

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072718\
 Data File : BG035943.D
 Acq On : 27 Jul 2018 18:42
 Operator : JU/SJ
 Sample : J4192-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

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-BG071218.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

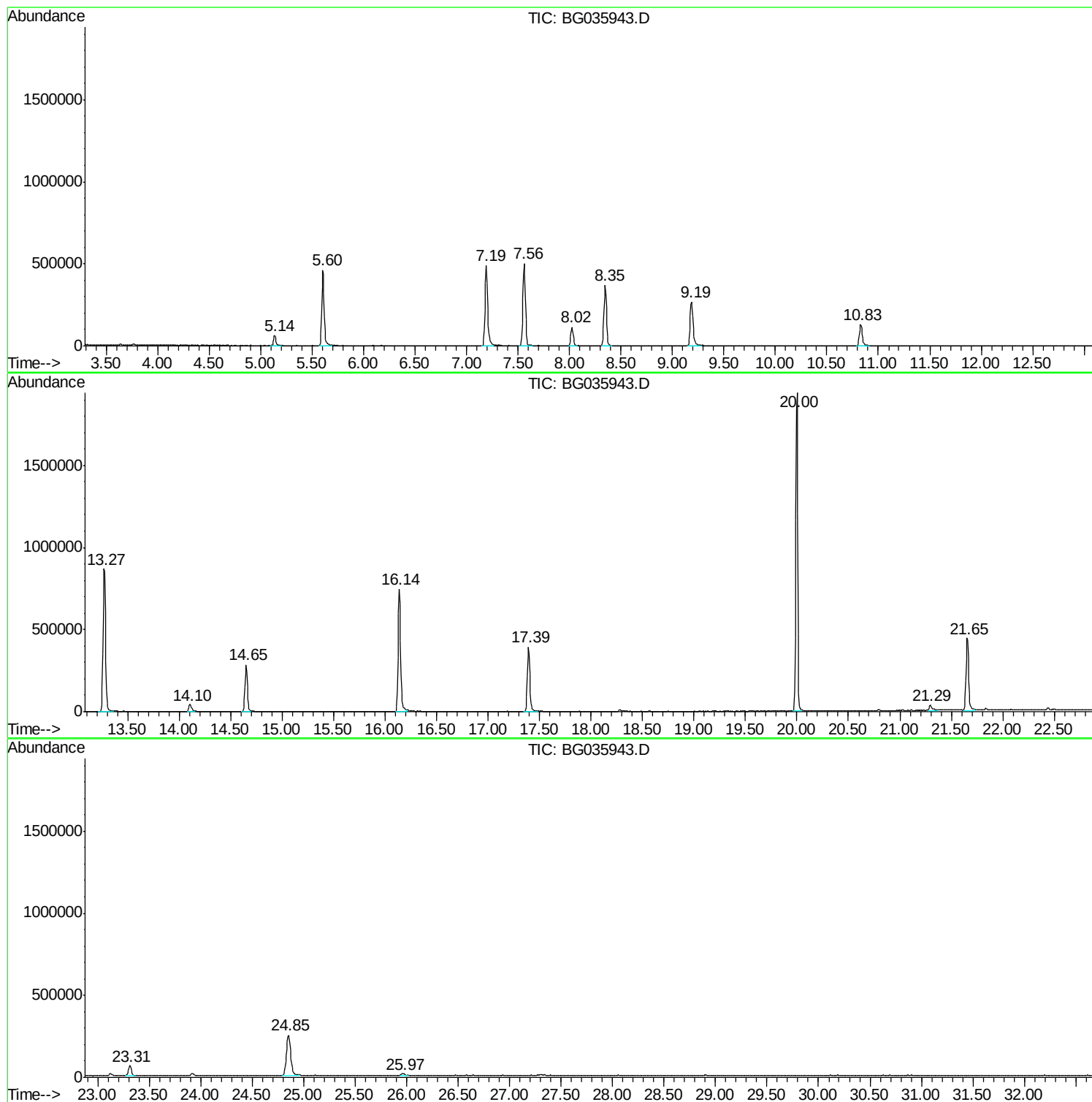
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.139	307	315	325	rVB	62898	102557	3.95%	0.816%
2	5.603	387	394	409	rBV	462002	795236	30.62%	6.330%
3	7.195	657	665	677	rBV	489411	928681	35.75%	7.392%
4	7.559	719	727	740	rBV	500618	856102	32.96%	6.814%
5	8.023	800	806	814	rBV	115721	191125	7.36%	1.521%
6	8.346	854	861	871	rBV	370075	640103	24.64%	5.095%
7	9.186	996	1004	1020	rBV2	267589	546060	21.02%	4.346%
8	10.825	1276	1283	1297	rBV	131810	268638	10.34%	2.138%
9	13.269	1690	1699	1714	rBV	869600	1453244	55.95%	11.567%
10	14.103	1836	1841	1849	rBV3	44008	85969	3.31%	0.684%
11	14.649	1926	1934	1942	rBV2	284958	468498	18.04%	3.729%
12	16.136	2181	2187	2200	rBV	747322	1222618	47.07%	9.731%
13	17.393	2393	2401	2416	rBV2	393955	678371	26.12%	5.399%
14	20.001	2838	2845	2852	rBV	1939428	2597461	100.00%	20.675%
15	21.293	3061	3065	3078	rBV4	32876	70874	2.73%	0.564%
16	21.652	3119	3126	3138	rBV	441790	780958	30.07%	6.216%
17	23.308	3401	3408	3416	rVB3	61926	124227	4.78%	0.989%
18	24.853	3660	3671	3688	rBV2	246419	720105	27.72%	5.732%
19	25.969	3855	3861	3867	rBV8	12173	32764	1.26%	0.261%

Sum of corrected areas: 12563591

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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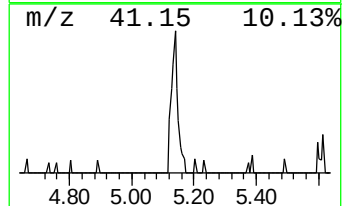
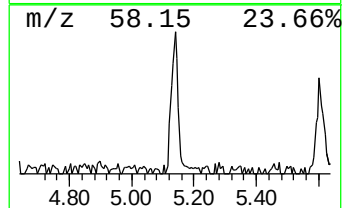
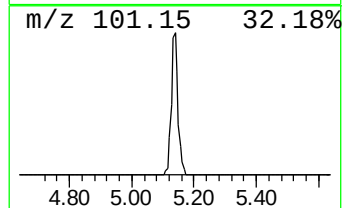
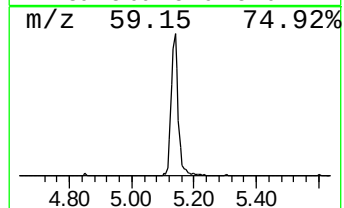
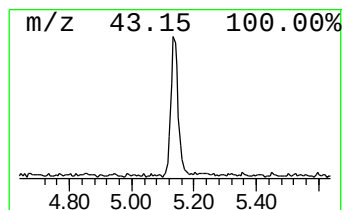
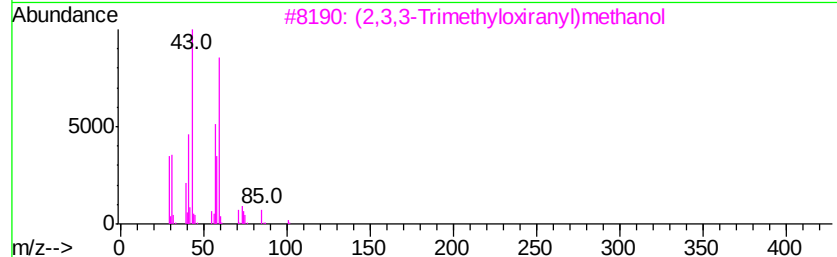
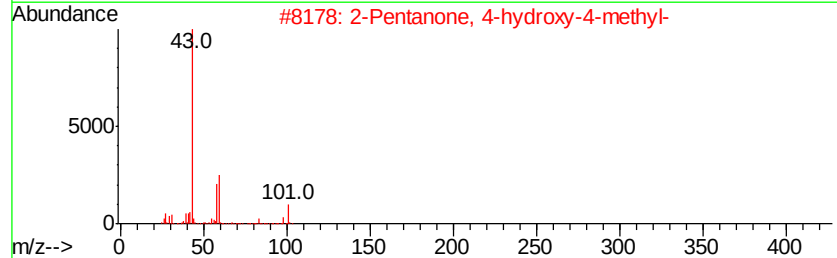
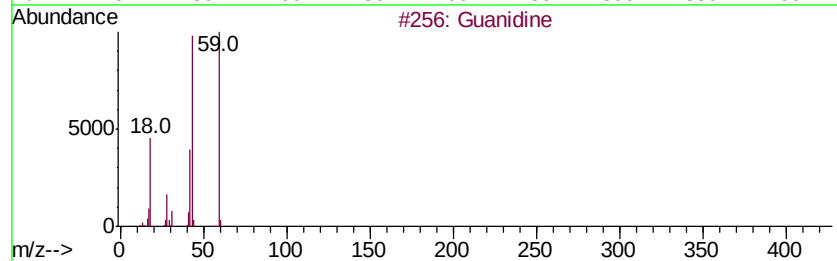
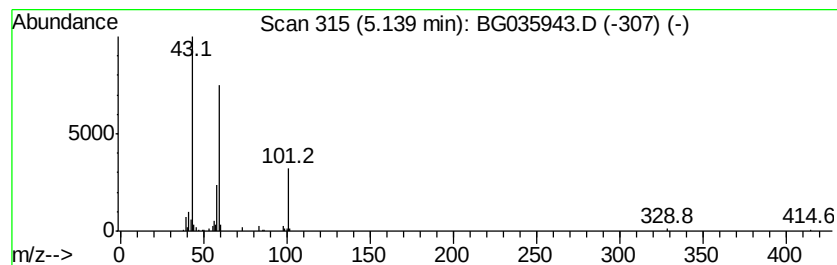
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Peak Number 1 Guanine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	10.73 ng	102557	1,4-Dichlorobenzene-d4	8.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanine		59	CH5N3	000113-00-8	50
2	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
3	(2,3,3-Trimethyloxiranvl)methanol		116	C6H12O2	1000306-64-7	39
4	Propane, 1,1-dipropoxy-		160	C9H20O2	004744-11-0	39
5	2-Acetoxyisobutyryl chloride		164	C6H9ClO3	040635-66-3	37



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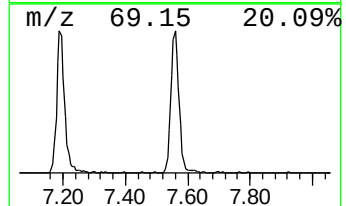
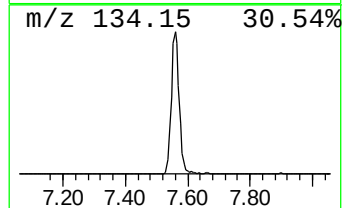
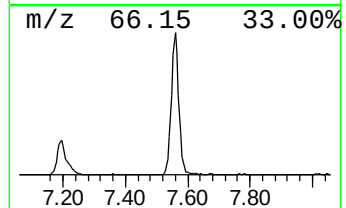
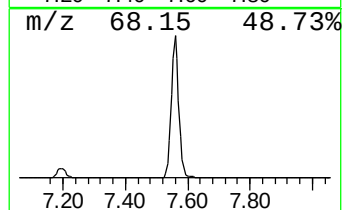
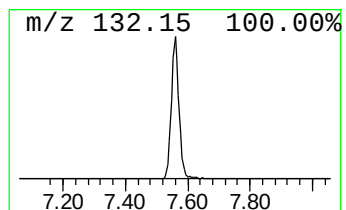
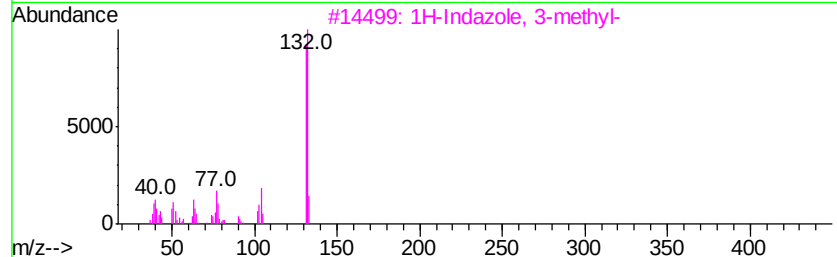
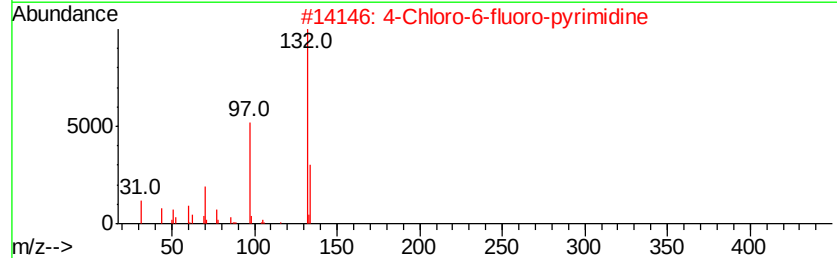
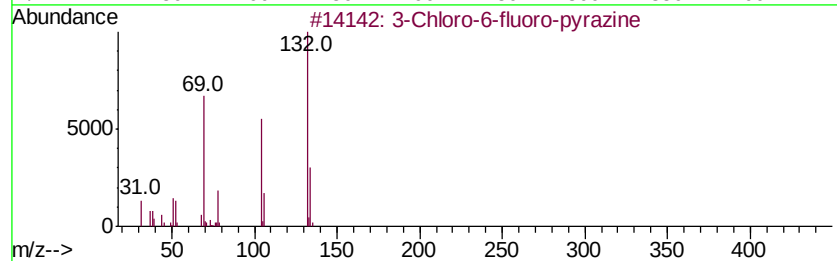
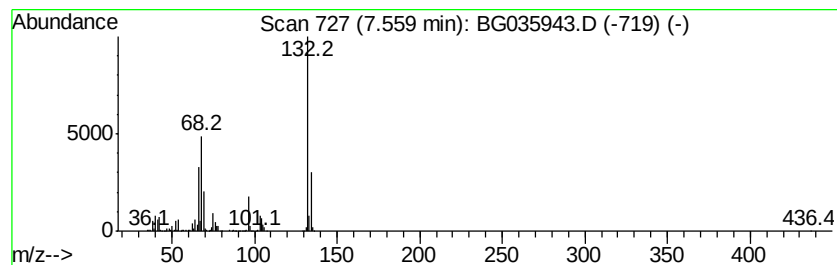
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Peak Number 2 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	89.59 ng	856102	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	16	
3	1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	14	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
5	5-Aminoindole	132	C8H8N2	005192-03-0	12	



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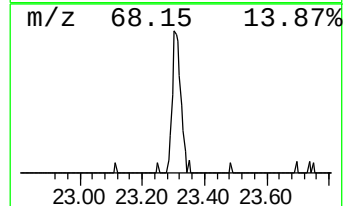
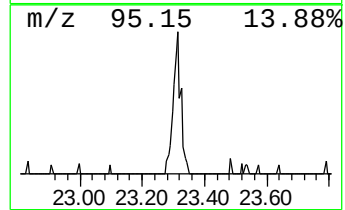
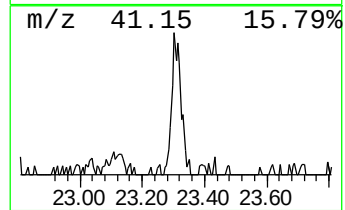
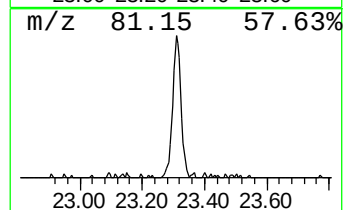
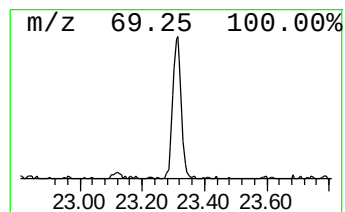
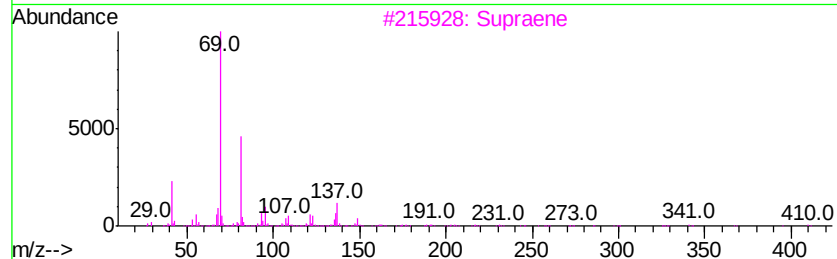
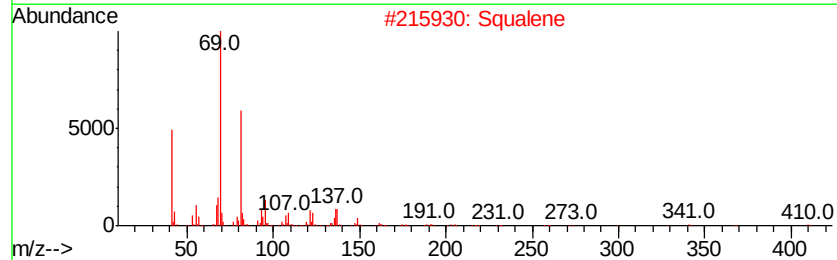
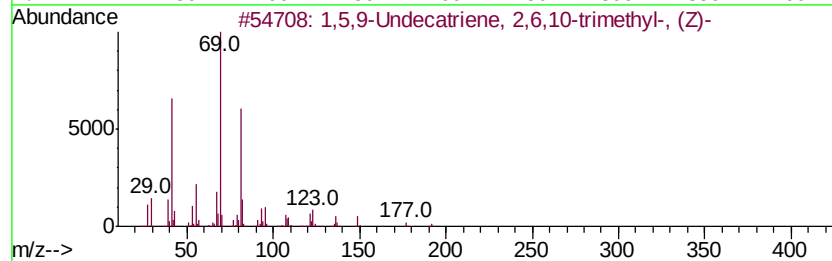
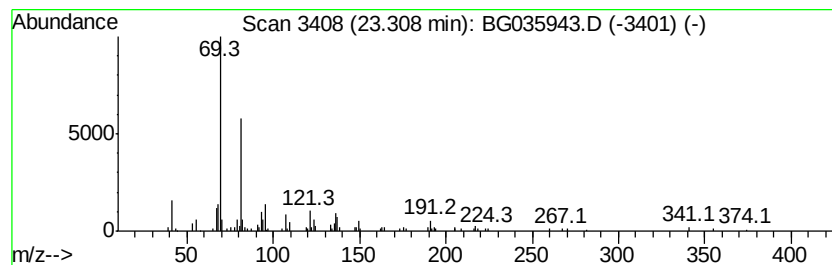
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Peak Number 4 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	3.45 ng	124227	Perylene-d12	24.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
2		Squalene	410	C30H50	000111-02-4	83
3		Supraene	410	C30H50	007683-64-9	83
4		Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	64
5		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Guanidine	5.14	10.7	ng	102557	1	8.02	191125	20.0
unknown7.56	7.56	89.6	ng	856102	1	8.02	191125	20.0
1,5,9-Undecatrien...	23.31	3.5	ng	124227	6	24.85	720105	20.0