

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139184.D
 Acq On : 27 Aug 2024 13:47
 Operator : RC/JU
 Sample : P3717-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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: BF139184.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	7	13	22	rVB	746111	1169380	85.79%	9.481%
2	3.375	210	218	243	rBV	15514	49115	3.60%	0.398%
3	5.099	500	511	519	rVB	53035	80759	5.93%	0.655%
4	5.504	574	580	585	rBV	897926	1170627	85.88%	9.491%
5	6.510	745	751	756	rBV	937029	1204922	88.40%	9.769%
6	6.893	811	816	821	rBV	407971	505076	37.06%	4.095%
7	7.446	905	910	916	rBV	569515	737150	54.08%	5.977%
8	7.704	949	954	958	rVB	23370	26553	1.95%	0.215%
9	8.175	1028	1034	1039	rBV	494846	626795	45.99%	5.082%
10	8.481	1081	1086	1096	rBV	43454	55700	4.09%	0.452%
11	9.245	1211	1216	1221	rBV	1141497	1363018	100.00%	11.051%
12	9.363	1232	1236	1239	rBV	30162	36461	2.68%	0.296%
13	9.581	1270	1273	1278	rVB	15848	19252	1.41%	0.156%
14	9.775	1302	1306	1310	rBV	25346	30320	2.22%	0.246%
15	9.839	1313	1317	1325	rVB	65452	94619	6.94%	0.767%
16	9.922	1325	1331	1335	rBV	564893	777613	57.05%	6.305%
17	9.951	1335	1336	1339	rVV	180685	195139	14.32%	1.582%
18	9.981	1339	1341	1345	rVV	134554	147506	10.82%	1.196%
19	10.016	1345	1347	1350	rVV	22491	34000	2.49%	0.276%
20	10.045	1350	1352	1356	rVB	26877	26877	1.97%	0.218%
21	10.598	1436	1446	1449	rBV4	12793	23479	1.72%	0.190%
22	10.710	1453	1465	1469	rBV	588920	753574	55.29%	6.110%
23	10.792	1474	1479	1482	rVV4	28144	47730	3.50%	0.387%
24	10.828	1482	1485	1492	rVB	36778	47813	3.51%	0.388%
25	11.410	1579	1584	1592	rBV	506405	618989	45.41%	5.019%
26	11.933	1666	1673	1685	rBV	93101	143931	10.56%	1.167%
27	12.645	1786	1794	1802	rBV2	17560	49158	3.61%	0.399%
28	12.722	1802	1807	1820	rVV	34937	58135	4.27%	0.471%
29	12.992	1848	1853	1859	rVB	811651	1027998	75.42%	8.335%
30	13.904	2002	2008	2017	rBV2	36450	81178	5.96%	0.658%
31	14.045	2027	2032	2040	rBV	382552	492637	36.14%	3.994%
32	14.527	2110	2114	2126	rBV3	14862	37634	2.76%	0.305%
33	14.910	2176	2179	2186	rVB	12268	18376	1.35%	0.149%
34	15.180	2221	2225	2229	rBV	22213	34738	2.55%	0.282%
35	15.521	2277	2283	2289	rBV	268279	394964	28.98%	3.202%
36	15.774	2322	2326	2332	rVB4	12354	20300	1.49%	0.165%

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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

37	16.016	2362	2367	2372	rBV	17786	30031	2.20%	0.243%
38	17.627	2635	2641	2653	rVB10	19257	55279	4.06%	0.448%
39	18.192	2730	2737	2745	rVB8	18016	46837	3.44%	0.380%

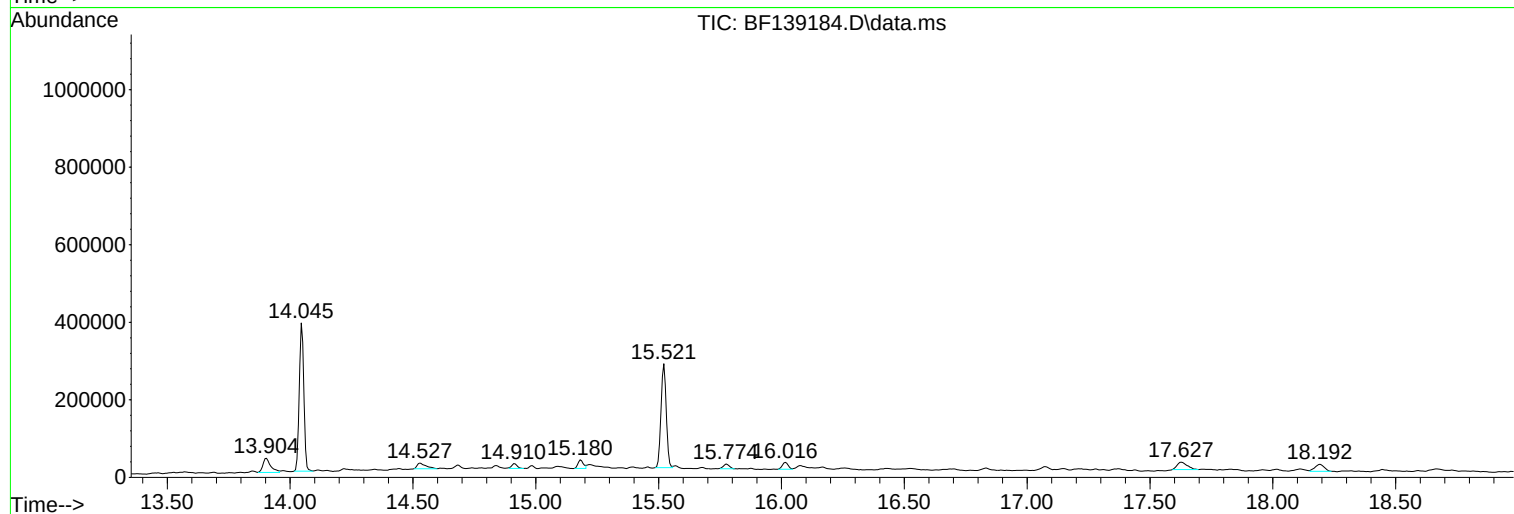
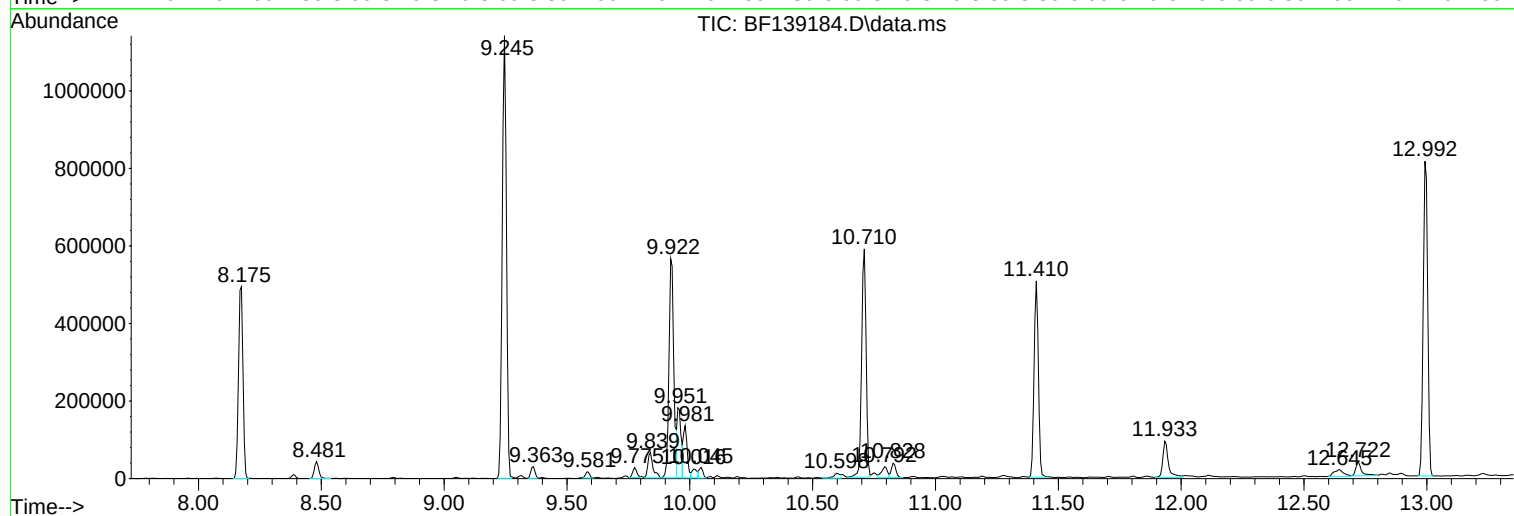
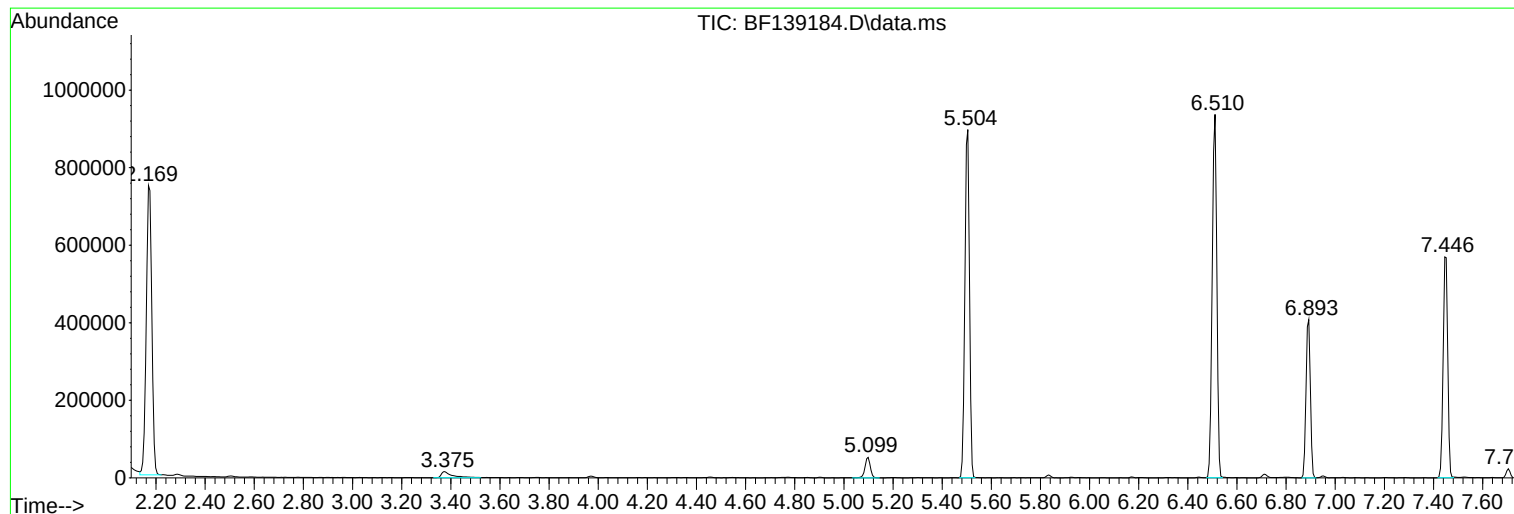
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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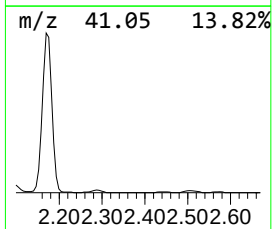
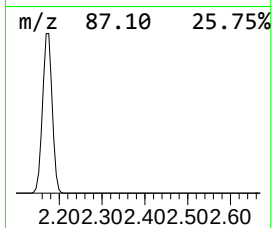
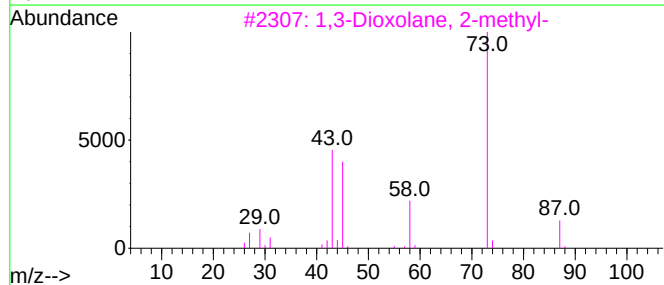
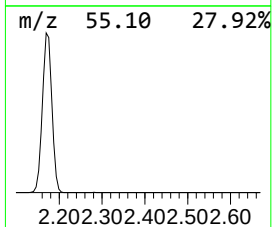
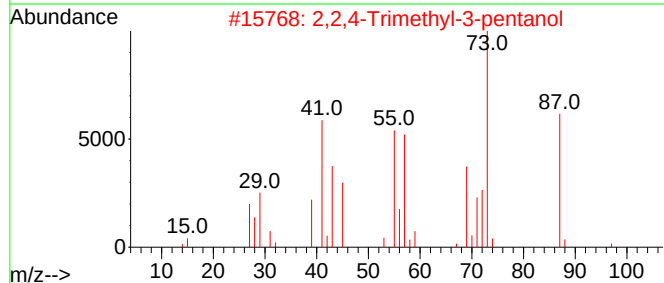
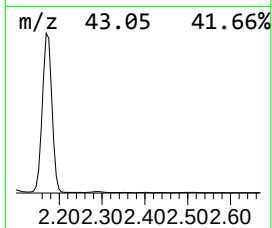
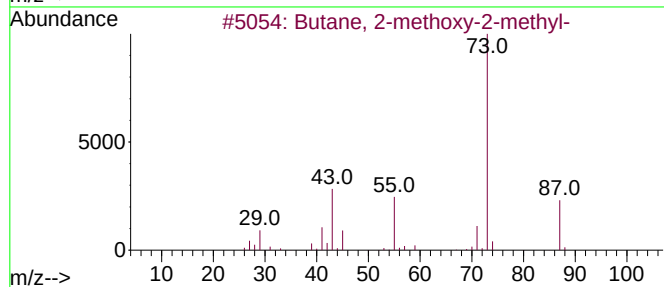
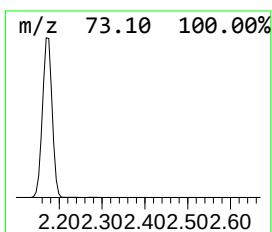
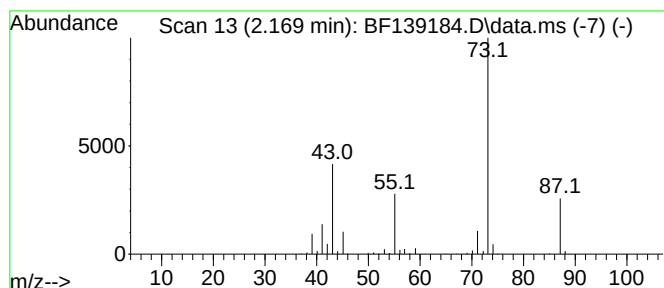
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	46.31 ng	1169380	1,4-Dichlorobenzene-d4	6.893

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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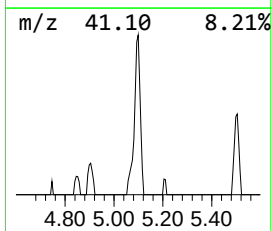
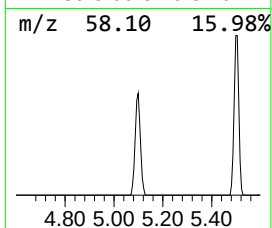
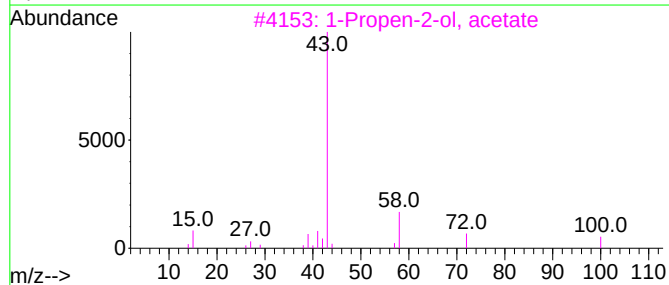
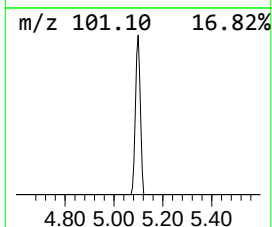
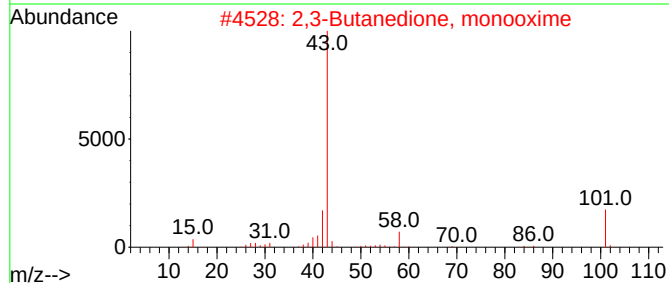
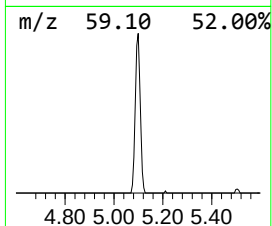
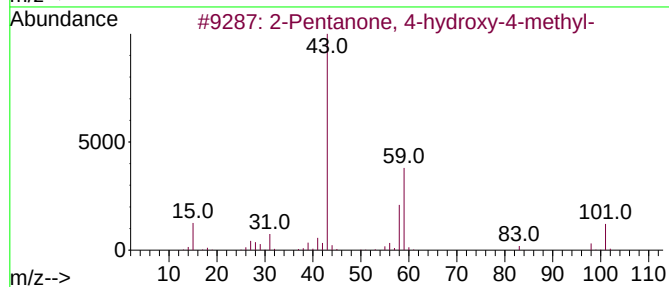
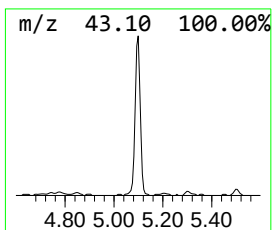
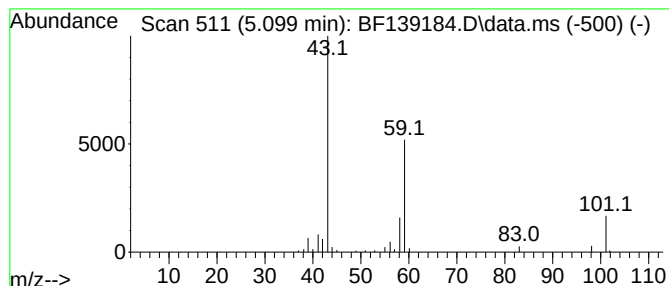
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	3.20 ng	80759	1,4-Dichlorobenzene-d4	6.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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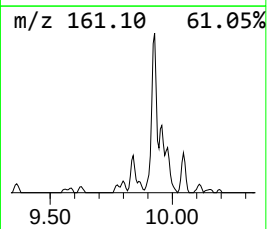
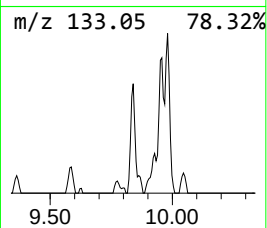
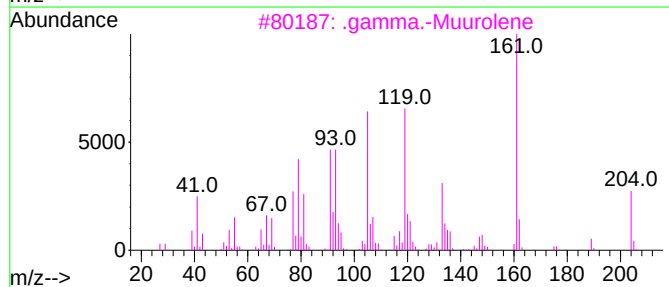
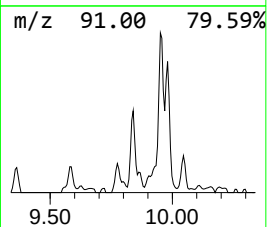
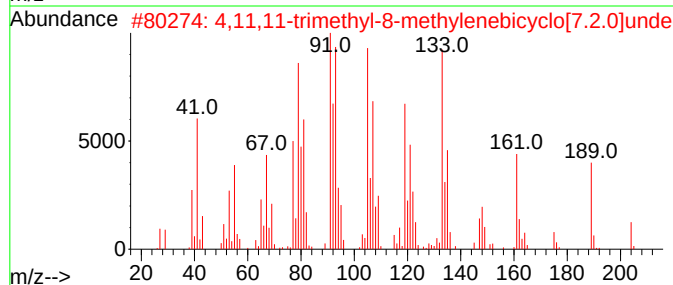
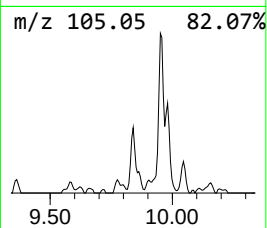
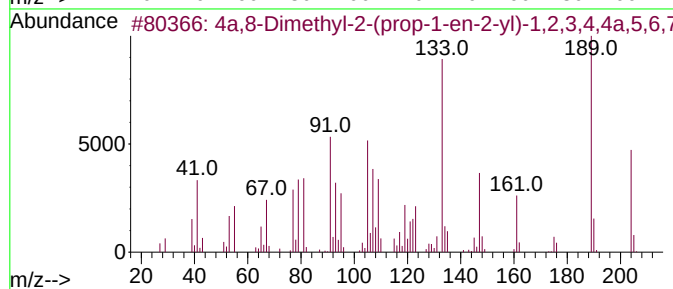
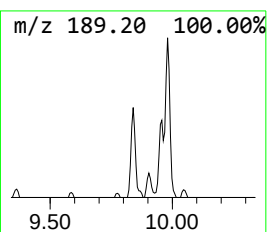
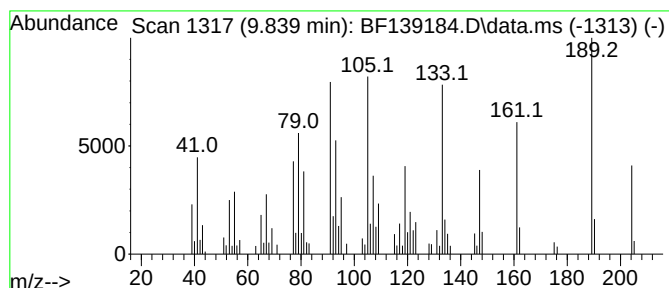
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4a,8-Dimethyl-2-(prop-1-en-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.839	2.43 ng	94619	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	96
2			4,11,11-trimethyl-8-methylenebic...	204	C15H24	889360-49-0	90
3			.gamma.-Muurolene	204	C15H24	030021-74-0	89
4			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	87
5			Cycloisolongifolene	204	C15H24	1000151-99-7	86



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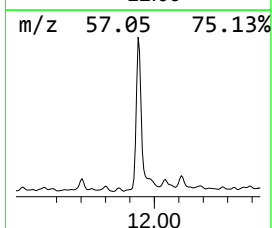
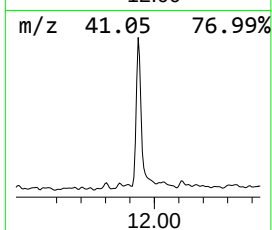
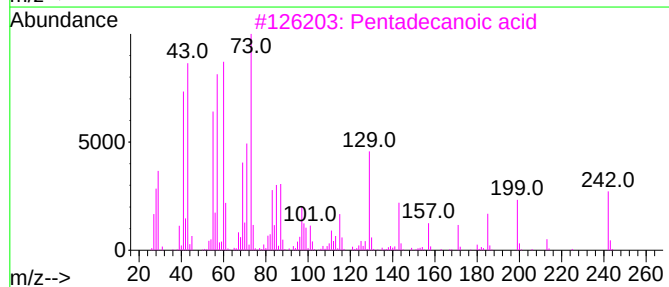
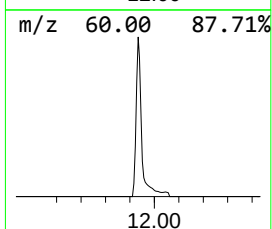
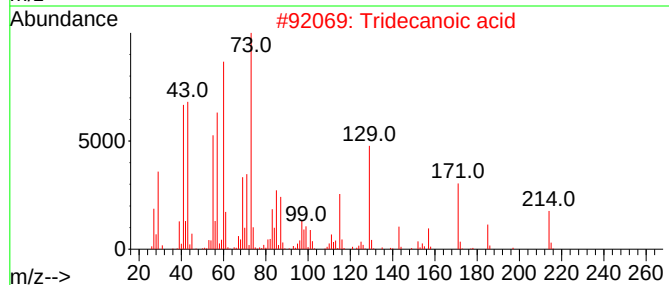
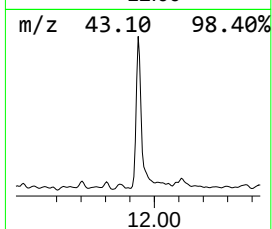
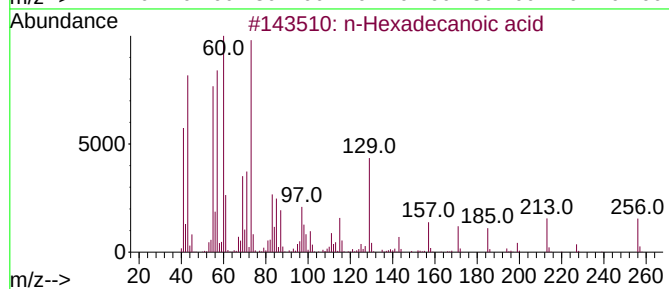
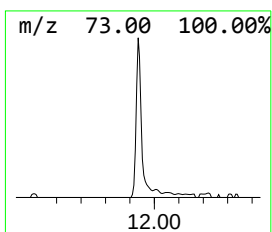
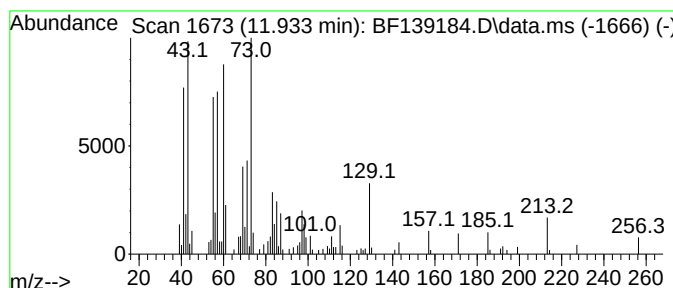
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.934	4.65 ng	143931	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, propyl tridecyl ester	314	C18H34O4	1000309-26-6	18



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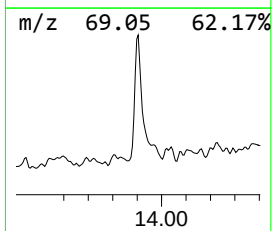
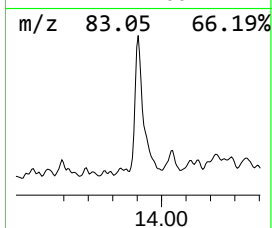
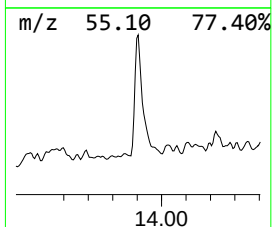
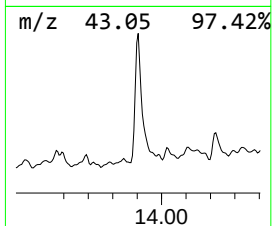
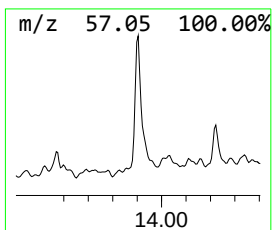
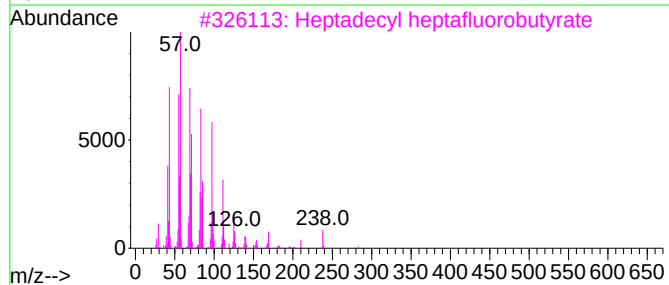
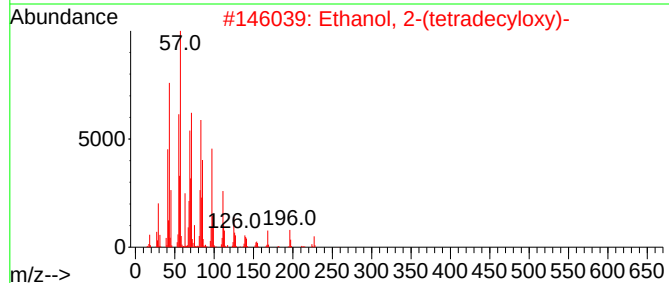
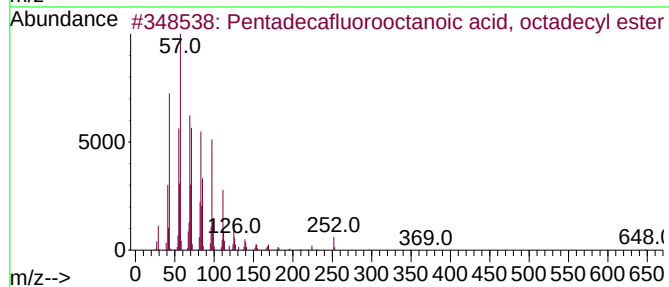
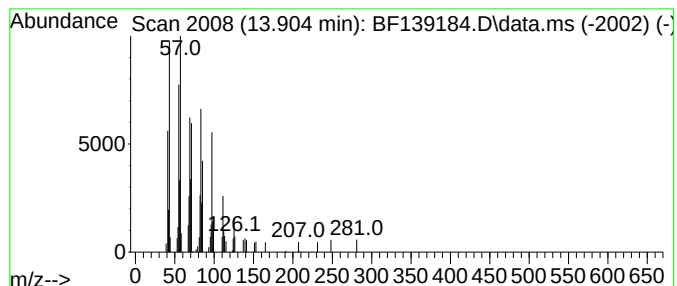
Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	3.30 ng	81178	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, octadecyl ester	666	C26H37F15O2	1000406-04-8	95
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4	Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	87
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139184.D
Acq On : 27 Aug 2024 13:47
Operator : RC/JU
Sample : P3717-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

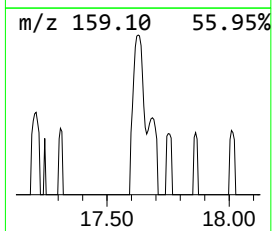
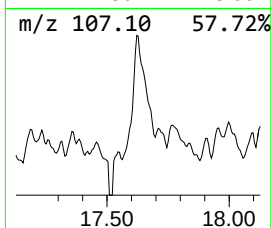
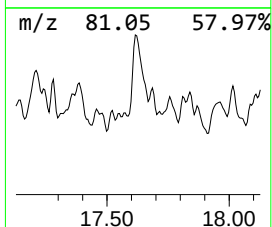
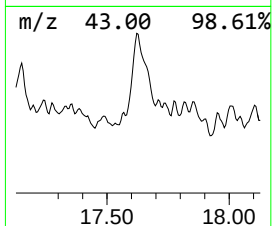
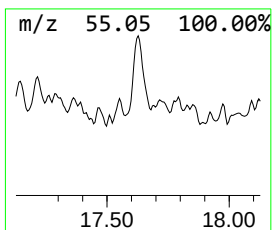
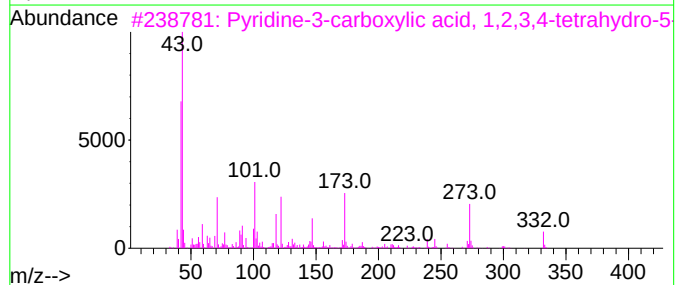
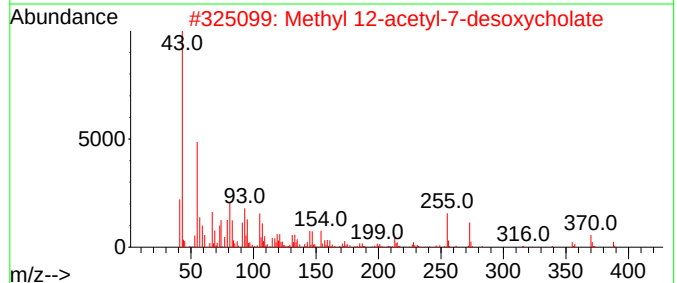
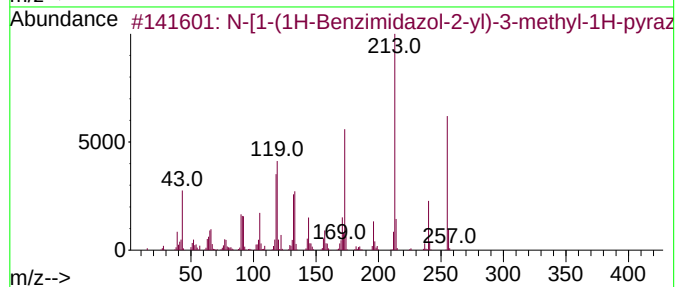
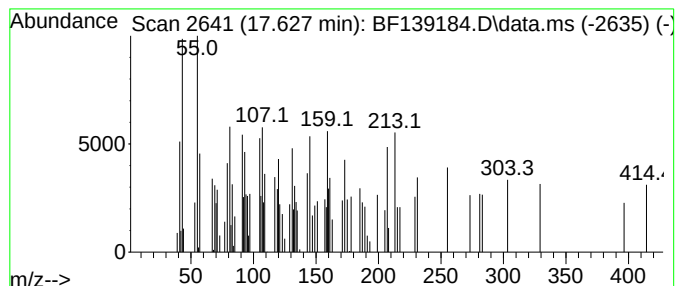
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.627 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.627	2.80 ng	55279	Perylene-d12	15.522	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[1-(1H-Benzimidazol-2-yl)-3-me...	255	C13H13N5O	433697-54-2	30
2	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	9
3	Pyridine-3-carboxylic acid, 1,2,...	332	C16H16N2O4S	1000268-49-8	9
4	6-Methyl(pentamethylene)silyloxy...	326	C20H42OSi	1010278-79-4	9
5	cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139184.D
Acq On : 27 Aug 2024 13:47
Operator : RC/JU
Sample : P3717-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

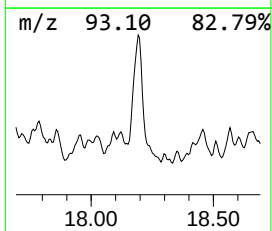
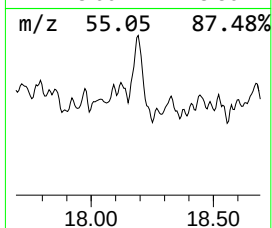
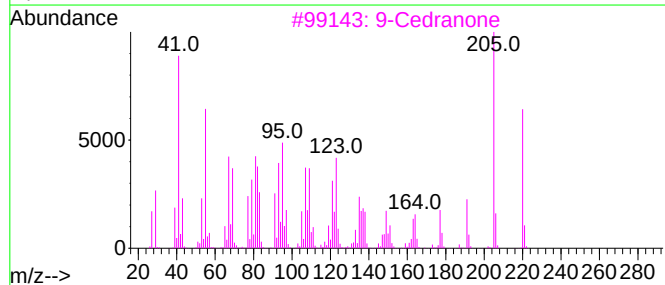
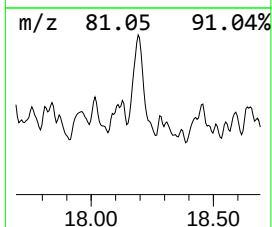
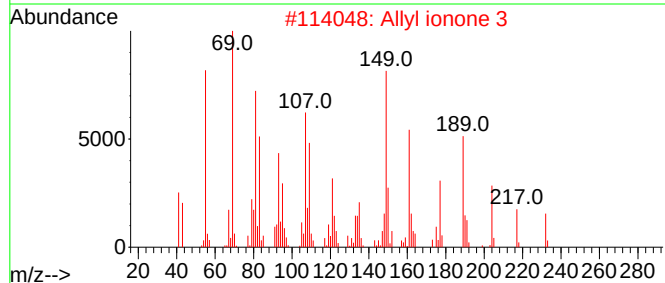
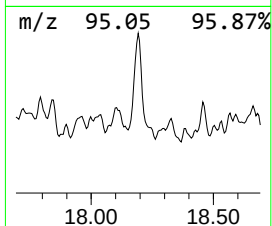
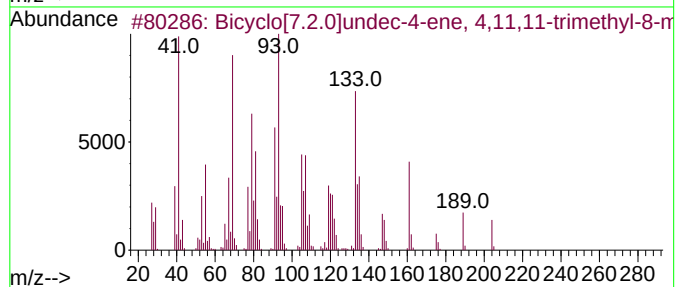
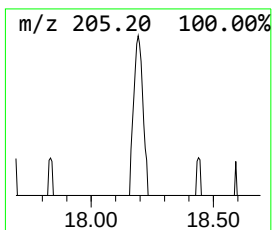
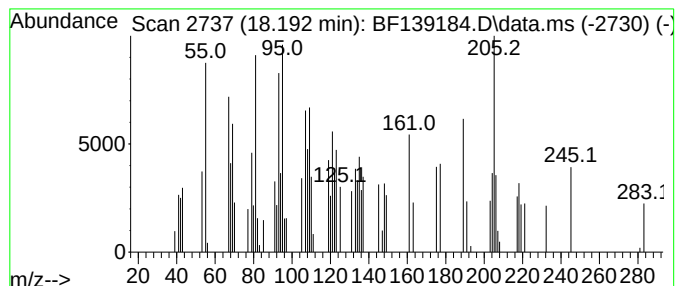
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.192 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	2.37 ng	46837	Perylene-d12	15.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	44
2			Allyl ionone 3	232	C16H24O	1000284-92-9	42
3			9-Cedranone	220	C15H24O	1000156-23-2	30
4			.beta.-Humulene	204	C15H24	000116-04-1	25
5			2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139184.D
Acq On : 27 Aug 2024 13:47
Operator : RC/JU
Sample : P3717-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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
Butane, 2-metho...	2.169	46.3	ng	1169380	1	6.893	505076	20.0
2-Pentanone, 4-...	5.099	3.2	ng	80759	1	6.893	505076	20.0
4a,8-Dimethyl-2...	9.839	2.4	ng	94619	3	9.922	777613	20.0
Spiro[5.5]undec...	9.981	3.8	ng	147506	3	9.922	777613	20.0
n-Hexadecanoic ...	11.934	4.7	ng	143931	4	11.410	618989	20.0
Pentadecafluoro...	13.904	3.3	ng	81178	5	14.045	492637	20.0
unknown17.627	17.627	2.8	ng	55279	6	15.522	394964	20.0
unknown18.192	18.192	2.4	ng	46837	6	15.522	394964	20.0