

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125439.D
 Acq On : 13 Sep 2021 12:06
 Operator : JU/CG
 Sample : PB139002BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB139002BL

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-BF081821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	23	31	39	rVB	124164	170241	2.77%	0.443%
2	4.022	322	329	335	rVB	47819	62657	1.02%	0.163%
3	5.528	579	585	588	rBV	4212069	4721991	76.84%	12.285%
4	6.528	749	755	758	rBV	3993923	4631047	75.36%	12.048%
5	6.886	812	816	819	rBV	1381291	1194261	19.43%	3.107%
6	7.451	906	912	915	rBV	2813745	3172585	51.63%	8.254%
7	8.169	1029	1034	1053	rBV	1718098	1624061	26.43%	4.225%
8	9.245	1211	1217	1221	rBV	5060224	5452337	88.73%	14.185%
9	9.927	1327	1333	1348	rBV	2150501	1841011	29.96%	4.790%
10	10.721	1463	1468	1471	rBV	3859698	3573422	58.15%	9.297%
11	11.421	1582	1587	1594	rBV	1951982	1919884	31.24%	4.995%
12	12.821	1821	1825	1828	rBV	188218	169098	2.75%	0.440%
13	13.010	1852	1857	1860	rBV	6065872	6145179	100.00%	15.988%
14	13.527	1941	1945	1950	rBV2	133765	143168	2.33%	0.372%
15	14.068	2032	2037	2040	rBV	1783657	1647194	26.80%	4.285%
16	15.568	2285	2292	2303	rBV	1187331	1581421	25.73%	4.114%
17	17.256	2569	2579	2596	rVB5	86490	387748	6.31%	1.009%

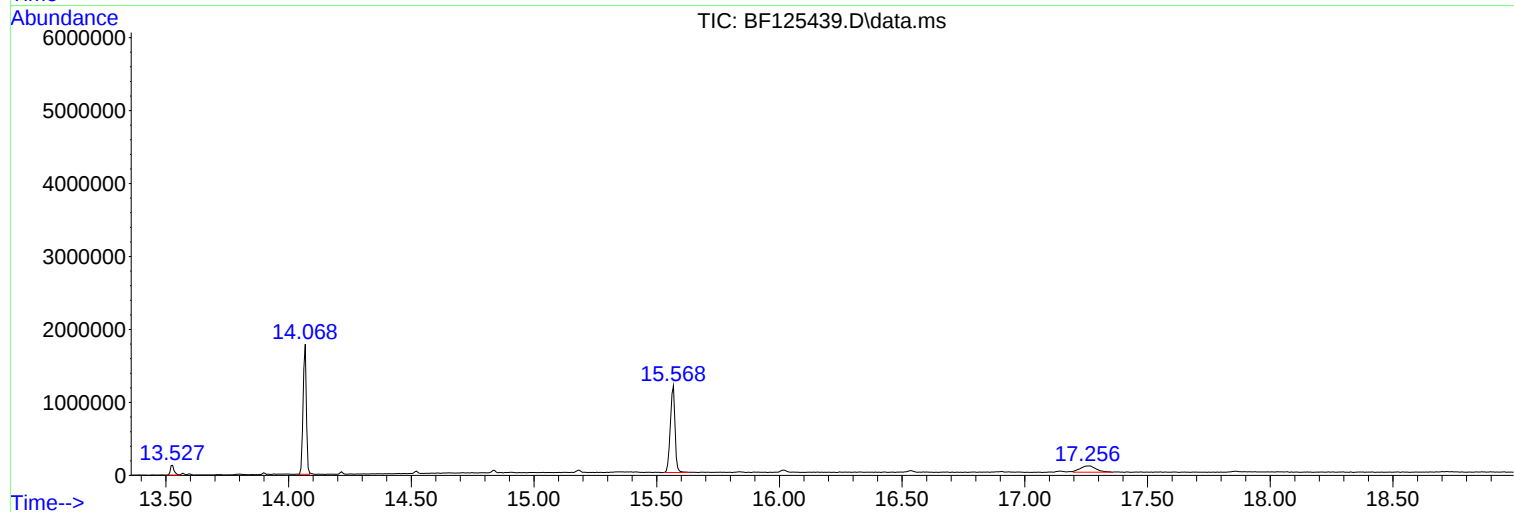
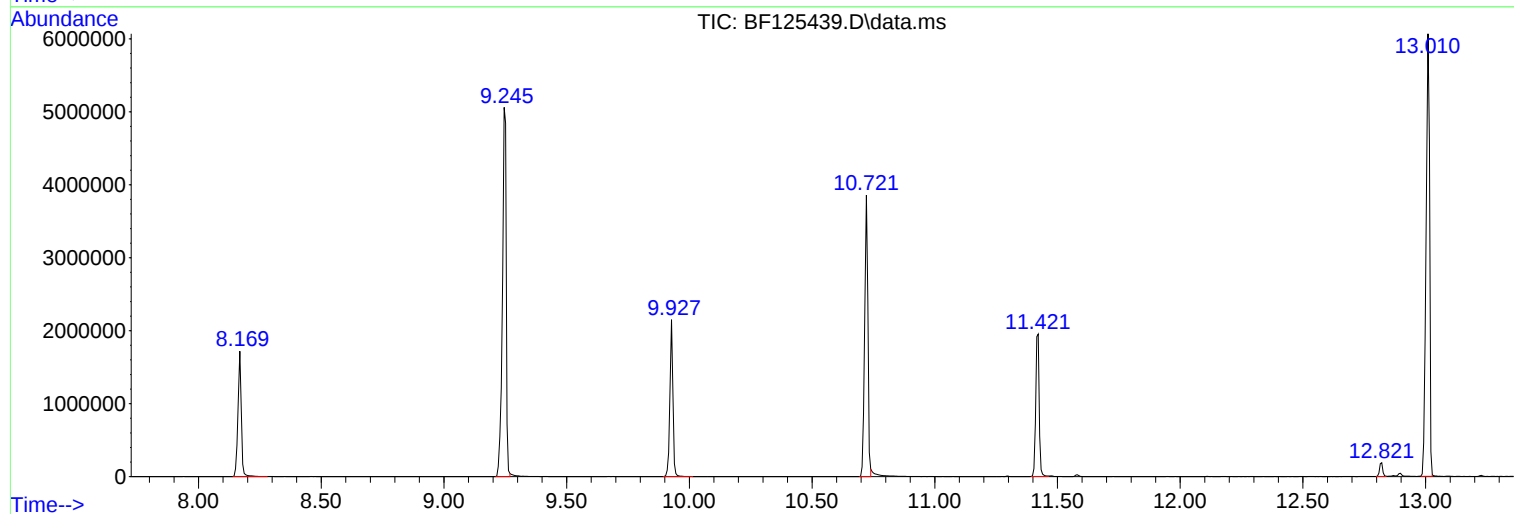
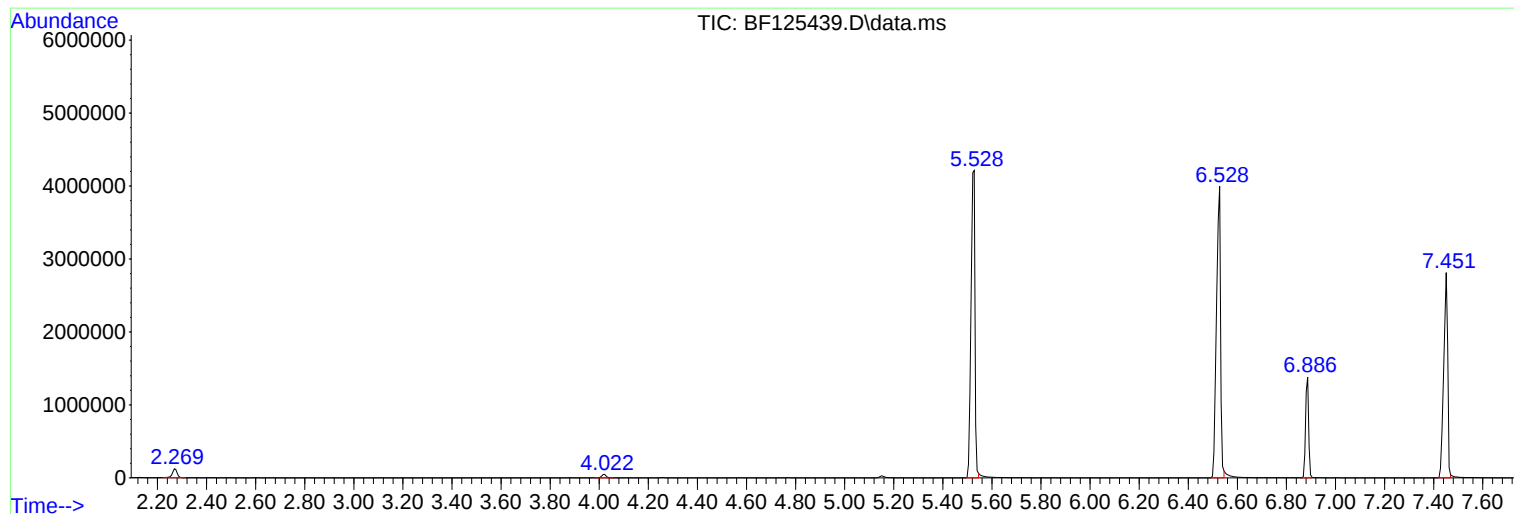
Sum of corrected areas: 38437305

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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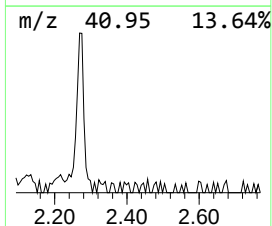
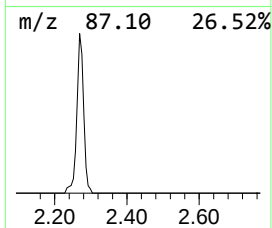
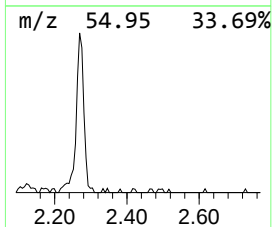
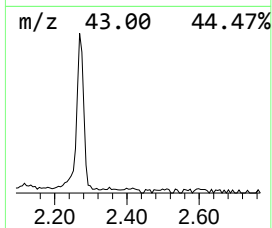
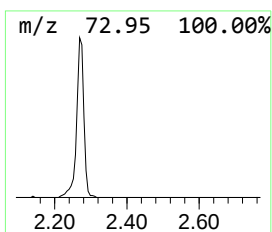
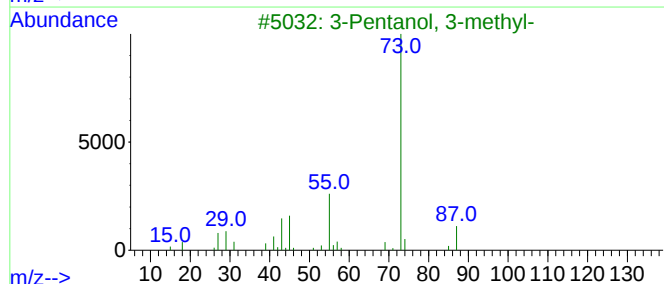
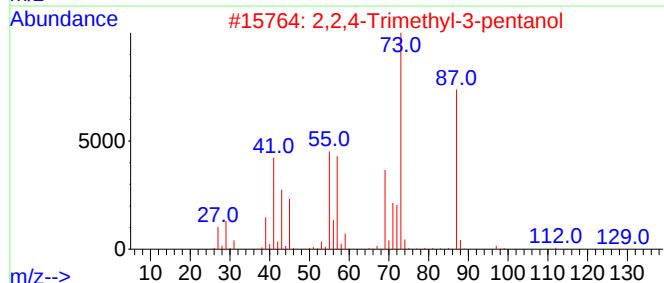
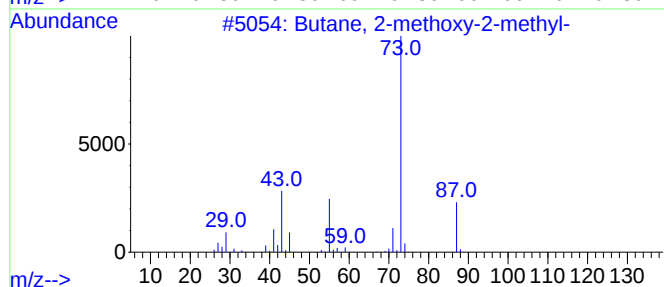
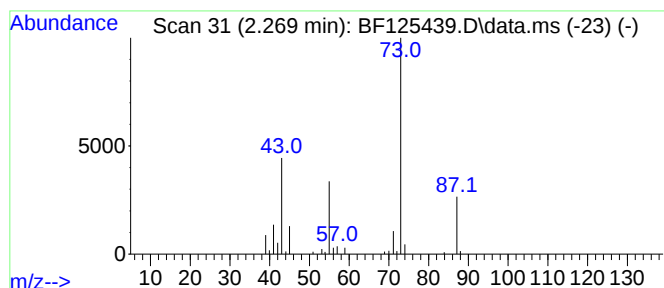
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.85 ng	170241	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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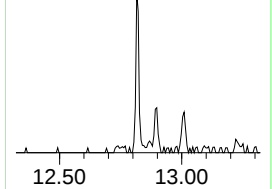
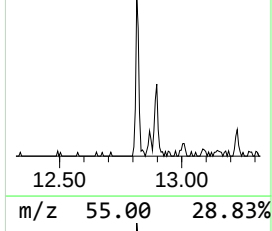
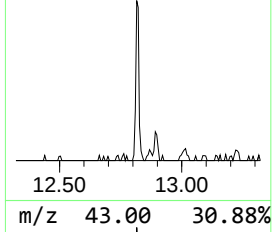
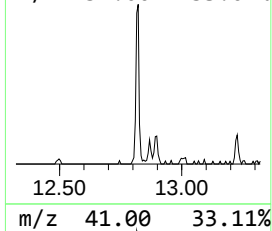
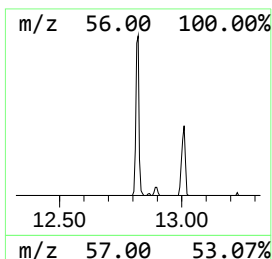
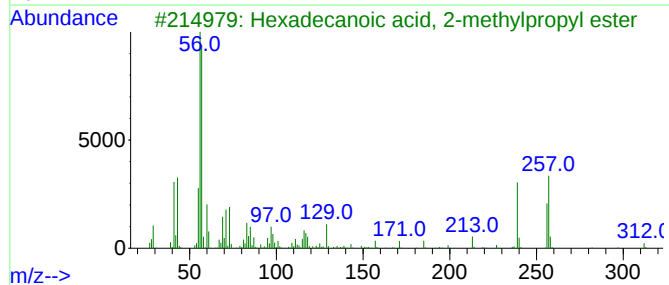
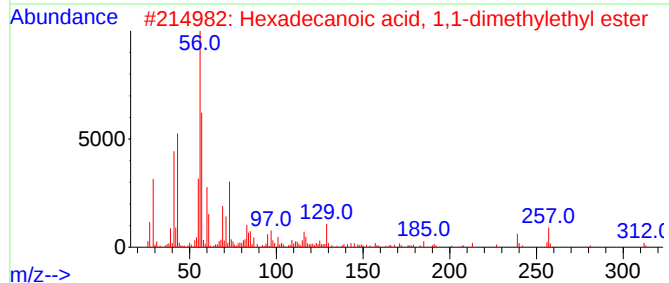
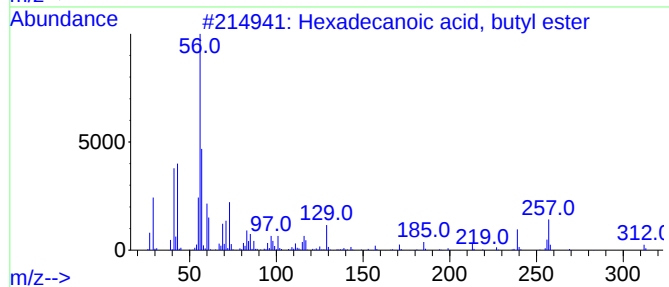
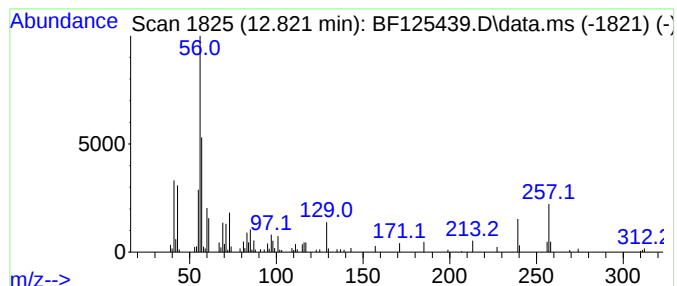
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.821	2.05 ng	169098	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	90
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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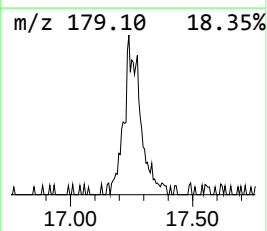
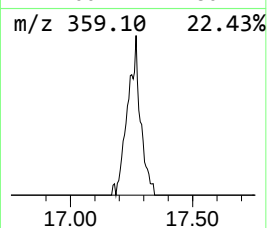
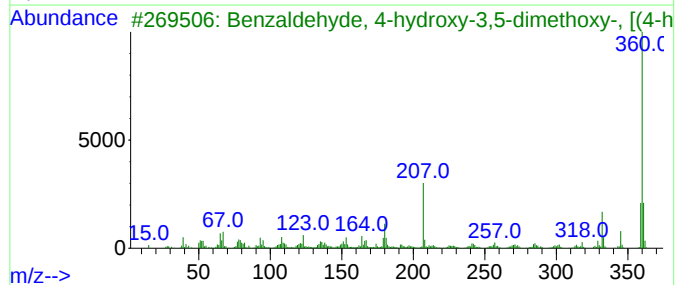
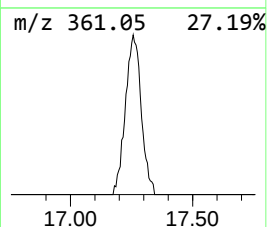
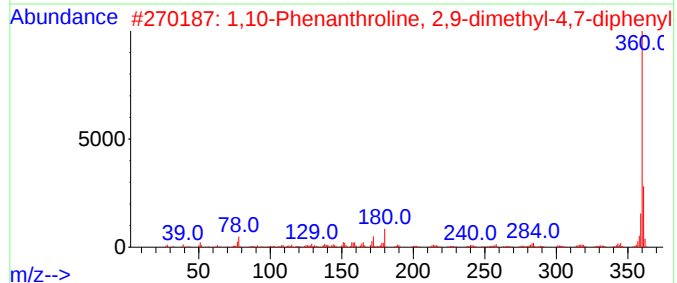
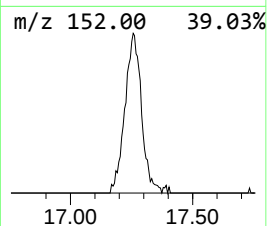
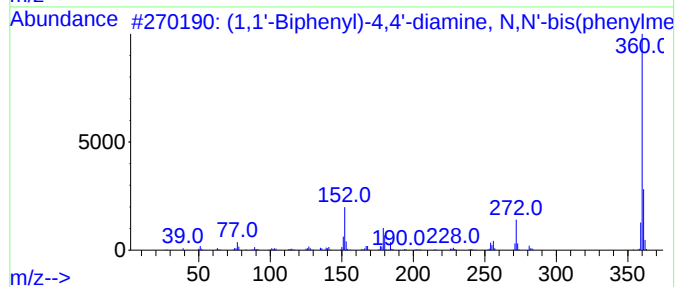
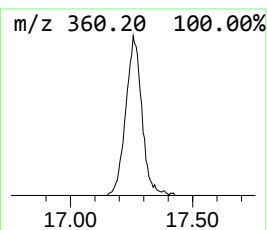
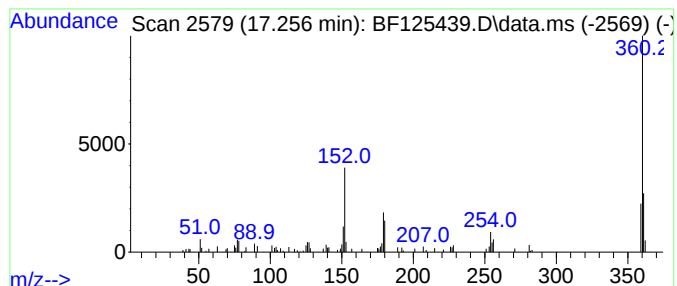
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Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.256	4.90 ng	387748	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	90
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	52
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	52
4			1H-isoindole-1,3(2H)-dione, 2-[5...	360	C21H16N2O4	1000398-48-8	47
5			Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.269	2.9	ng	170241	1	6.886	1194260	20.0
Hexadecanoic ac...	12.821	2.0	ng	169098	5	14.068	1647190	20.0
(1,1'-Biphenyl)...	17.256	4.9	ng	387748	6	15.568	1581420	20.0