

Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
 Data File : BF102154.D
 Acq On : 17 Jan 2018 17:12
 Operator : SJ/JU
 Sample : PB105727BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB105727BL

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_F\METHODS\8270-BF010918.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	4.940	477	485	495	rBV	177869	286918	6.51%	0.865%
2	5.340	547	553	556	rBV	3630844	3947505	89.61%	11.897%
3	6.363	720	727	730	rBV	3439965	3800406	86.27%	11.453%
4	6.492	744	749	752	rBV	3973623	3989420	90.56%	12.023%
5	6.722	784	788	791	rBV	990284	817279	18.55%	2.463%
6	6.875	810	814	818	rBV	3183688	3139420	71.26%	9.461%
7	7.287	878	884	887	rBV	2331147	2546272	57.80%	7.674%
8	7.998	1001	1005	1009	rBV	1183763	1110377	25.20%	3.346%
9	9.081	1183	1189	1192	rBV	4527904	4405385	100.00%	13.277%
10	9.751	1298	1303	1307	rBV	1279382	1168566	26.53%	3.522%
11	10.545	1433	1438	1441	rBV	2357196	2301469	52.24%	6.936%
12	11.233	1551	1555	1559	rBV	1214536	1015563	23.05%	3.061%
13	12.821	1820	1825	1828	rBV	3172240	3123872	70.91%	9.415%
14	13.863	1998	2002	2006	rBV	713331	669017	15.19%	2.016%
15	15.280	2238	2243	2247	rBV2	567498	690412	15.67%	2.081%
16	16.745	2487	2492	2499	rVB8	40049	94101	2.14%	0.284%
17	17.539	2623	2627	2635	rVB9	32138	75361	1.71%	0.227%

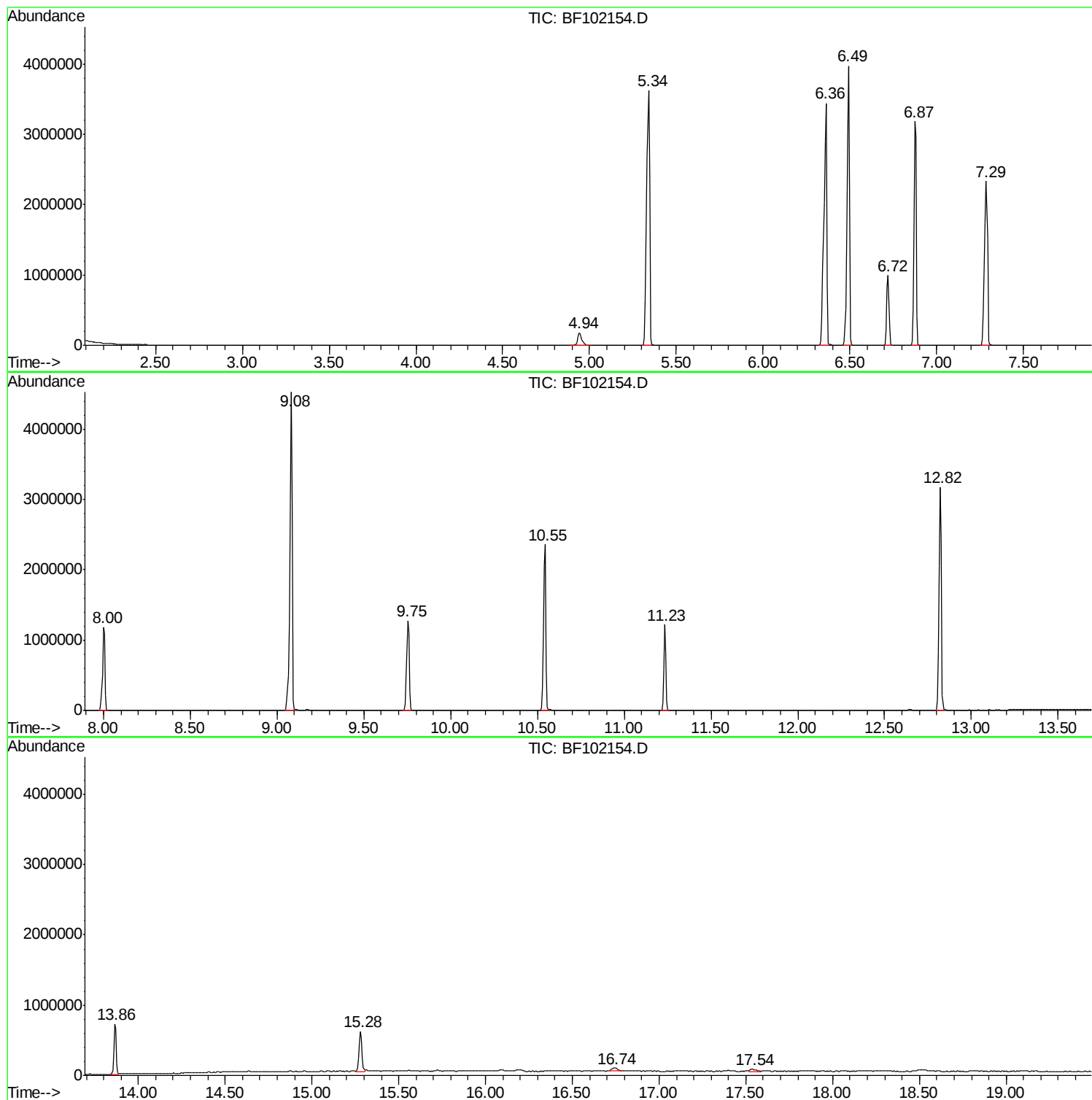
Sum of corrected areas: 33181343

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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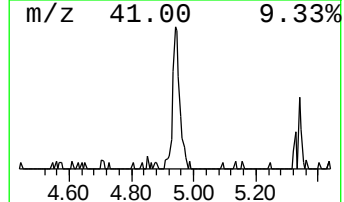
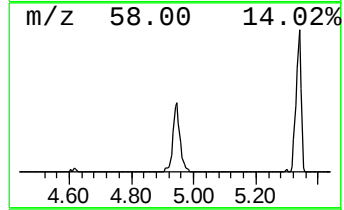
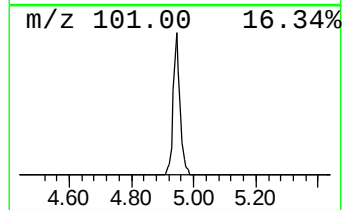
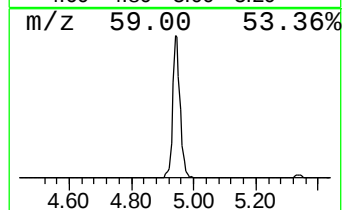
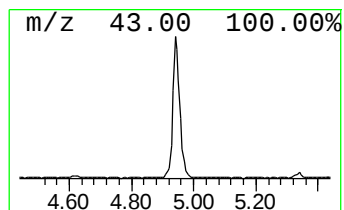
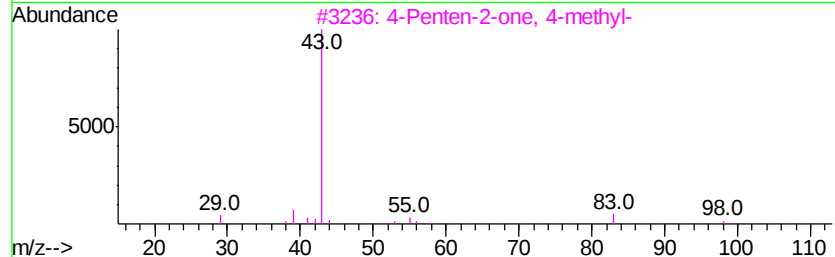
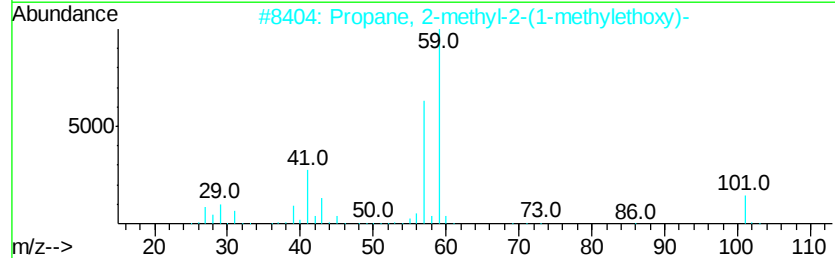
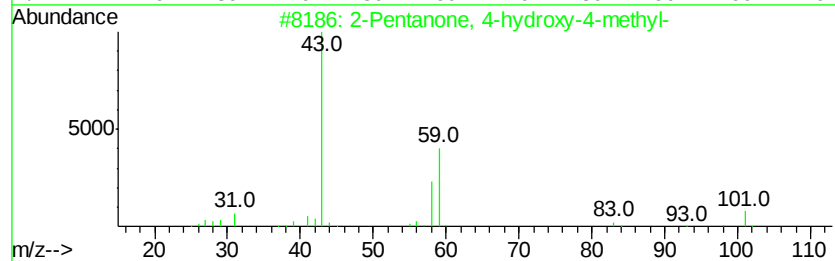
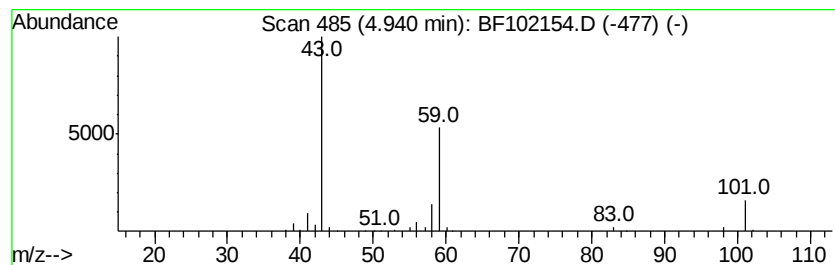
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	7.02 ng	286918	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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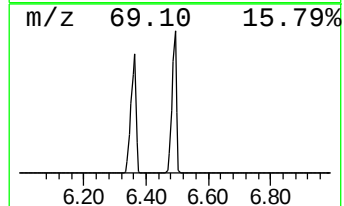
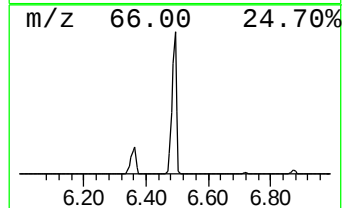
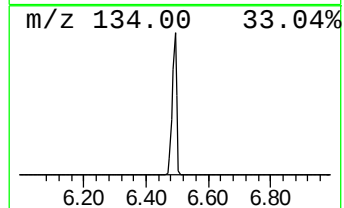
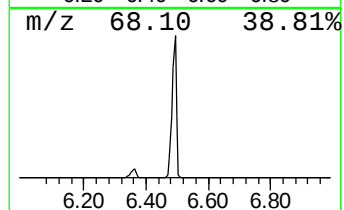
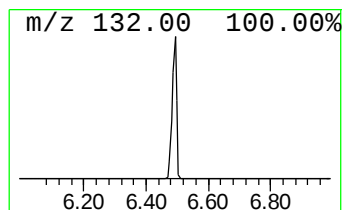
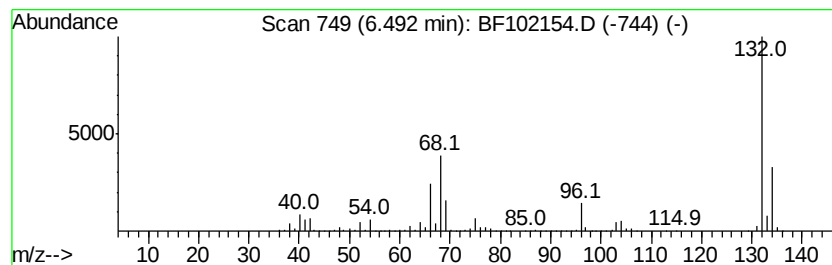
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	97.63 ng	3989420	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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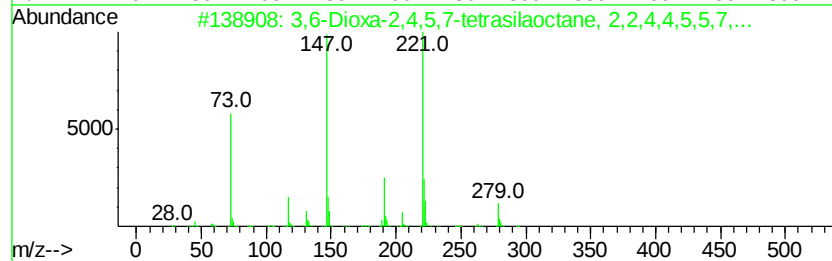
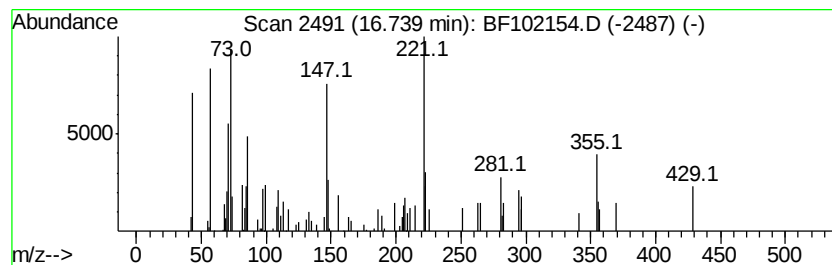
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Peak Number 4 unknown16.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.73 ng	94101	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
3		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
4		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32
5		2-((E)-([3-(2-Dimethylanilino)-1...	356	C23H20N2O2	073428-83-8	22



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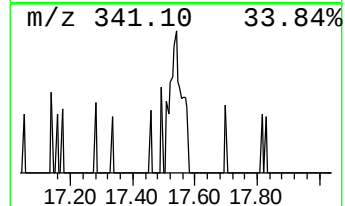
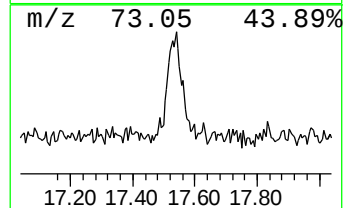
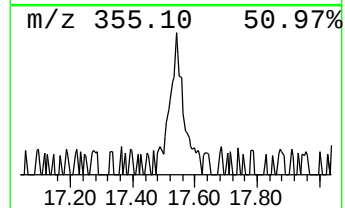
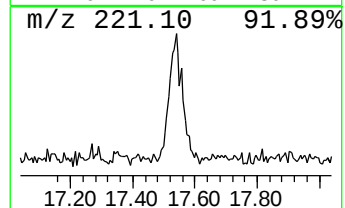
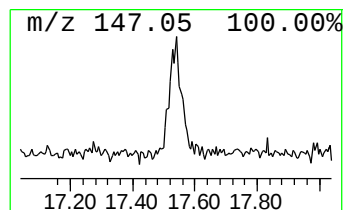
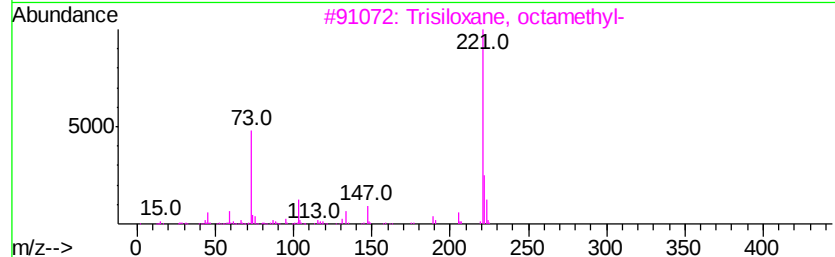
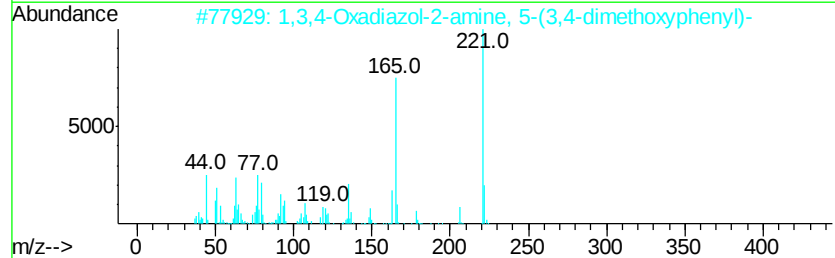
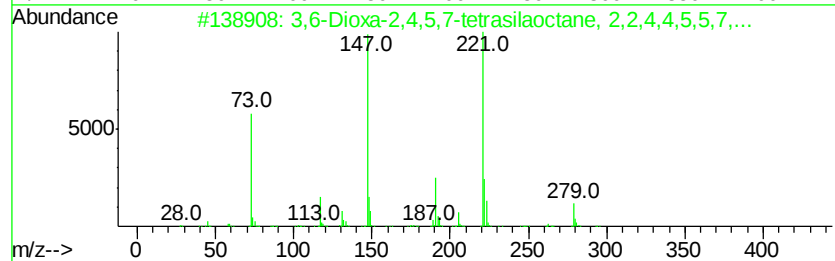
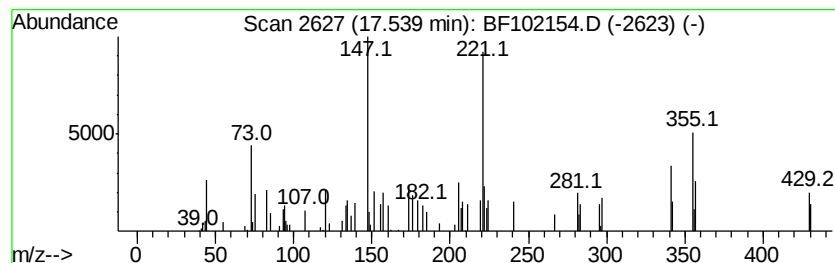
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Peak Number 5 unknown17.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.54	2.18 ng	75361	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
2		1,3,4-Oxadiazol-2-amine, 5-(3,4-...	221	C10H11N3O3	1000362-71-7	18
3		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	14
4		Tetrazole, 1-(2-fluorophenyl)-5-...	342	C18H19FN4S	1000272-52-4	14
5		5-Fluoro-4-chloro-2-aminopyrimidine	147	C4H3ClFN3	001683-75-6	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	7.0	ng	286918	1	6.72	817279	20.0
unknown6.49	6.49	97.6	ng	3989420	1	6.72	817279	20.0
unknown16.74	16.74	2.7	ng	94101	6	15.28	690412	20.0
unknown17.54	17.54	2.2	ng	75361	6	15.28	690412	20.0