

Data Path : Z:\HPCHEM1\BNA G\DATA\BG093017\
 Data File : BG028988.D
 Acq On : 30 Sep 2017 20:45
 Operator : SJ/JU
 Sample : I5457-19
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-3_092717

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:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	295	300	311	rBV	46090	75287	2.15%	0.516%
2	5.821	373	380	392	rBV	294766	503539	14.38%	3.452%
3	7.407	644	650	661	rBV	180074	338417	9.67%	2.320%
4	7.783	707	714	725	rBV	488580	886772	25.33%	6.079%
5	8.253	788	794	803	rBV2	114344	201140	5.75%	1.379%
6	8.576	842	849	858	rVB	442412	801540	22.90%	5.495%
7	9.422	986	993	1006	rBV	375196	720653	20.59%	4.940%
8	11.073	1267	1274	1283	rBV	143597	284677	8.13%	1.952%
9	13.494	1676	1686	1696	rBV	1292712	2067566	59.06%	14.174%
10	14.317	1819	1826	1835	rBV	82106	131870	3.77%	0.904%
11	14.875	1914	1921	1930	rVB2	292340	483136	13.80%	3.312%
12	16.367	2167	2175	2190	rBV	1136090	1824006	52.11%	12.504%
13	16.532	2194	2203	2216	rVV3	143672	418159	11.95%	2.867%
14	17.624	2383	2389	2401	rBV	435803	685918	19.59%	4.702%
15	20.216	2824	2830	2840	rBV	2732241	3500633	100.00%	23.998%
16	21.937	3116	3123	3132	rVB	453440	830044	23.71%	5.690%
17	25.368	3694	3707	3720	rBV2	262116	833780	23.82%	5.716%

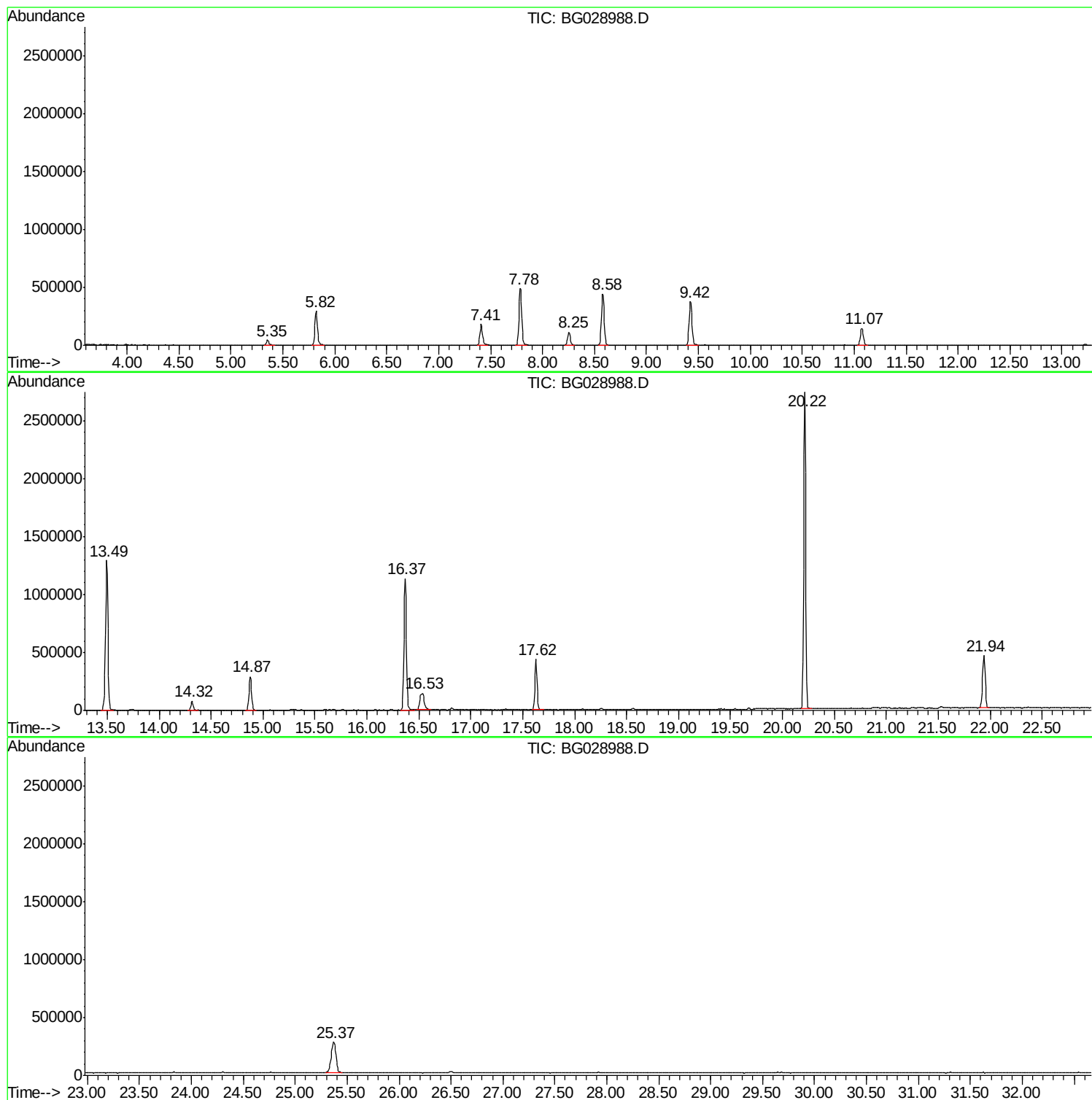
Sum of corrected areas: 14587137

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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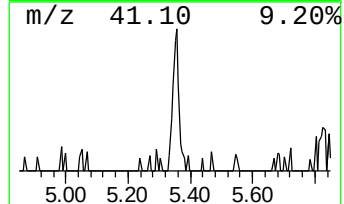
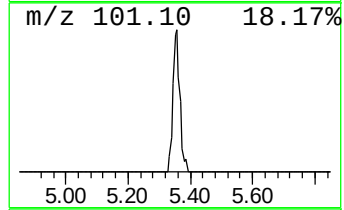
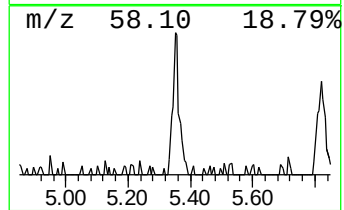
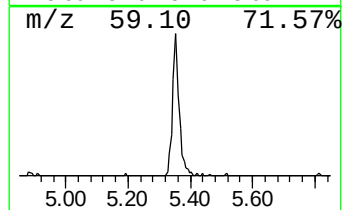
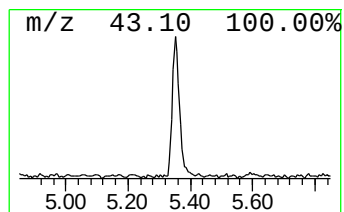
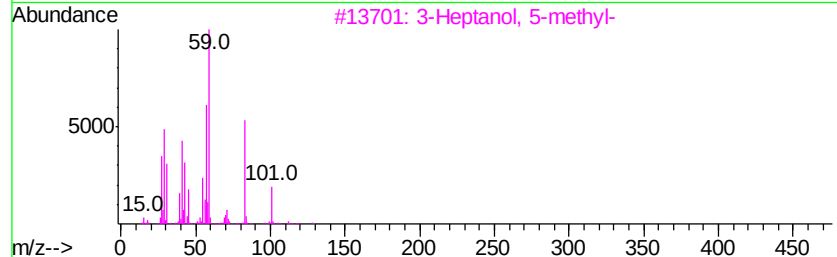
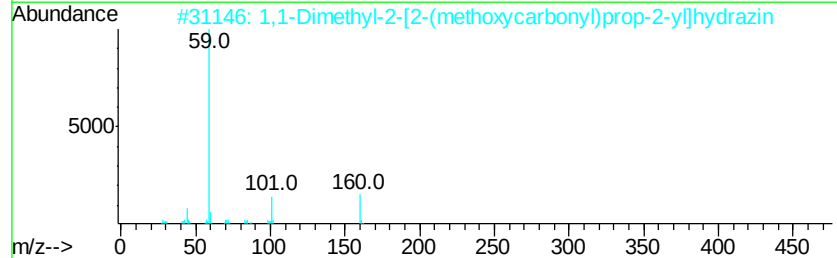
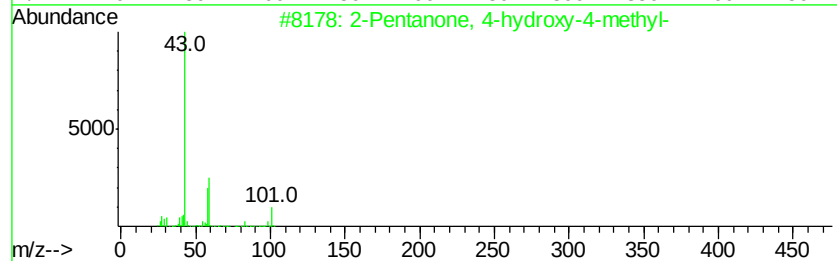
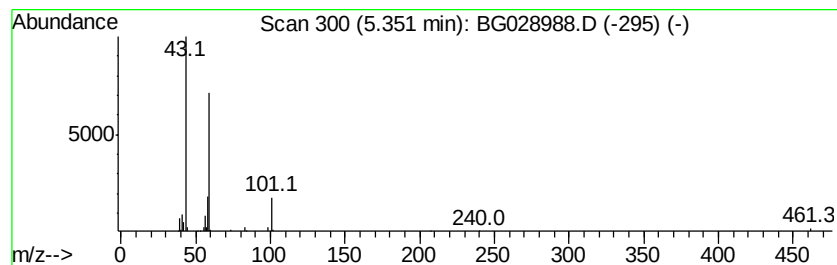
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.35	7.49 ng	75287	1,4-Dichlorobenzene-d4	8.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1,1-Dimethyl-2-[2-(methoxycarbonyl)prop-2-yl]hydrazin	160	C7H16N2O2	097812-30-1	28
3			3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	28
4			Tetraolyme	222	C10H22O5	000143-24-8	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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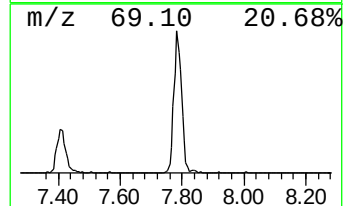
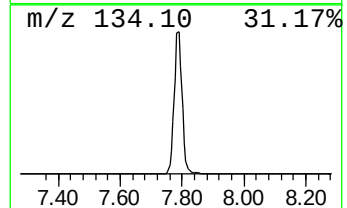
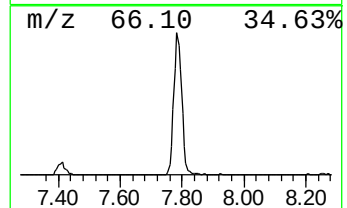
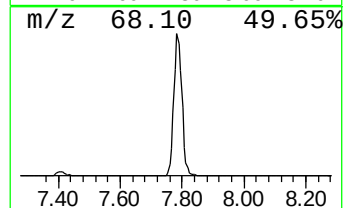
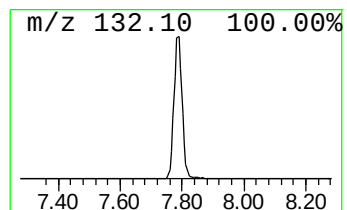
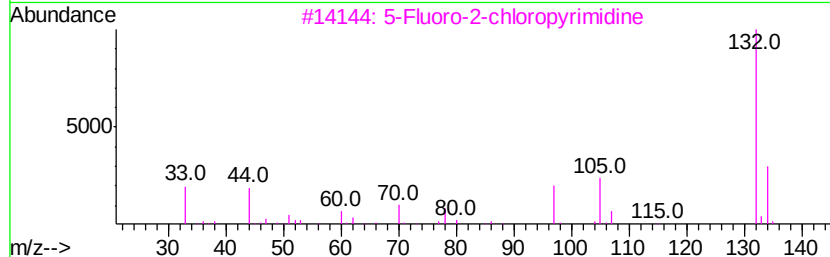
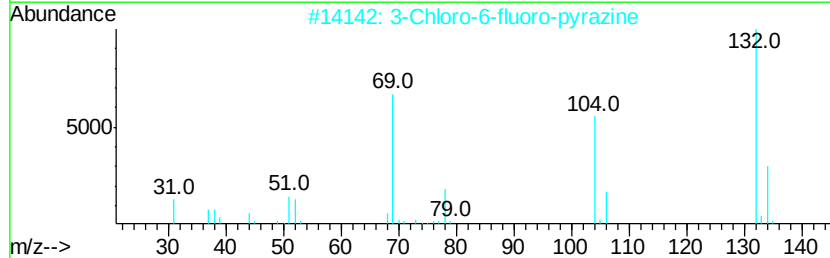
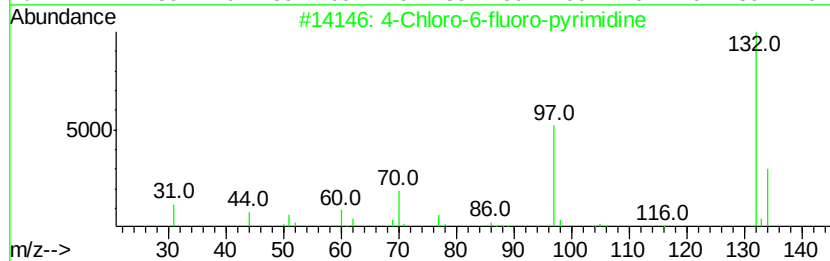
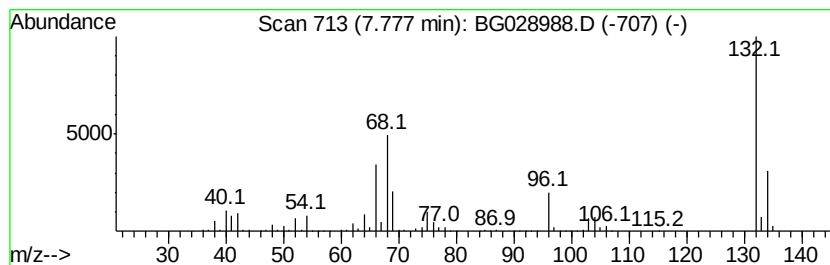
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Peak Number 2 unknown7.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	88.17 ng	886772	1,4-Dichlorobenzene-d4	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	9



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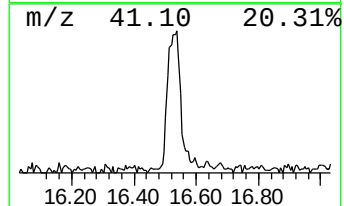
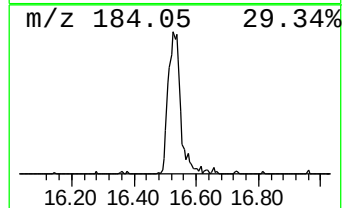
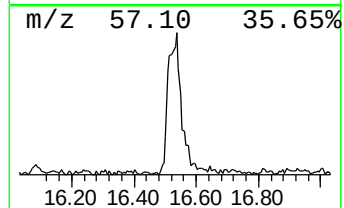
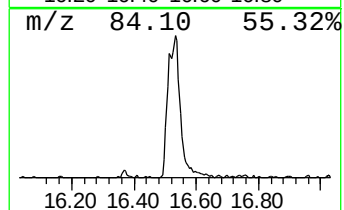
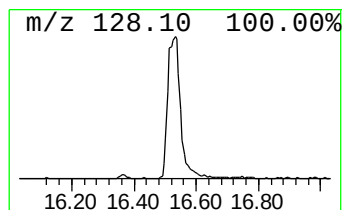
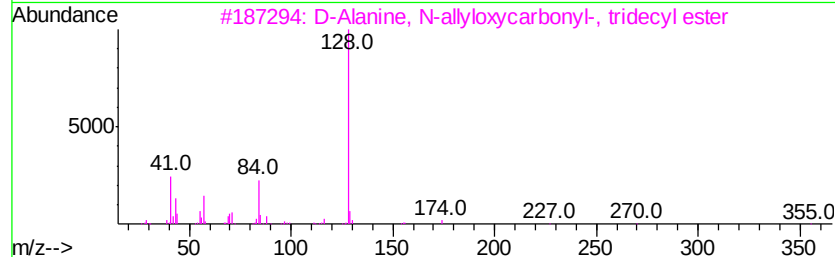
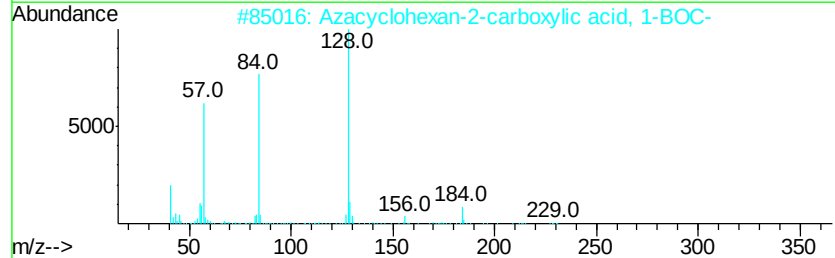
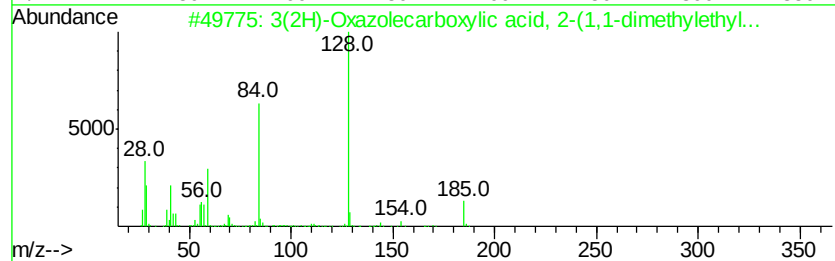
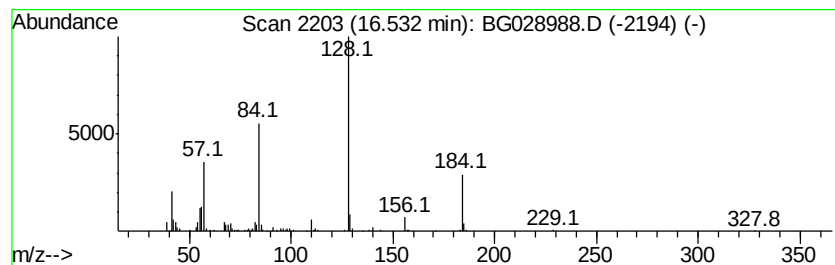
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Peak Number 4 3(2H)-Oxazolecarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.53	12.19 ng	418159	Phenanthrene-d10	17.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3(2H)-Oxazolecarboxylic acid, 2-...	185	C9H15N03	104173-34-4	64
2		Azacyclohexan-2-carboxylic acid,...	229	C11H19N04	1000126-80-6	59
3		D-Alanine, N-allyloxycarbonyl-, ...	355	C20H37N04	1000347-73-6	53
4		l-Alanine, N-allyloxycarbonyl-, ...	257	C13H23N04	1000313-42-7	53
5		l-Alanine, N-allyloxycarbonyl-, ...	369	C21H39N04	1000313-43-5	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.35	7.5	ng	75287	1	8.25	201140	20.0
unknown7.78	7.78	88.2	ng	886772	1	8.25	201140	20.0
3(2H)-Oxazolecarb...	16.53	12.2	ng	418159	4	17.62	685918	20.0