

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139180.D
 Acq On : 27 Aug 2024 11:46
 Operator : RC/JU
 Sample : P3717-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF082724.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	16	23	rVB	1109796	1739838	85.11%	11.037%
2	3.387	214	220	237	rBV	30994	77343	3.78%	0.491%
3	5.104	503	512	519	rVB	75101	114159	5.58%	0.724%
4	5.504	574	580	586	rBV	1277098	1712964	83.80%	10.867%
5	6.510	745	751	756	rBV	1330476	1777100	86.94%	11.273%
6	6.710	781	785	800	rBV	17511	26847	1.31%	0.170%
7	6.892	811	816	821	rVB	405503	497974	24.36%	3.159%
8	7.451	905	911	916	rBV	875105	1124483	55.01%	7.133%
9	7.704	949	954	958	rVB	40948	47894	2.34%	0.304%
10	8.169	1028	1033	1039	rBV	492537	626305	30.64%	3.973%
11	8.481	1081	1086	1095	rBV	72005	95410	4.67%	0.605%
12	9.245	1210	1216	1221	rBV	1687684	2044150	100.00%	12.968%
13	9.922	1326	1331	1336	rVB	573977	692365	33.87%	4.392%
14	10.016	1341	1347	1355	rBV	28439	45009	2.20%	0.286%
15	10.710	1459	1465	1470	rBV	888121	1125513	55.06%	7.140%
16	10.833	1481	1486	1494	rVB3	15279	27947	1.37%	0.177%
17	11.410	1579	1584	1589	rBV	515374	645841	31.59%	4.097%
18	11.933	1667	1673	1689	rBV	160641	253788	12.42%	1.610%
19	12.722	1802	1807	1820	rBV	72519	119424	5.84%	0.758%
20	12.992	1848	1853	1858	rBV	1316092	1628455	79.66%	10.330%
21	13.898	2002	2007	2022	rBV	49815	112406	5.50%	0.713%
22	14.045	2026	2032	2038	rVV	338291	447122	21.87%	2.836%
23	14.521	2109	2113	2126	rBV2	18107	35440	1.73%	0.225%
24	14.833	2162	2166	2172	rBV	17094	23732	1.16%	0.151%
25	14.910	2175	2179	2184	rVB2	18737	25014	1.22%	0.159%
26	15.180	2220	2225	2230	rBV	25950	40235	1.97%	0.255%
27	15.515	2276	2282	2287	rBV	322051	482980	23.63%	3.064%
28	15.562	2287	2290	2300	rVB	25601	44181	2.16%	0.280%
29	16.010	2361	2366	2372	rBV	28693	49173	2.41%	0.312%
30	16.527	2449	2454	2463	rVB	20328	44077	2.16%	0.280%
31	17.139	2553	2558	2568	rVB	16623	36463	1.78%	0.231%

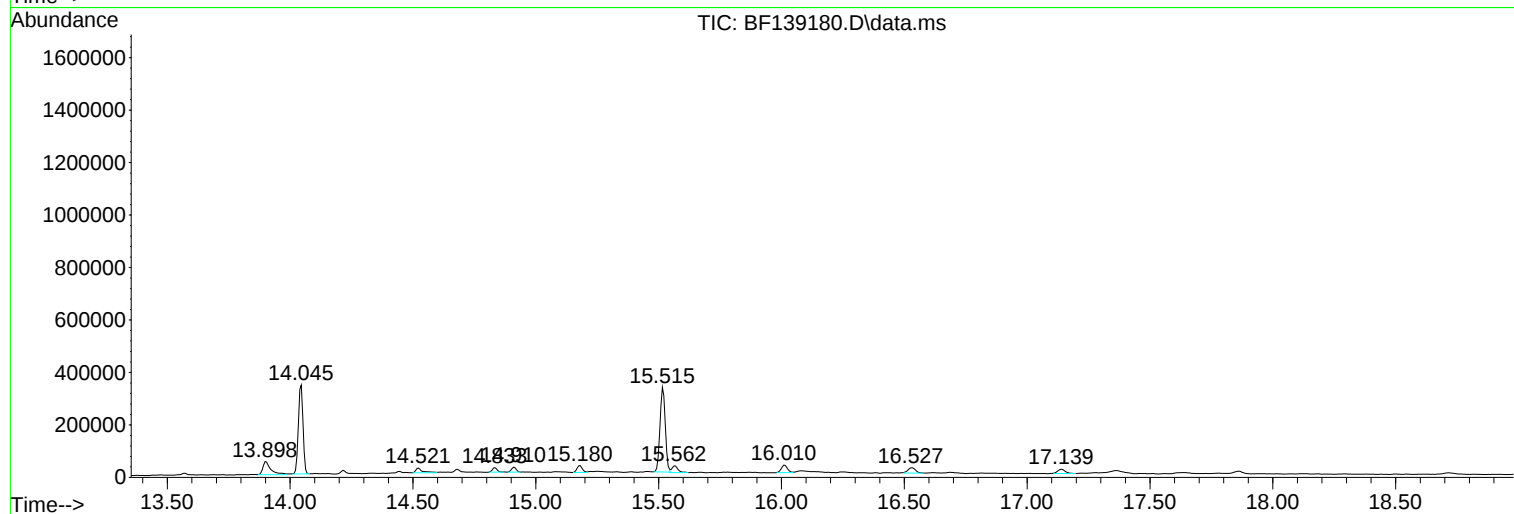
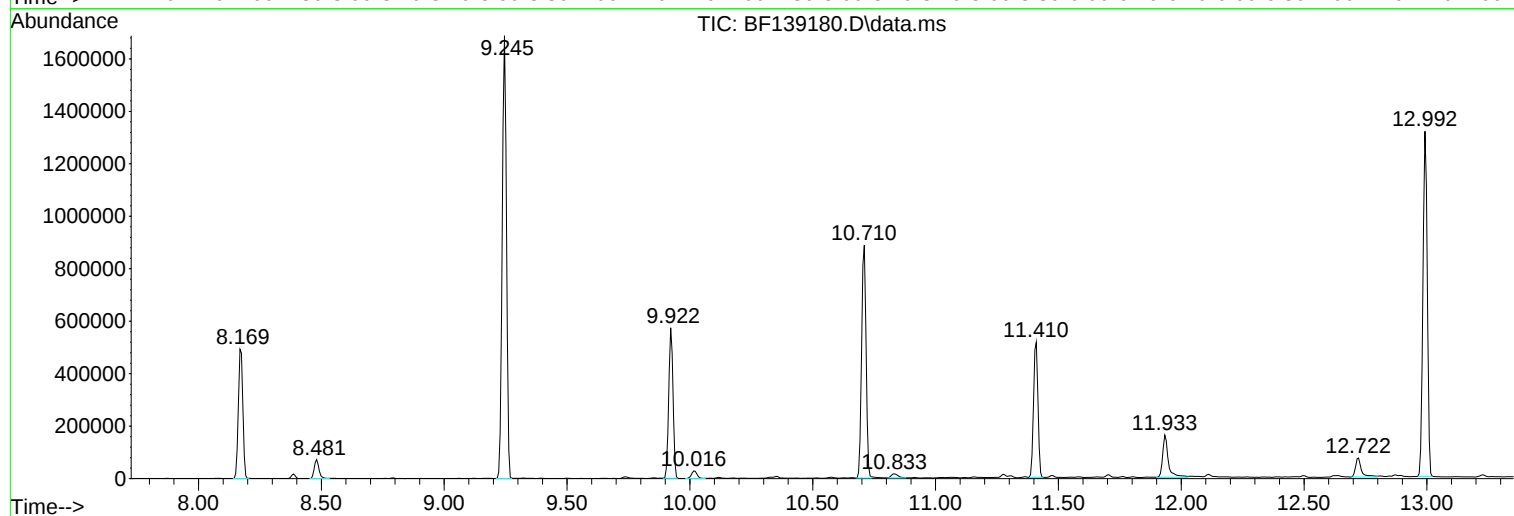
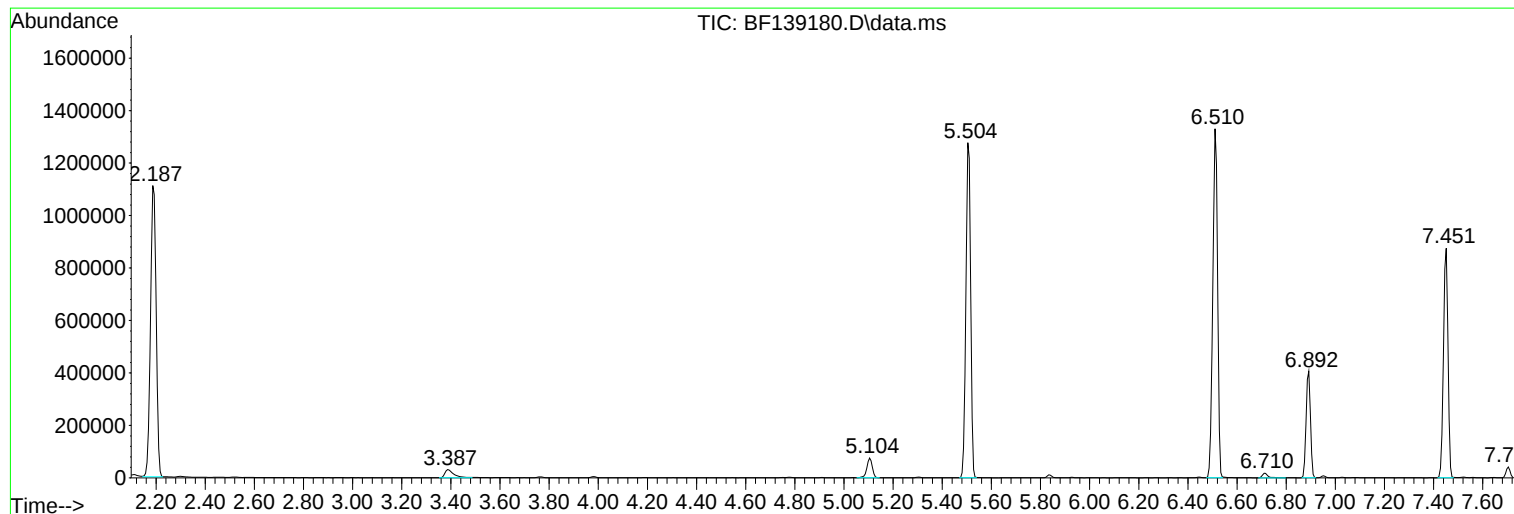
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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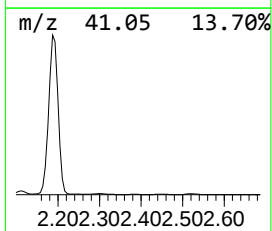
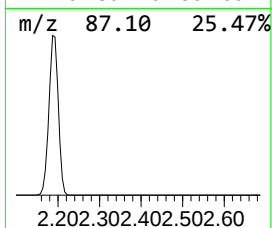
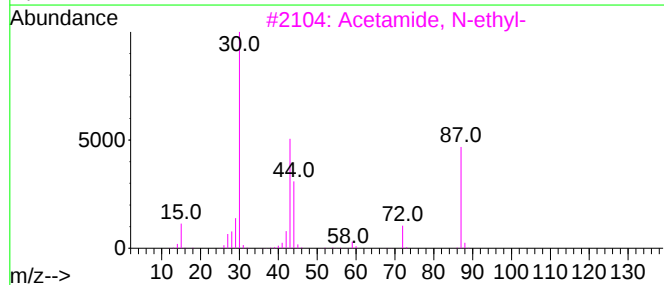
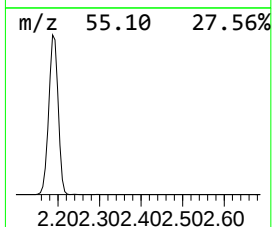
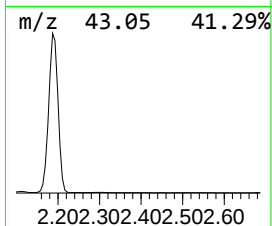
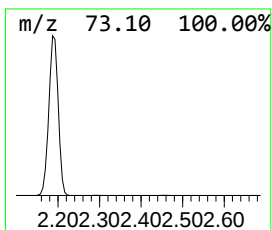
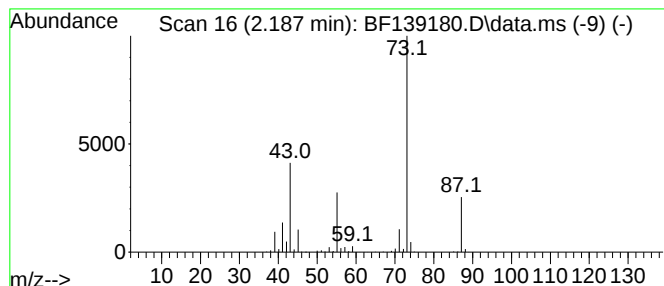
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	69.88 ng	1739840	1,4-Dichlorobenzene-d4	6.892

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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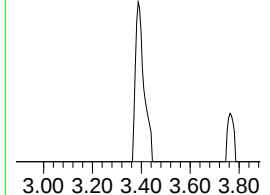
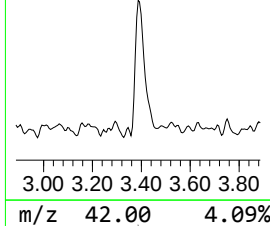
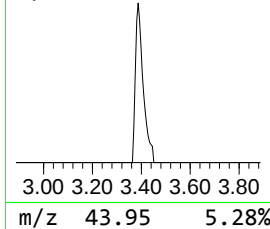
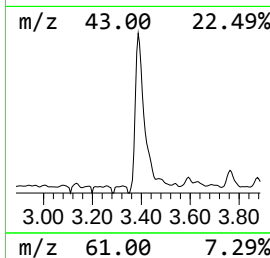
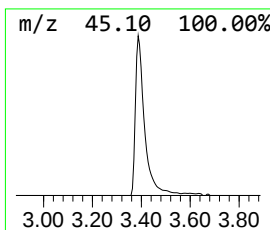
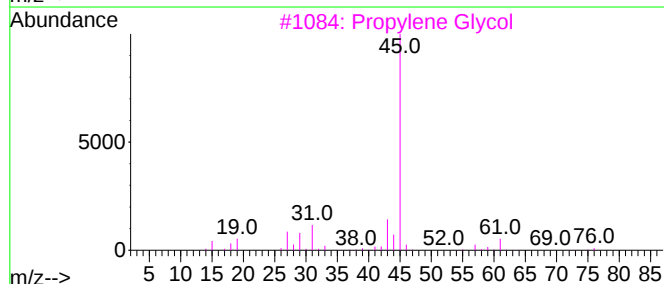
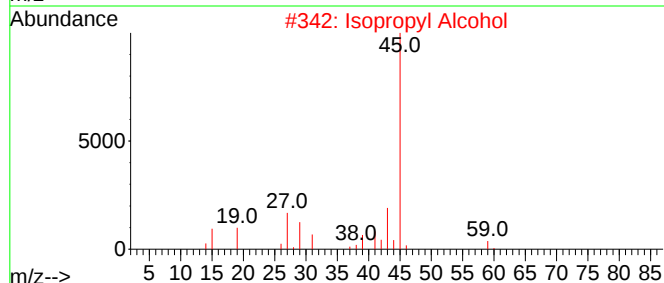
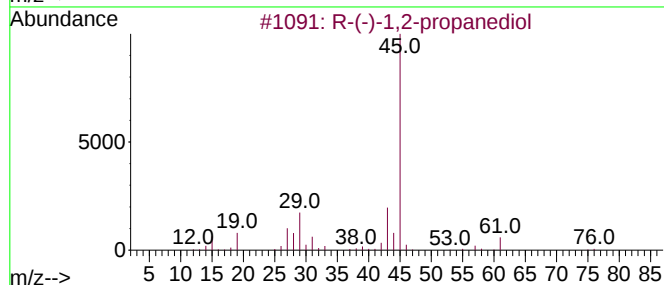
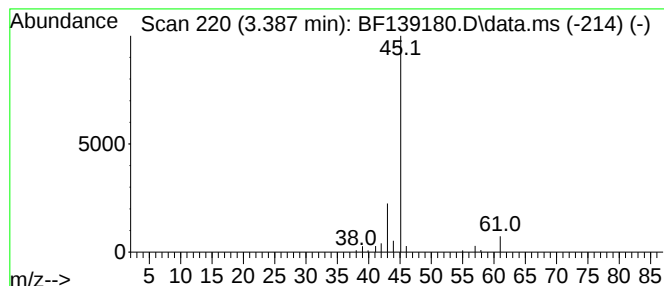
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Peak Number 2 unknown3.387 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	3.11 ng	77343	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	9
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Formamide			45	CH3NO	000075-12-7	5
5	Thiirane			60	C2H4S	000420-12-2	4



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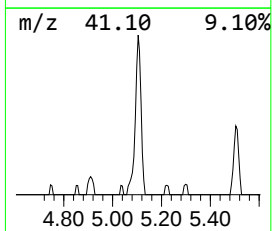
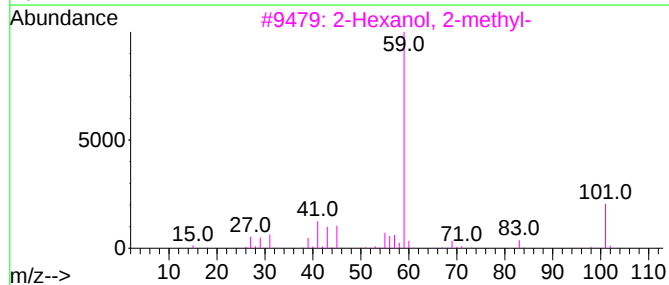
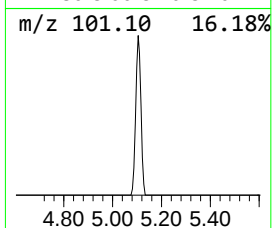
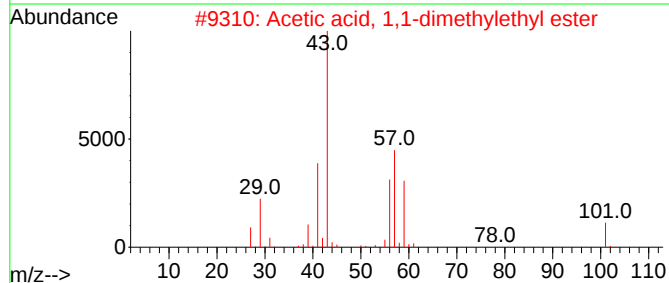
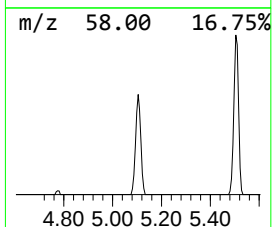
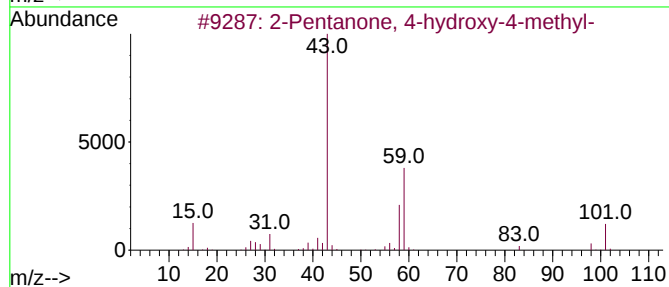
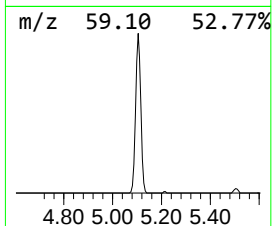
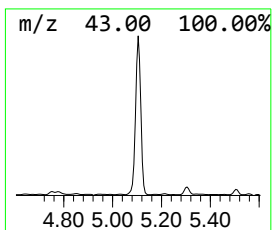
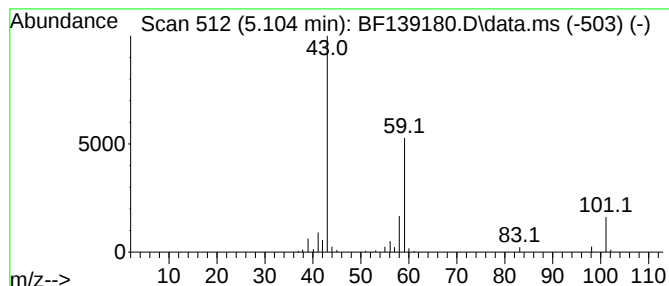
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.58 ng	114159	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Acetone	58	C3H6O	000067-64-1	12		



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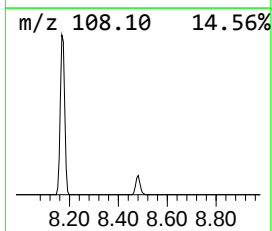
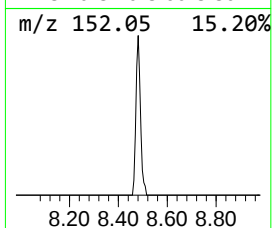
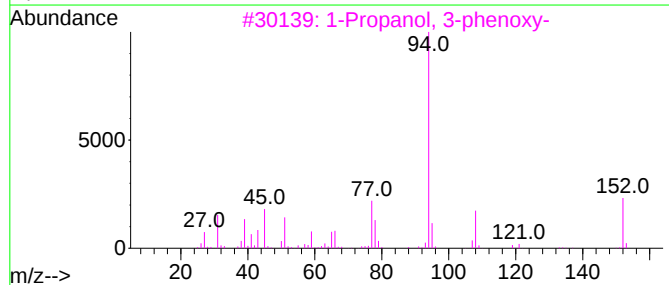
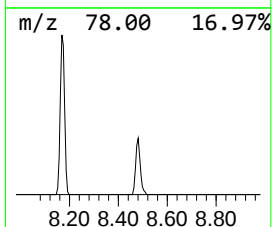
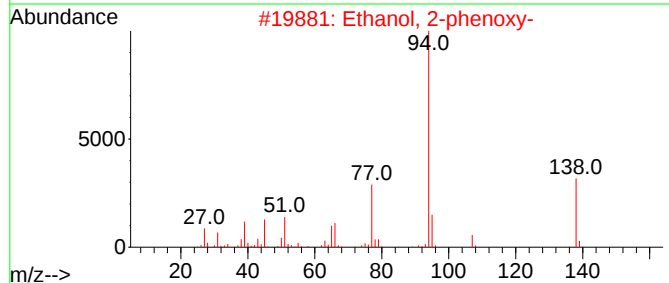
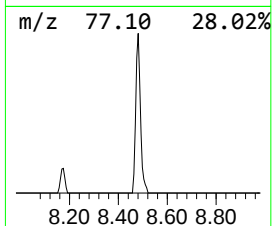
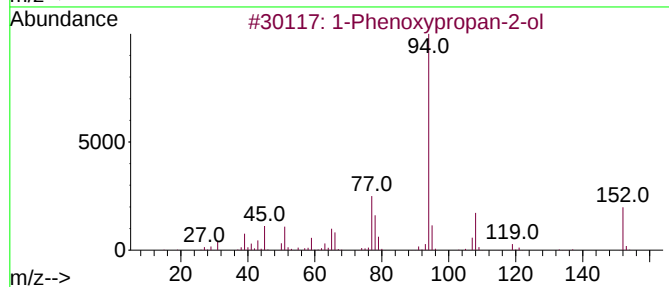
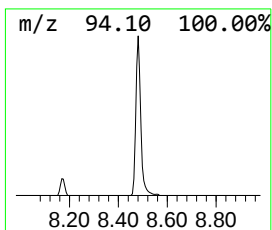
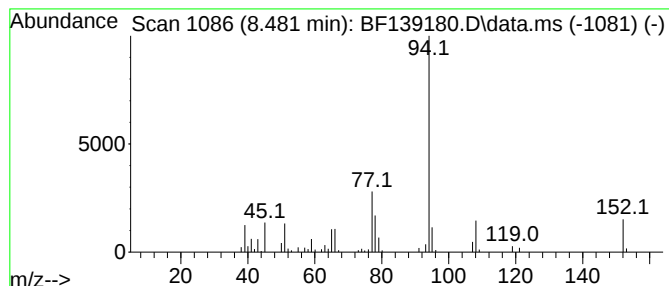
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	3.05 ng	95410	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4		Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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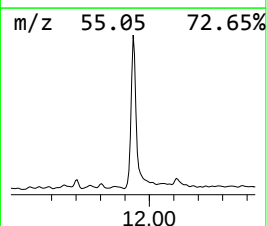
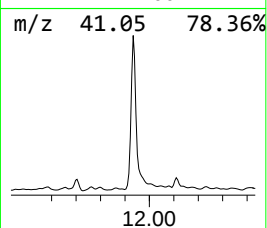
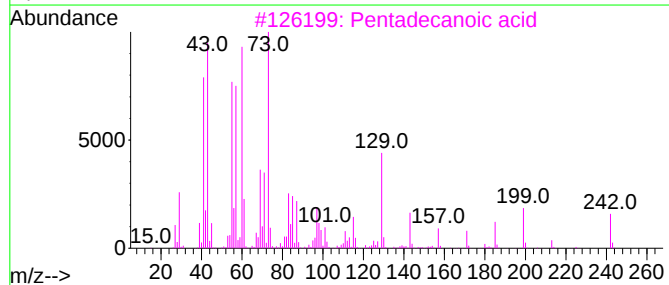
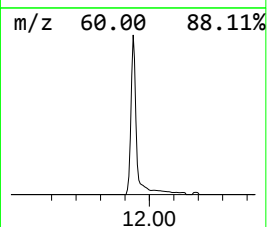
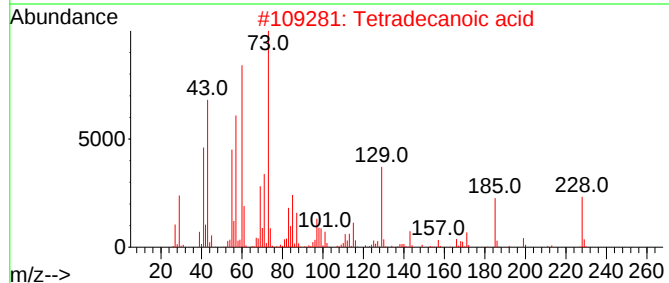
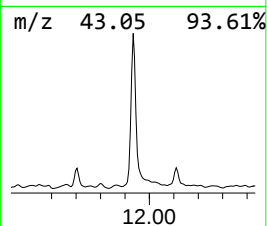
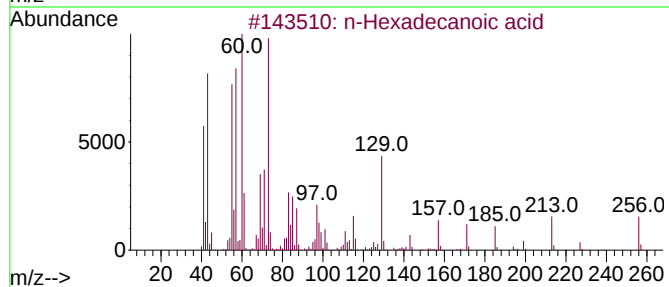
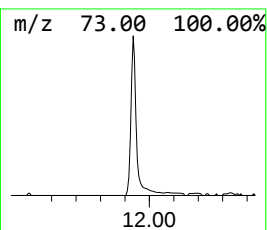
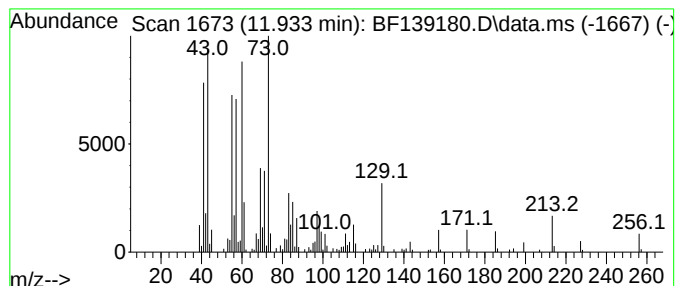
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	7.86 ng	253788	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59



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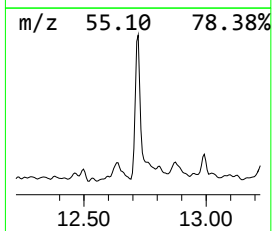
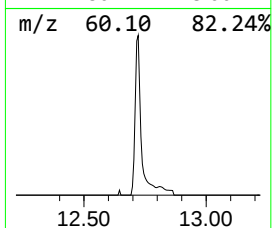
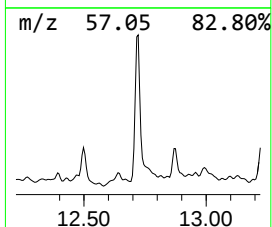
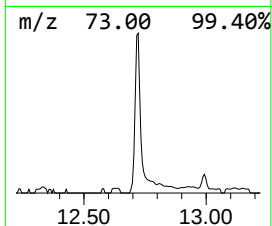
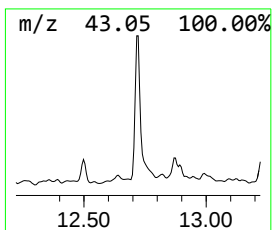
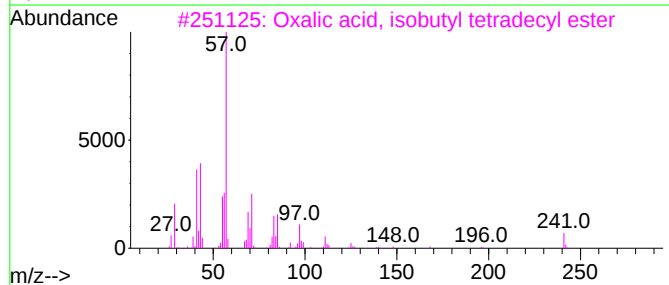
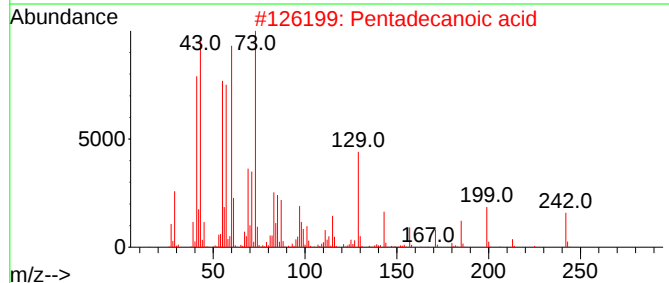
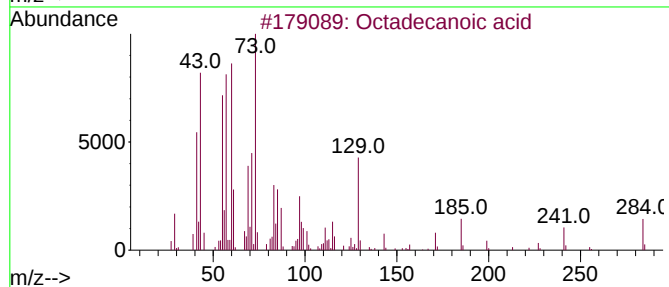
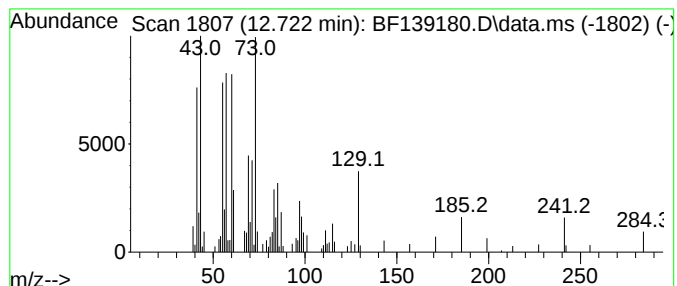
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	3.70 ng	119424	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25
4			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25
5			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139180.D
Acq On : 27 Aug 2024 11:46
Operator : RC/JU
Sample : P3717-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

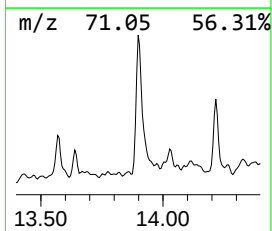
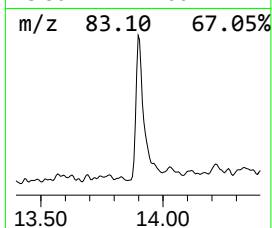
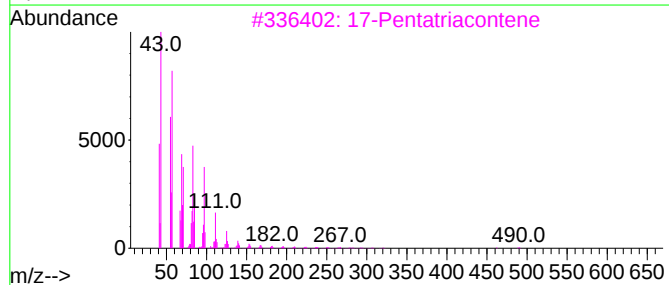
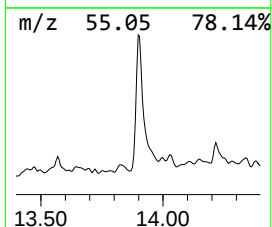
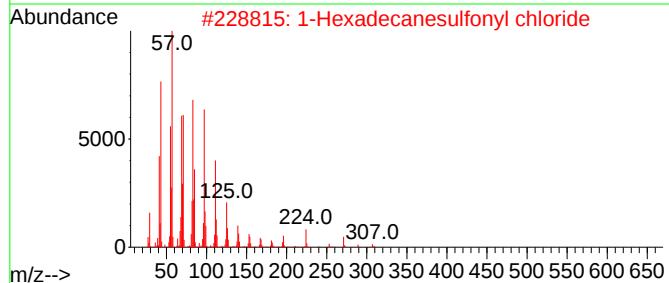
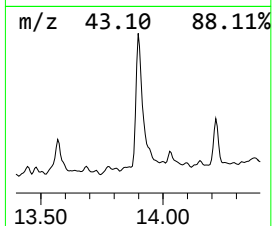
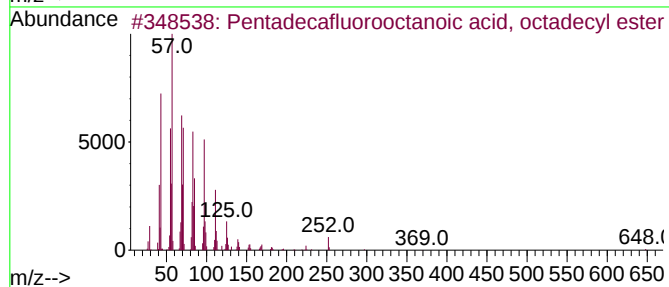
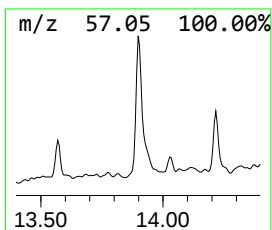
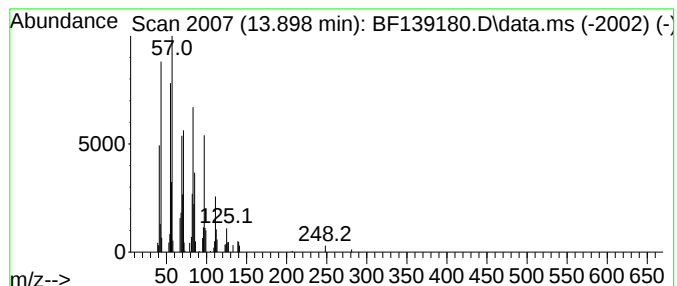
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.03 ng	112406	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139180.D
Acq On : 27 Aug 2024 11:46
Operator : RC/JU
Sample : P3717-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

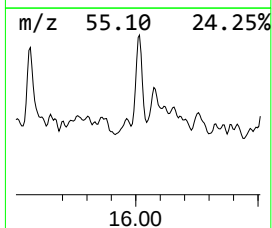
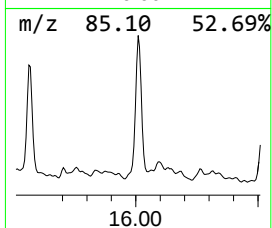
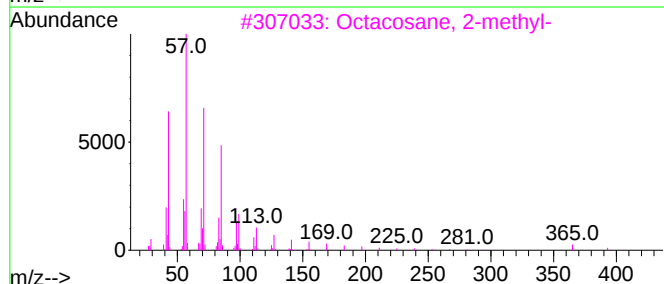
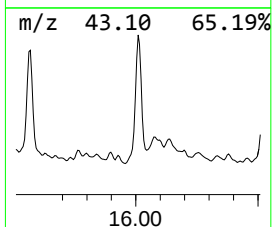
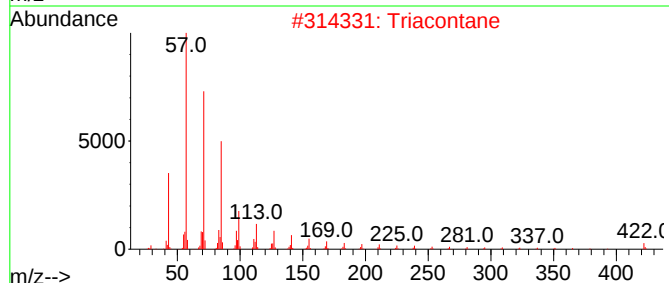
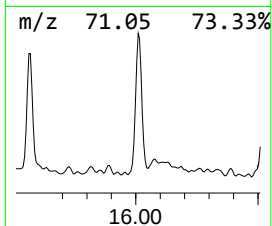
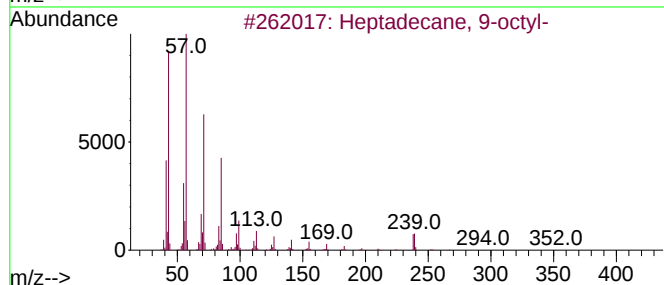
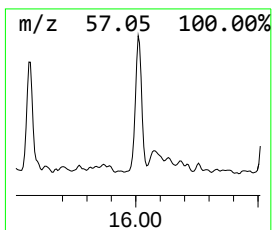
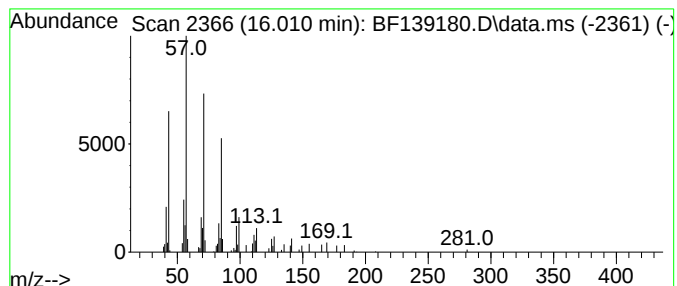
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.04 ng	49173	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Triacontane	422	C30H62	000638-68-6	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139180.D
Acq On : 27 Aug 2024 11:46
Operator : RC/JU
Sample : P3717-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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...	2.187	69.9	ng	1739840	1	6.892	497974	20.0
unknown3.387	3.387	3.1	ng	77343	1	6.892	497974	20.0
2-Pentanone, 4-...	5.104	4.6	ng	114159	1	6.892	497974	20.0
1-Phenoxypropan...	8.481	3.0	ng	95410	2	8.169	626305	20.0
n-Hexadecanoic ...	11.933	7.9	ng	253788	4	11.410	645841	20.0
Octadecanoic acid	12.722	3.7	ng	119424	4	11.410	645841	20.0
Pentadecafluoro...	13.898	5.0	ng	112406	5	14.045	447122	20.0
Heptadecane, 9-...	16.009	2.0	ng	49173	6	15.515	482980	20.0