

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131421.D
 Acq On : 28 Nov 2022 10:05
 Operator : CG\JU
 Sample : PB149277BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149277BL

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131421.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	28	36	43	rVB	63442	87091	2.24%	0.405%
2	5.187	522	527	536	rBV	470919	630076	16.22%	2.928%
3	5.575	587	593	595	rBV	2379237	2687570	69.20%	12.489%
4	6.575	756	763	765	rBV	2202476	2682225	69.06%	12.464%
5	6.951	823	827	830	rBV	669658	526856	13.57%	2.448%
6	7.516	917	923	926	rBV	1576162	1760539	45.33%	8.181%
7	8.239	1041	1046	1049	rBV	822179	682934	17.58%	3.174%
8	9.322	1224	1230	1233	rBV	3293379	3166620	81.54%	14.715%
9	10.004	1341	1346	1350	rBV	960409	817813	21.06%	3.800%
10	10.798	1475	1481	1485	rBV	2090861	2163145	55.70%	10.052%
11	11.504	1597	1601	1604	rBV	1033134	864105	22.25%	4.015%
12	13.104	1868	1873	1876	rBV	3958003	3883720	100.00%	18.047%
13	14.163	2048	2053	2056	rBV	865719	804775	20.72%	3.740%
14	14.257	2064	2069	2075	rBV	34633	41874	1.08%	0.195%
15	15.698	2308	2314	2319	rBV	489235	607161	15.63%	2.821%
16	17.880	2674	2685	2701	rVB3	28395	113158	2.91%	0.526%

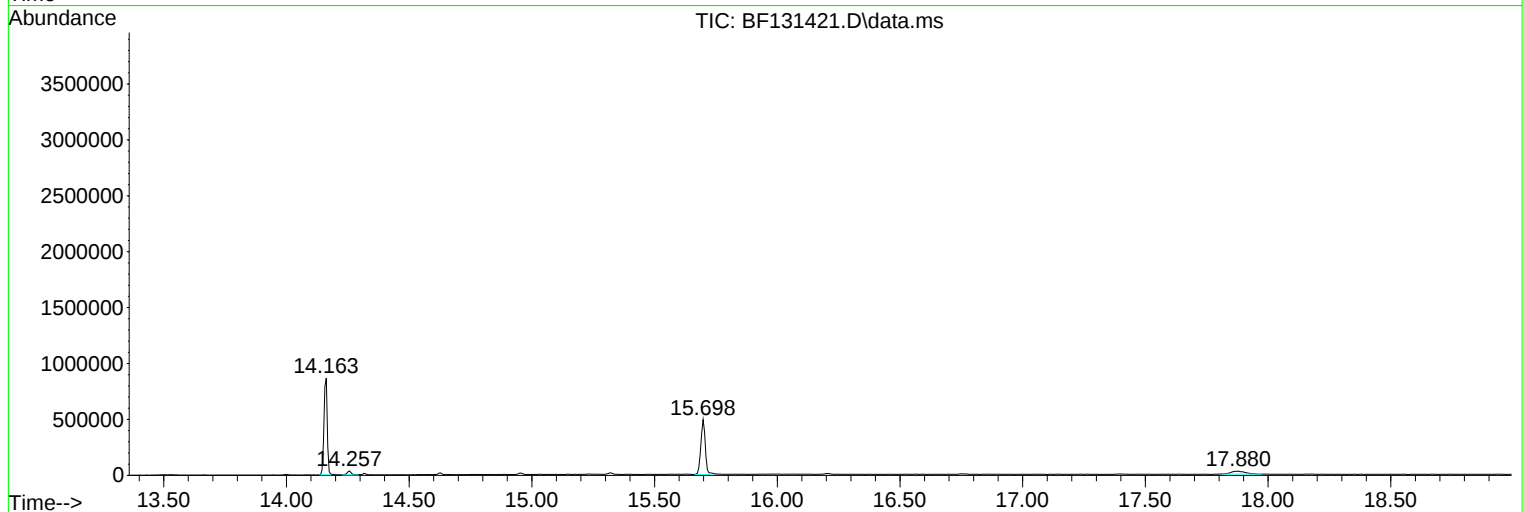
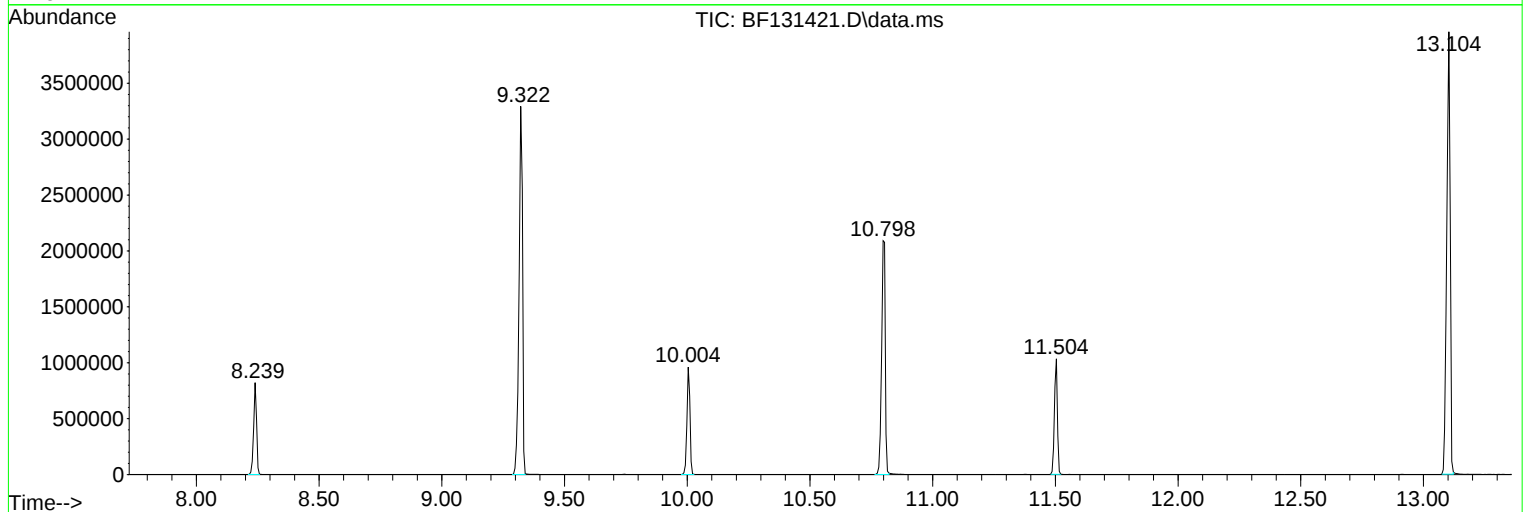
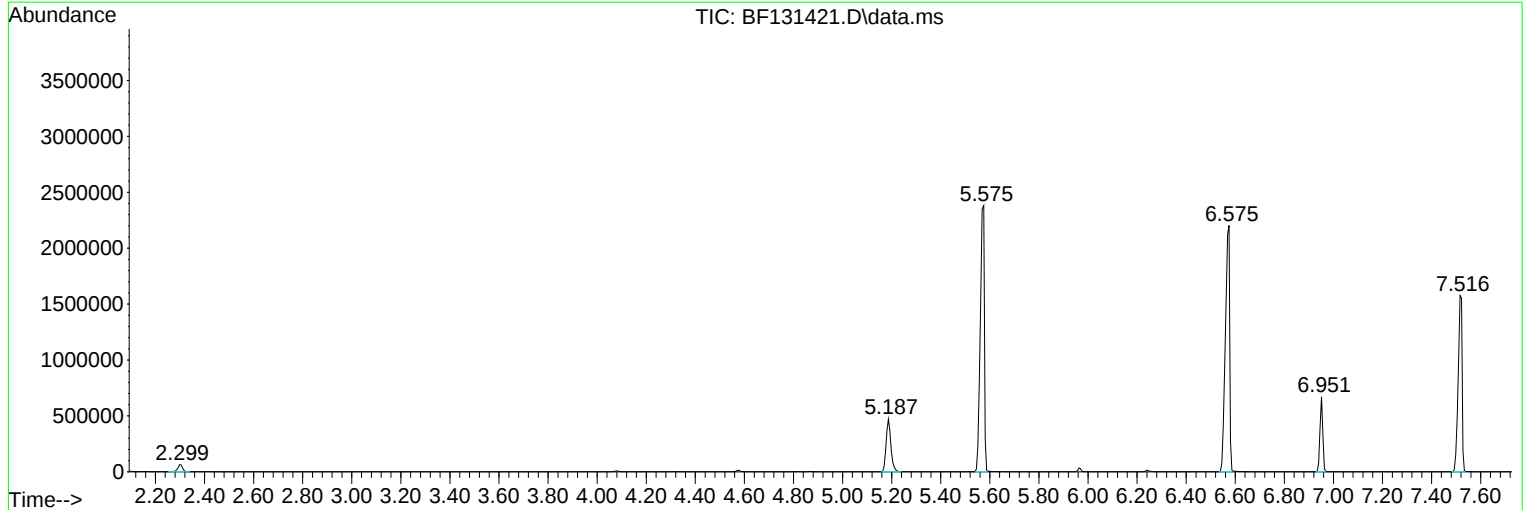
Sum of corrected areas: 21519662

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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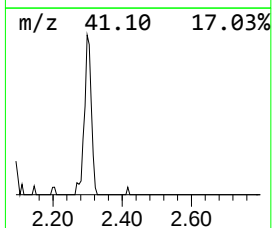
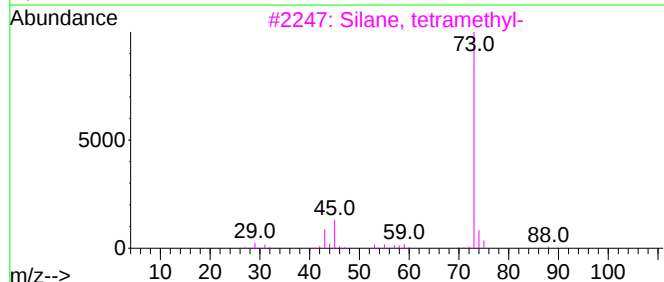
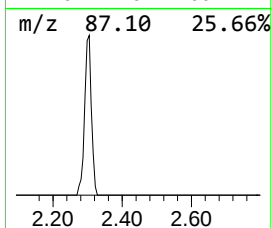
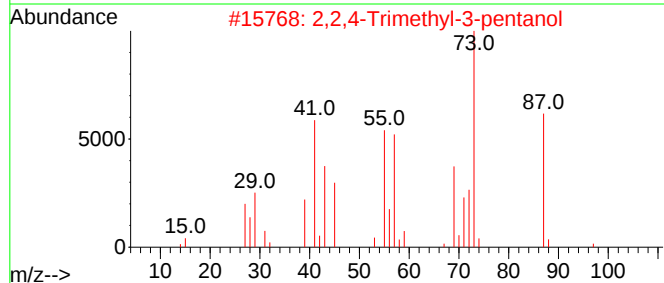
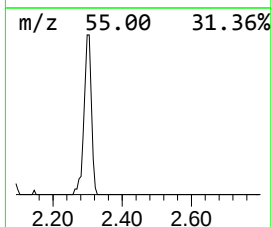
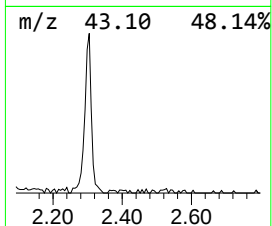
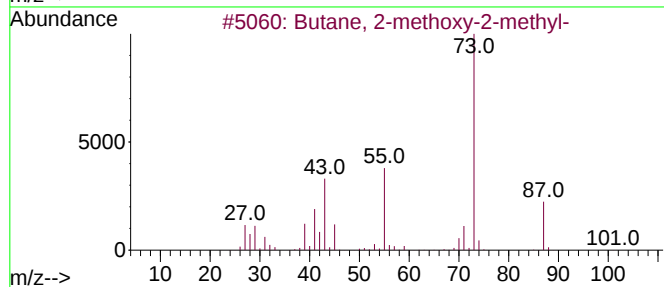
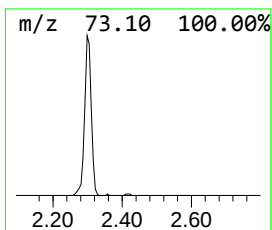
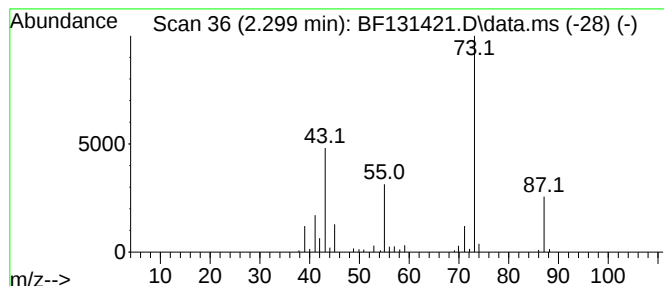
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	3.31 ng	87091	1,4-Dichlorobenzene-d4	6.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12



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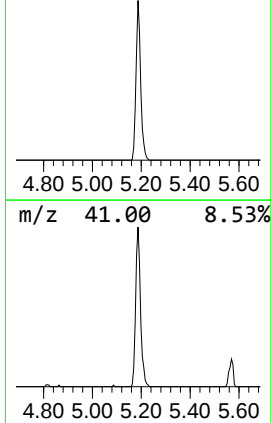
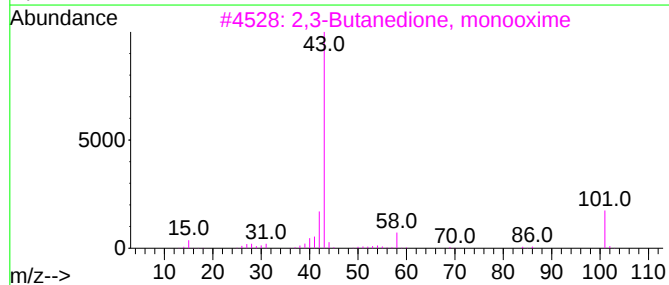
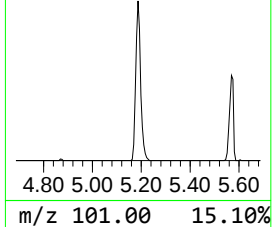
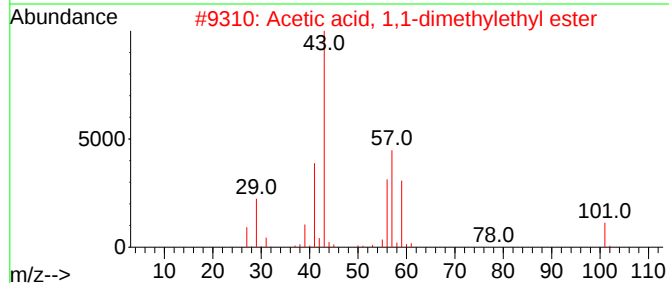
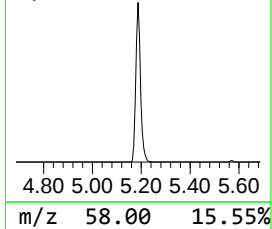
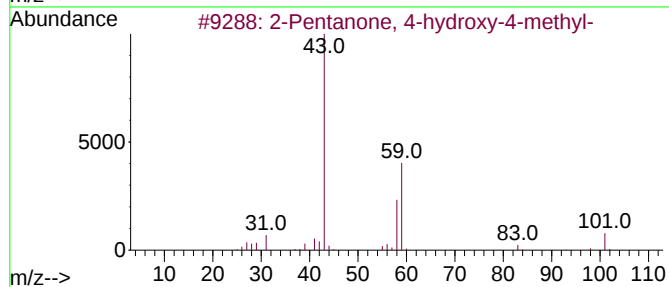
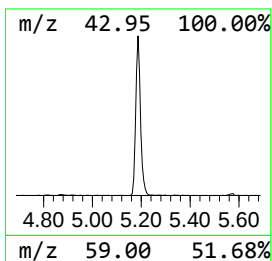
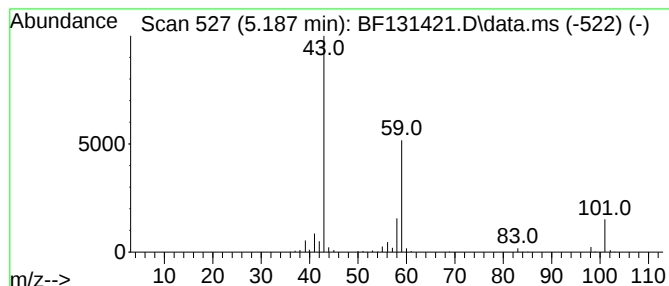
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	23.92 ng	630076	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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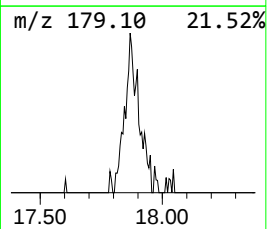
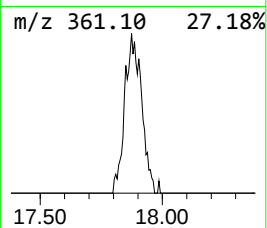
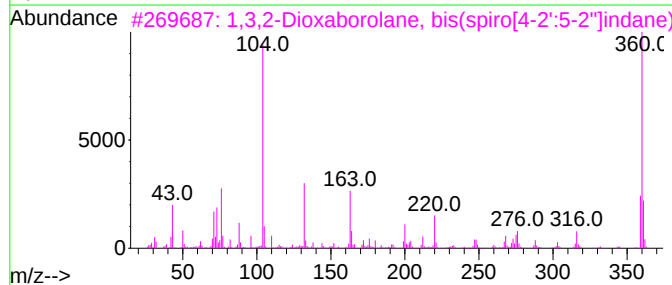
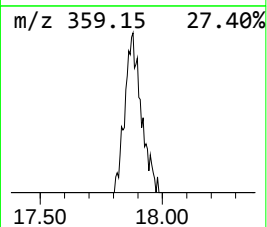
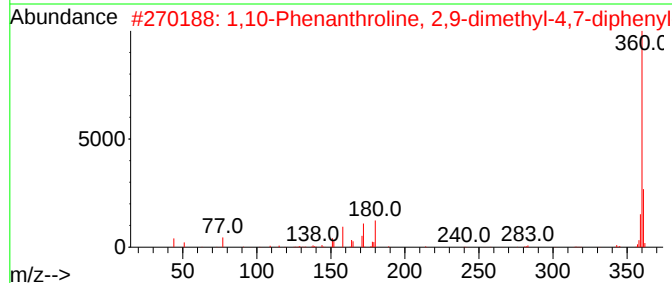
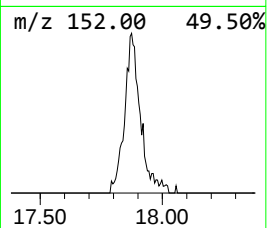
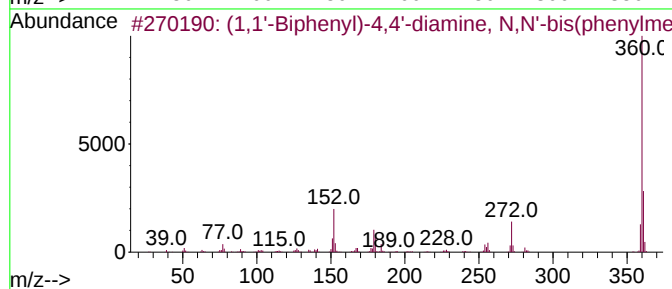
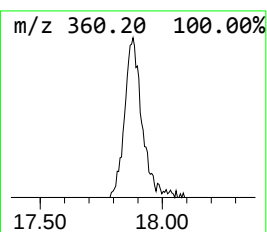
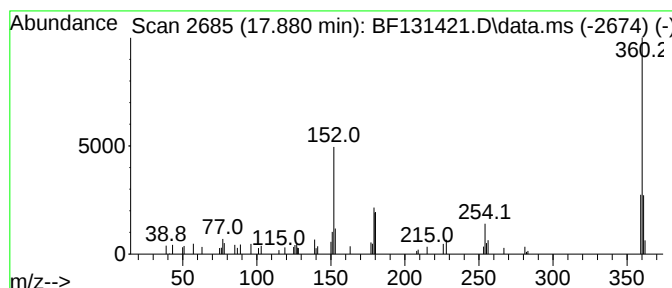
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TIC Integration Parameters: LSCINT.P

Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.880	3.73 ng	113158	Perylene-d12	15.698	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N'-bis(2,2,2-trifluoroethyl)carbamate	360	C26H20N2	006311-48-4	76
2	1,10-Phenanthroline, 2,9-dimethyl-, 1,10-bis(2,2,2-trifluoroethyl)carbamate	360	C26H20N2	004733-39-5	47
3	1,3,2-Dioxaborolane, bis(spiro[4.5]undec-5-en-2-ylidene)-	360	C20H13B06	1000150-23-7	38
4	Jaceidin	360	C18H16O8	010173-01-0	38
5	1H-isindole-1,3(2H)-dione, 2-[5-(2,2,2-trifluoroethyl)-1H-imidazol-1-yl]-	360	C21H16N2O4	1000398-48-8	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.299	3.3	ng	87091	1	6.951	526856	20.0
2-Pentanone, 4-...	5.187	23.9	ng	630076	1	6.951	526856	20.0
(1,1'-Biphenyl)...	17.880	3.7	ng	113158	6	15.698	607161	20.0