

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082418\
 Data File : BG036409.D
 Acq On : 24 Aug 2018 11:49
 Operator : JU/SJ
 Sample : J4568-06
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 081718-DBRI-E-D-S

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_G\METHODS\8270-BG082318.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	5.633	392	399	410	rBV	361455	567668	12.77%	2.983%
2	7.214	660	668	677	rBV	234319	392075	8.82%	2.060%
3	7.596	724	733	740	rBV	613500	1029203	23.15%	5.409%
4	8.066	807	813	820	rBV	184592	313665	7.06%	1.648%
5	8.389	861	868	876	rVB	799719	1390244	31.28%	7.306%
6	9.229	1002	1011	1021	rBV	664360	1209892	27.22%	6.358%
7	10.874	1280	1291	1298	rBV	260268	451030	10.15%	2.370%
8	13.318	1699	1707	1715	rBV	1875568	2912179	65.51%	15.304%
9	14.687	1933	1940	1951	rVB2	425174	701305	15.78%	3.686%
10	15.504	2070	2079	2083	rBV2	37854	59716	1.34%	0.314%
11	15.986	2155	2161	2169	rBV	310978	388089	8.73%	2.040%
12	16.174	2185	2193	2205	rBV	1005879	1529456	34.41%	8.038%
13	17.431	2401	2407	2415	rBV	588877	875495	19.70%	4.601%
14	18.319	2554	2558	2565	rBV4	34833	52348	1.18%	0.275%
15	20.040	2845	2851	2857	rBV	3326067	4445201	100.00%	23.361%
16	21.697	3126	3133	3143	rVB	689554	1106369	24.89%	5.814%
17	23.054	3357	3364	3378	rBV	241295	551987	12.42%	2.901%
18	24.911	3670	3680	3691	rBV	381672	1052628	23.68%	5.532%

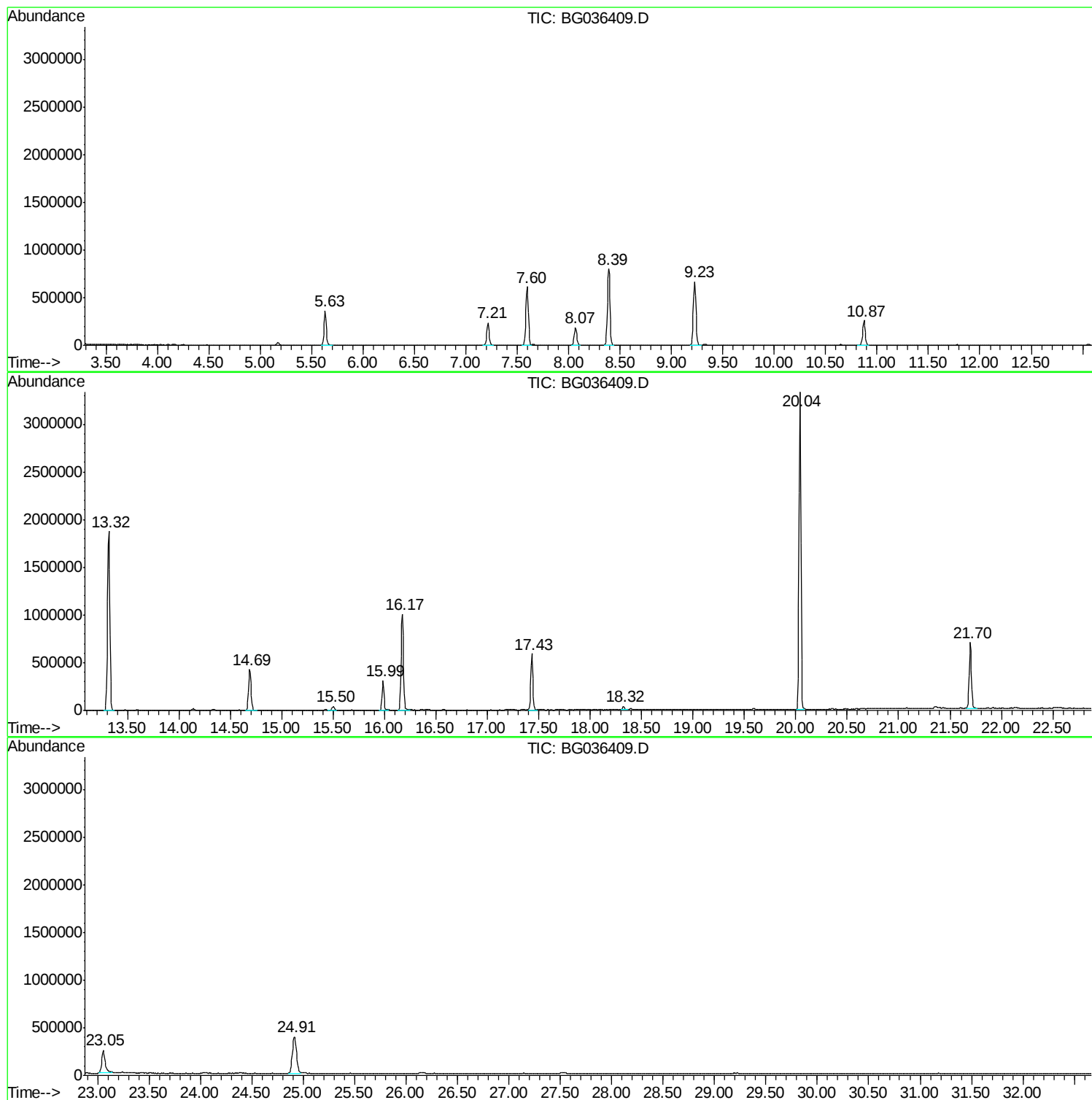
Sum of corrected areas: 19028550

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.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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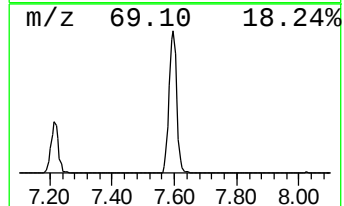
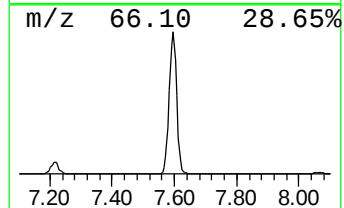
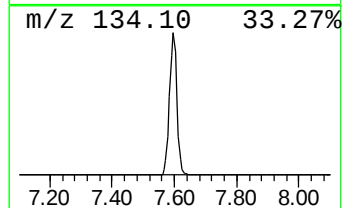
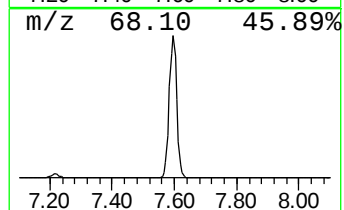
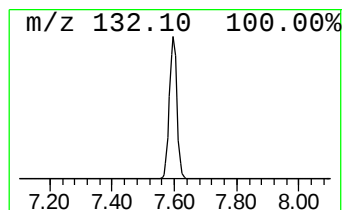
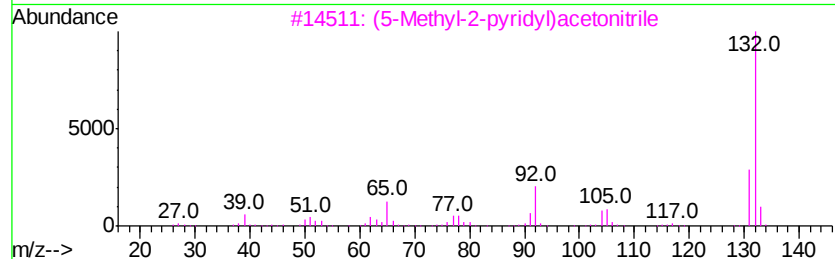
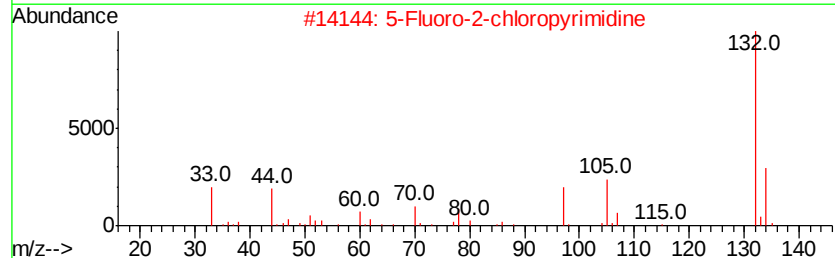
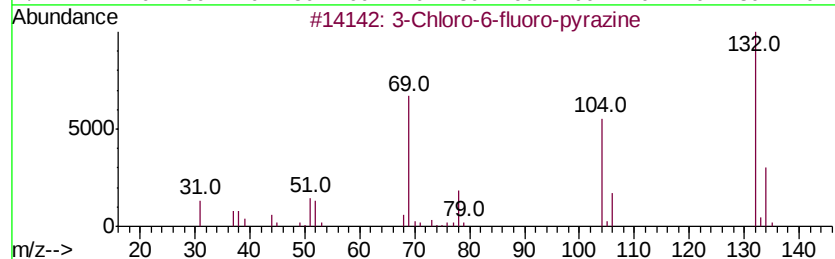
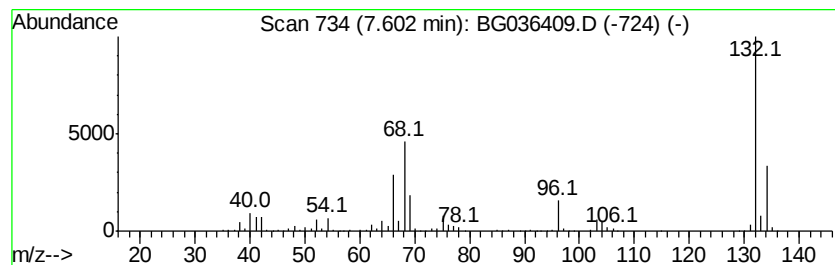
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TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	65.62 ng	1029200	1,4-Dichlorobenzene-d4	8.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-Methyl-2-pyridyl)acetonitrile			132	C8H8N2	1000241-93-9	10
4	Tranvlcypropine-propionyl			189	C12H15NO	1000123-86-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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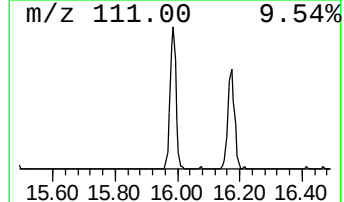
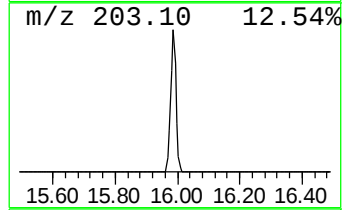
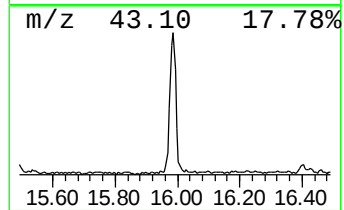
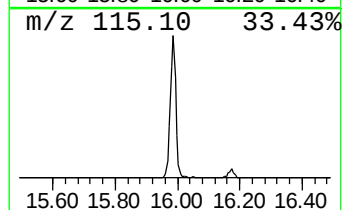
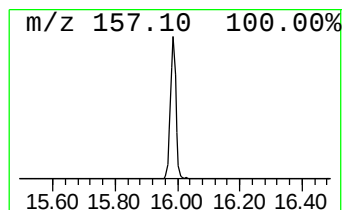
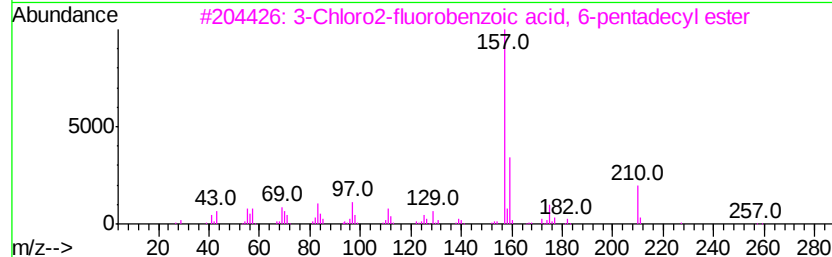
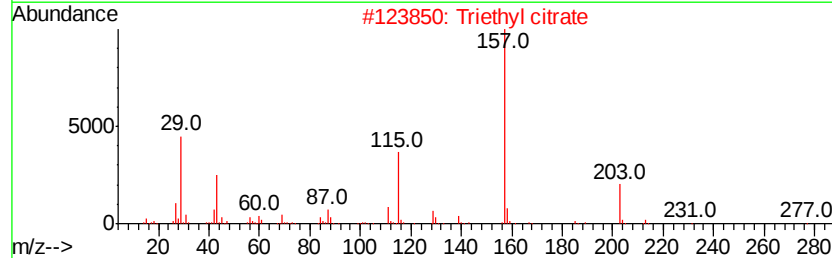
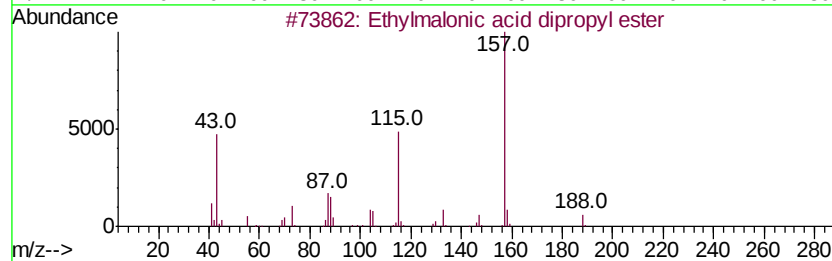
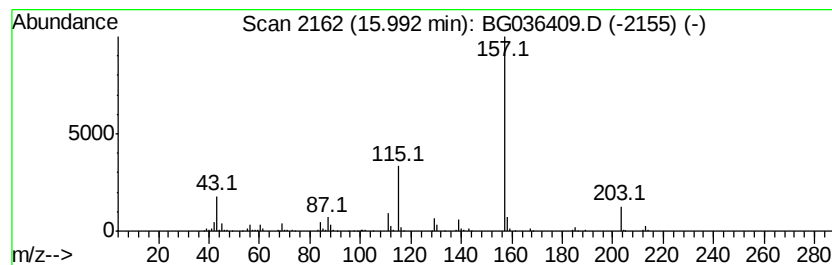
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Peak Number 3 Ethylmalonic acid dipropyl ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.99	11.07 ng	388089	Acenaphthene-d10	14.69		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
2		Triethyl citrate	276	C12H20O7	000077-93-0	58
3		3-Chloro2-fluorobenzoic acid, 6-...	384	C22H34ClF02	1000338-65-3	53
4		3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClF02	1000338-64-6	53
5		3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClF02	1000338-64-9	42



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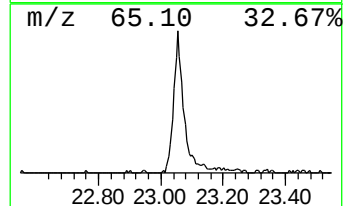
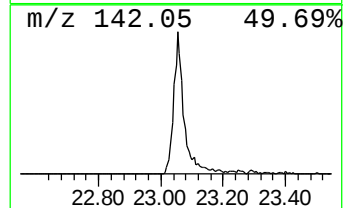
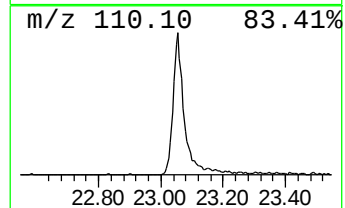
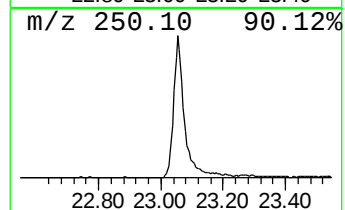
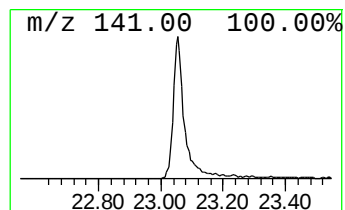
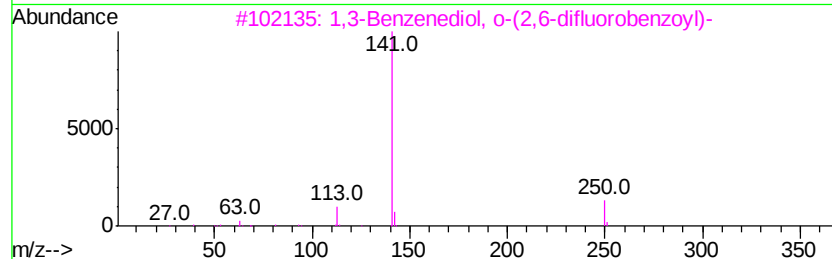
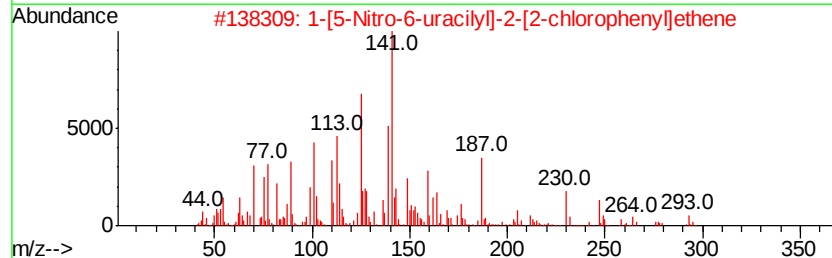
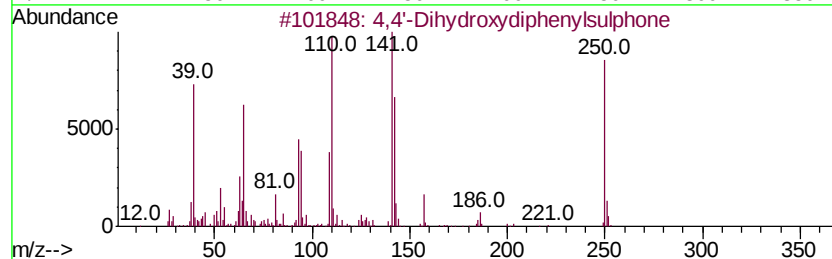
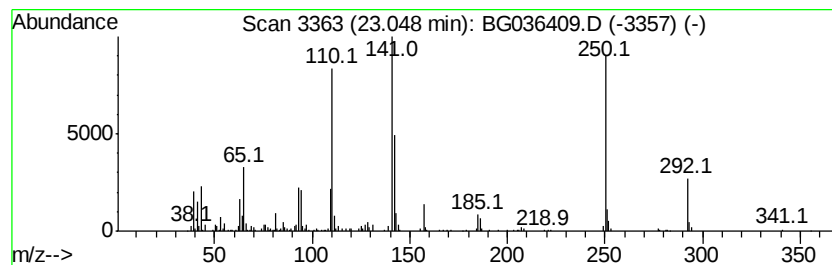
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Peak Number 4 4,4'-Dihydroxydiphenylsulphone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
23.05	9.98 ng	551987	Chrysene-d12	21.70		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	96	
2	1-[5-Nitro-6-uracilyl]-2-[2-chlo...	293	C12H8ClN3O4	296798-53-3	25	
3	1,3-Benzenediol, o-(2,6-difluoro...	250	C13H8F2O3	1000330-83-2	25	
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	14	
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	14	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.60	7.60	65.6	ng	1029200	1	8.07	313665	20.0
Ethylmalonic acid...	15.99	11.1	ng	388089	3	14.69	701305	20.0
4,4'-Dihydroxydip...	23.05	10.0	ng	551987	5	21.70	1106370	20.0