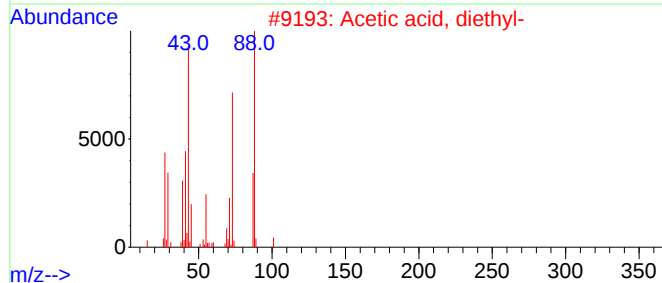
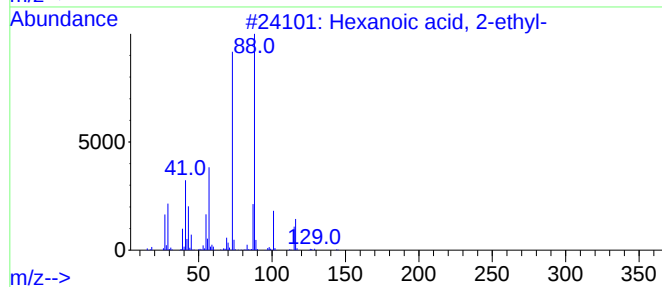
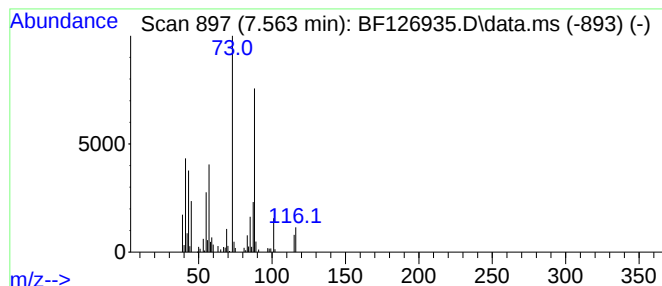
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	3.12 ng	94721	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	53
3			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
4			Lyxopyranoside, methyl 2,3,4-tri...	206	C9H18O5	002876-84-8	42
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
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Sample : N1573-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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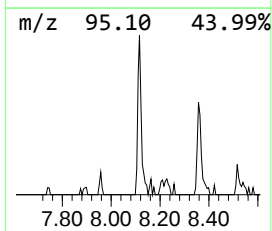
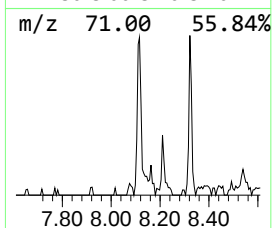
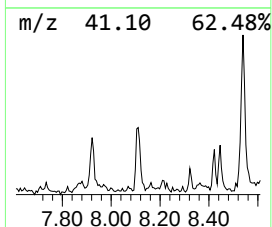
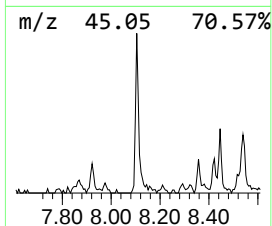
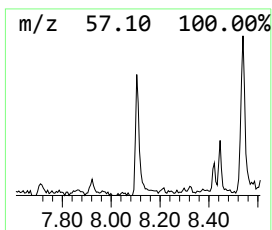
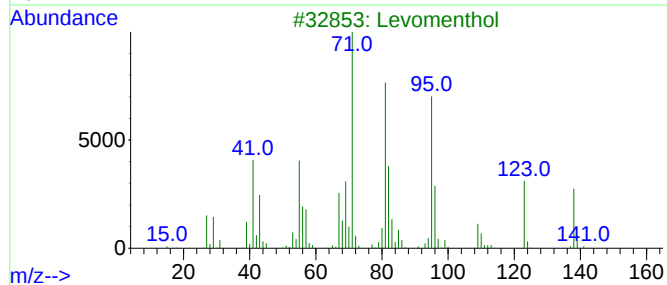
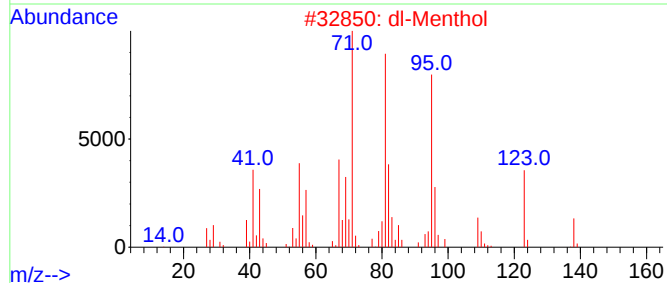
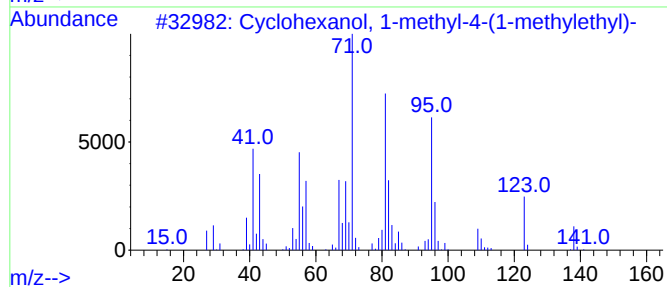
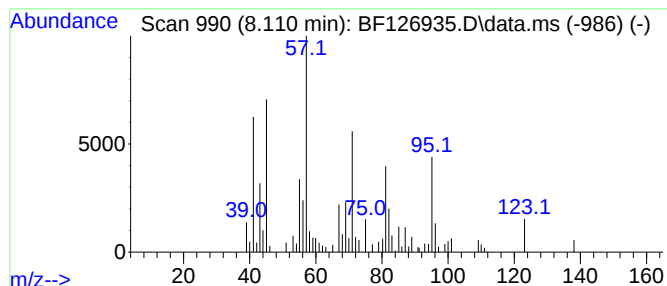
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexanol, 1-methyl-4-(1... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.08 ng	86257	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	021129-27-1	58
2			dl-Menthol	156	C10H20O	000089-78-1	52
3			Levomenthol	156	C10H20O	002216-51-5	49
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	023283-97-8	49
5			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
Operator : CG\JU
Sample : N1573-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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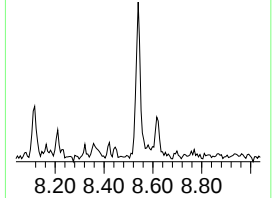
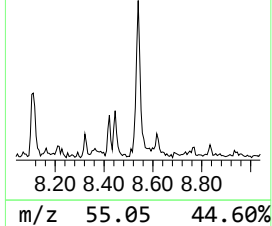
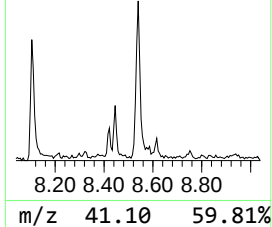
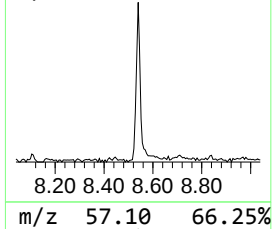
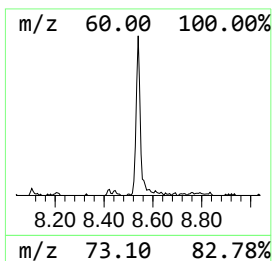
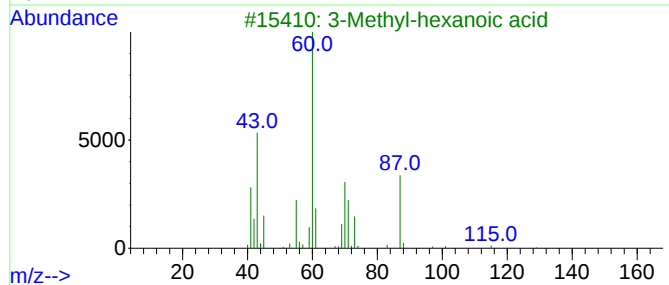
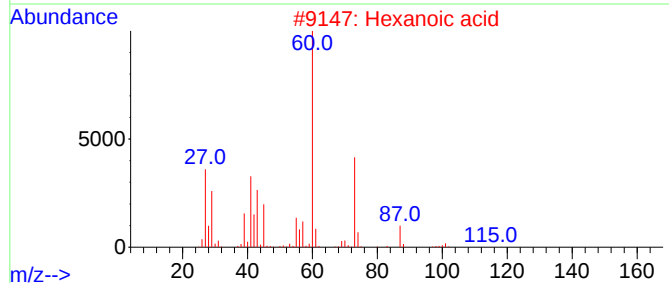
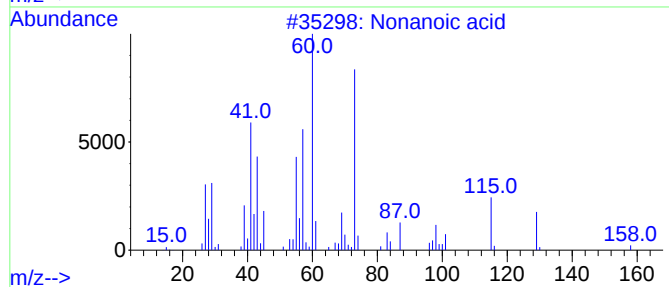
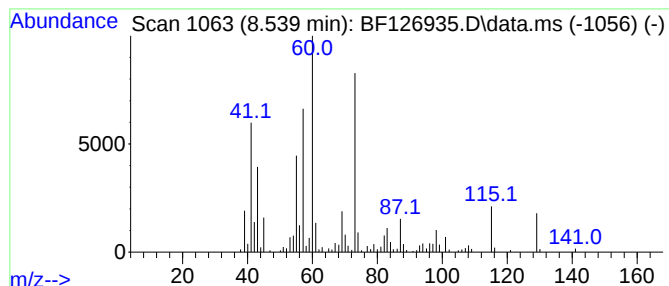
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	4.51 ng	187394	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Hexanoic acid	116	C6H12O2	000142-62-1	53
3			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	47
4			Butanoic acid	88	C4H8O2	000107-92-6	47
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
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Sample : N1573-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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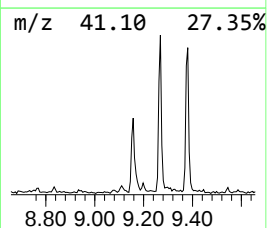
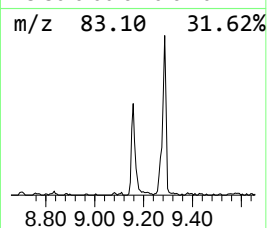
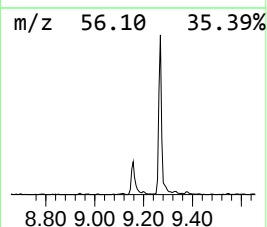
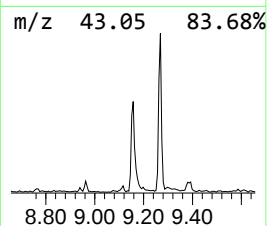
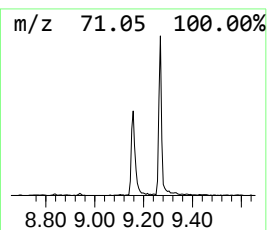
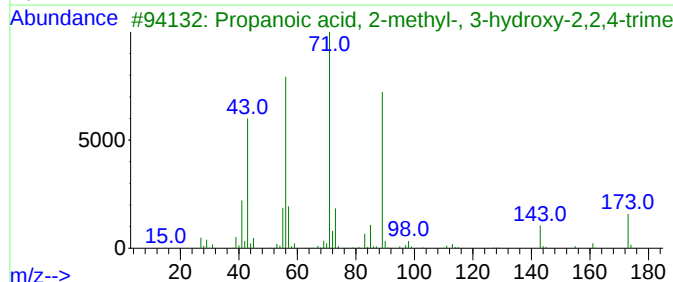
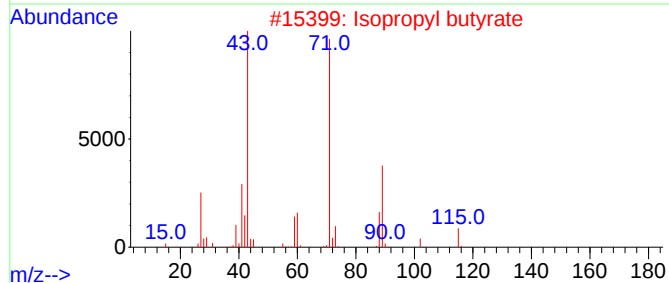
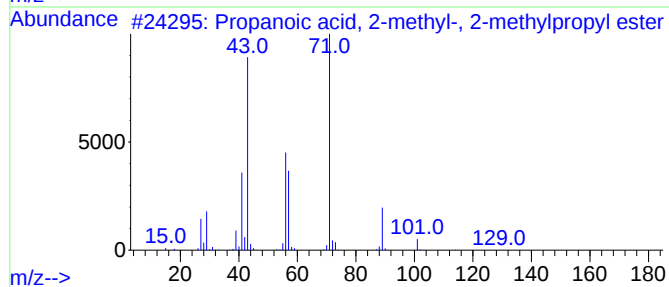
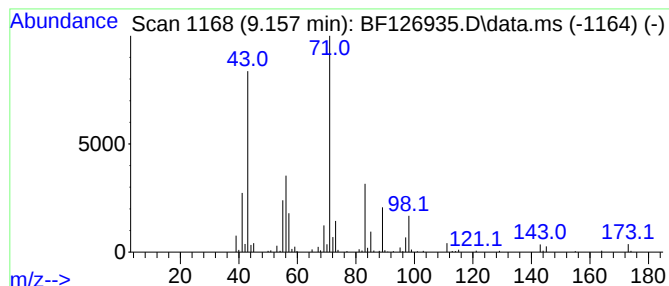
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	4.73 ng	207612	Acenaphthene-d10	9.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
2		Isopropyl butyrate	130	C7H14O2	000638-11-9	38
3		Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	38
4		1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	38
5		5-Nonanol, 2-methylpropionate	214	C13H26O2	1000463-47-6	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-12

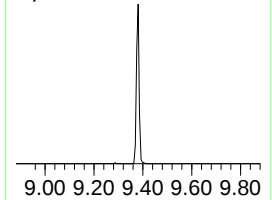
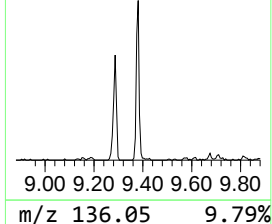
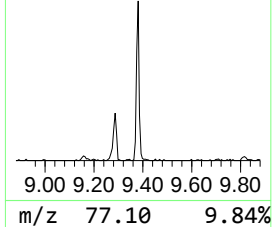
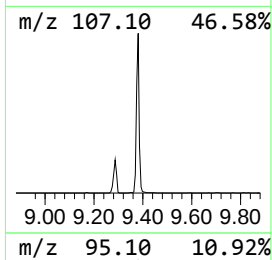
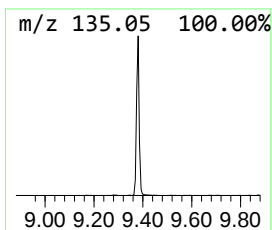
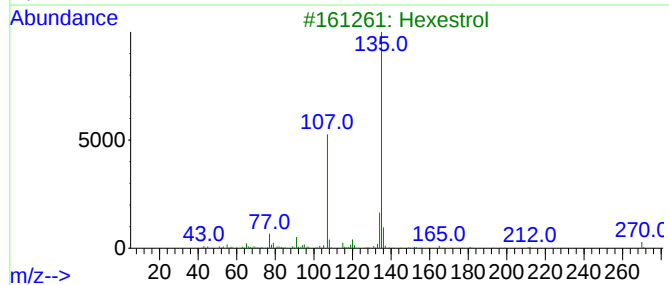
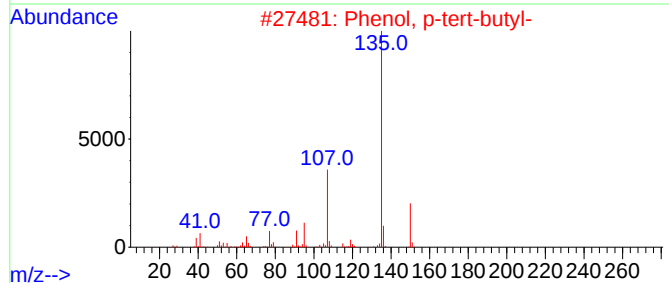
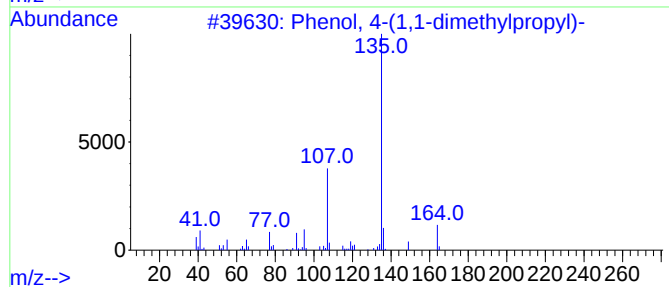
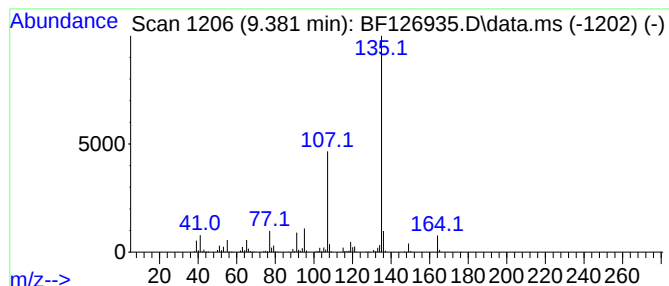
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.381	14.17 ng	621359	Acenaphthene-d10	9.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3		Hexestrol	270	C18H22O2	000084-16-2	72
4		Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
5		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

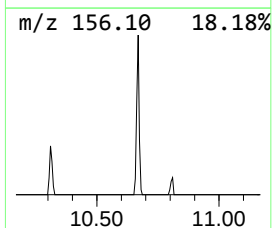
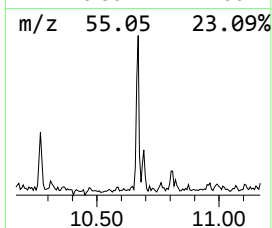
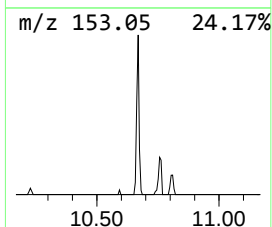
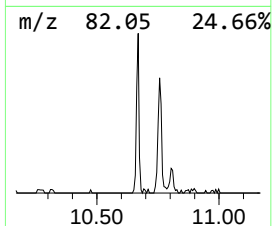
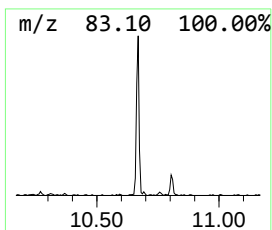
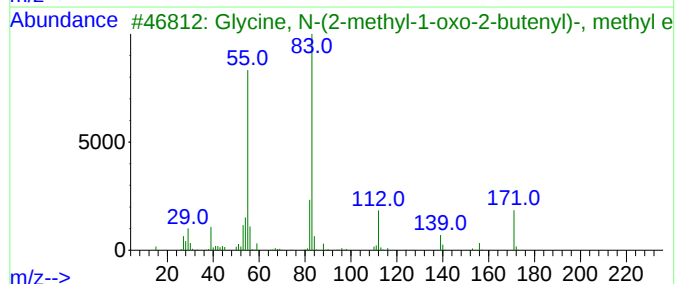
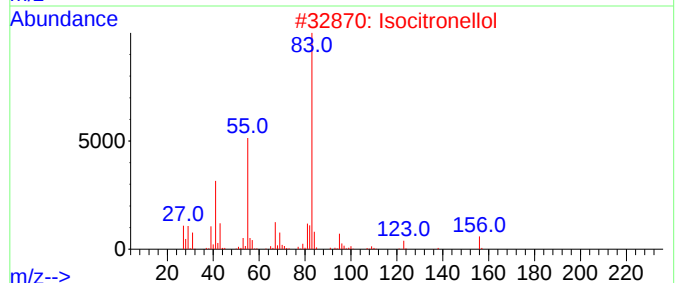
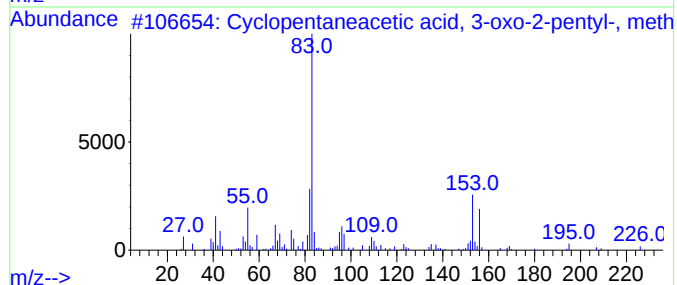
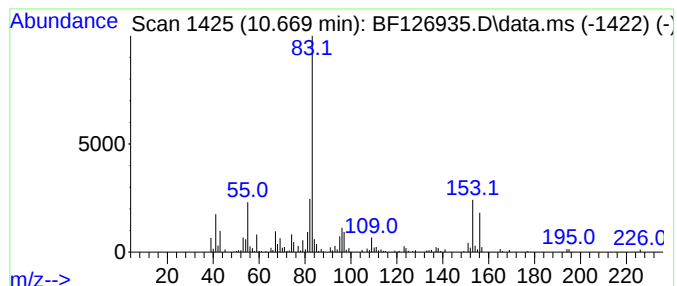
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.669	2.82 ng	123657	Acenaphthene-d10	9.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	94
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	Glycine, N-(2-methyl-1-oxo-2-but...	171	C8H13NO3	055649-53-1	47
4	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	47
5	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126935.D
Acq On : 17 Feb 2022 19:16
Operator : CG\JU
Sample : N1573-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Cyclopentanone	4.457	11.9	ng	361719	1	6.928	606586	20.0
unknown5.157	5.157	4.2	ng	125974	1	6.928	606586	20.0
2-Propanol, 1-(...	6.722	4.8	ng	144425	1	6.928	606586	20.0
1-Propanol, 2-(...	6.751	5.1	ng	154510	1	6.928	606586	20.0
2-Propanol, 1-(...	6.840	8.2	ng	249575	1	6.928	606586	20.0
1-Hexanol, 2-et...	6.981	2.8	ng	83704	1	6.928	606586	20.0
Hexanoic acid, ...	7.563	3.1	ng	94721	1	6.928	606586	20.0
Cyclohexanol, 1...	8.110	2.1	ng	86257	2	8.210	830495	20.0
Nonanoic acid	8.539	4.5	ng	187394	2	8.210	830495	20.0
Propanoic acid,...	9.157	4.7	ng	207612	3	9.969	877115	20.0
Phenol, 4-(1,1-...	9.381	14.2	ng	621359	3	9.969	877115	20.0
Cyclopentaneace...	10.669	2.8	ng	123657	3	9.969	877115	20.0
7,9-Di-tert-but...	11.833	2.5	ng	113347	4	11.457	906082	20.0