

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038674.D
 Acq On : 17 Dec 2018 23:00
 Operator : JU/SJ
 Sample : J6346-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DW-11

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-BG121218.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	5.138	345	349	356	rVB	22166	35304	2.03%	0.391%
2	5.608	422	429	444	rVB	418136	699492	40.19%	7.741%
3	7.212	695	702	714	rBV	433483	812392	46.68%	8.990%
4	7.588	756	766	779	rVB	398555	715414	41.10%	7.917%
5	8.058	840	846	856	rBV	72069	125526	7.21%	1.389%
6	8.381	894	901	909	rVB	292108	536838	30.84%	5.941%
7	9.239	1038	1047	1057	rBV	256056	482852	27.74%	5.343%
8	10.878	1317	1326	1334	rBV	91947	169109	9.72%	1.871%
9	13.317	1734	1741	1748	rBV	662012	1067708	61.35%	11.815%
10	14.139	1874	1881	1888	rBV	43482	65962	3.79%	0.730%
11	14.698	1969	1976	1985	rVB2	150692	256373	14.73%	2.837%
12	16.184	2222	2229	2240	rBV	587492	949292	54.54%	10.505%
13	17.441	2434	2443	2450	rBV	228836	352032	20.23%	3.896%
14	18.305	2585	2590	2596	rBV2	43899	70136	4.03%	0.776%
15	19.568	2802	2805	2813	rBV4	18770	28286	1.63%	0.313%
16	20.044	2880	2886	2892	rBV	1345003	1740459	100.00%	19.260%
17	21.319	3100	3103	3114	rVB9	12386	25911	1.49%	0.287%
18	21.725	3165	3172	3178	rBV2	225205	388855	22.34%	4.303%
19	25.021	3722	3733	3743	rVB2	126709	373011	21.43%	4.128%
20	26.801	4024	4036	4048	rBV5	38306	141700	8.14%	1.568%

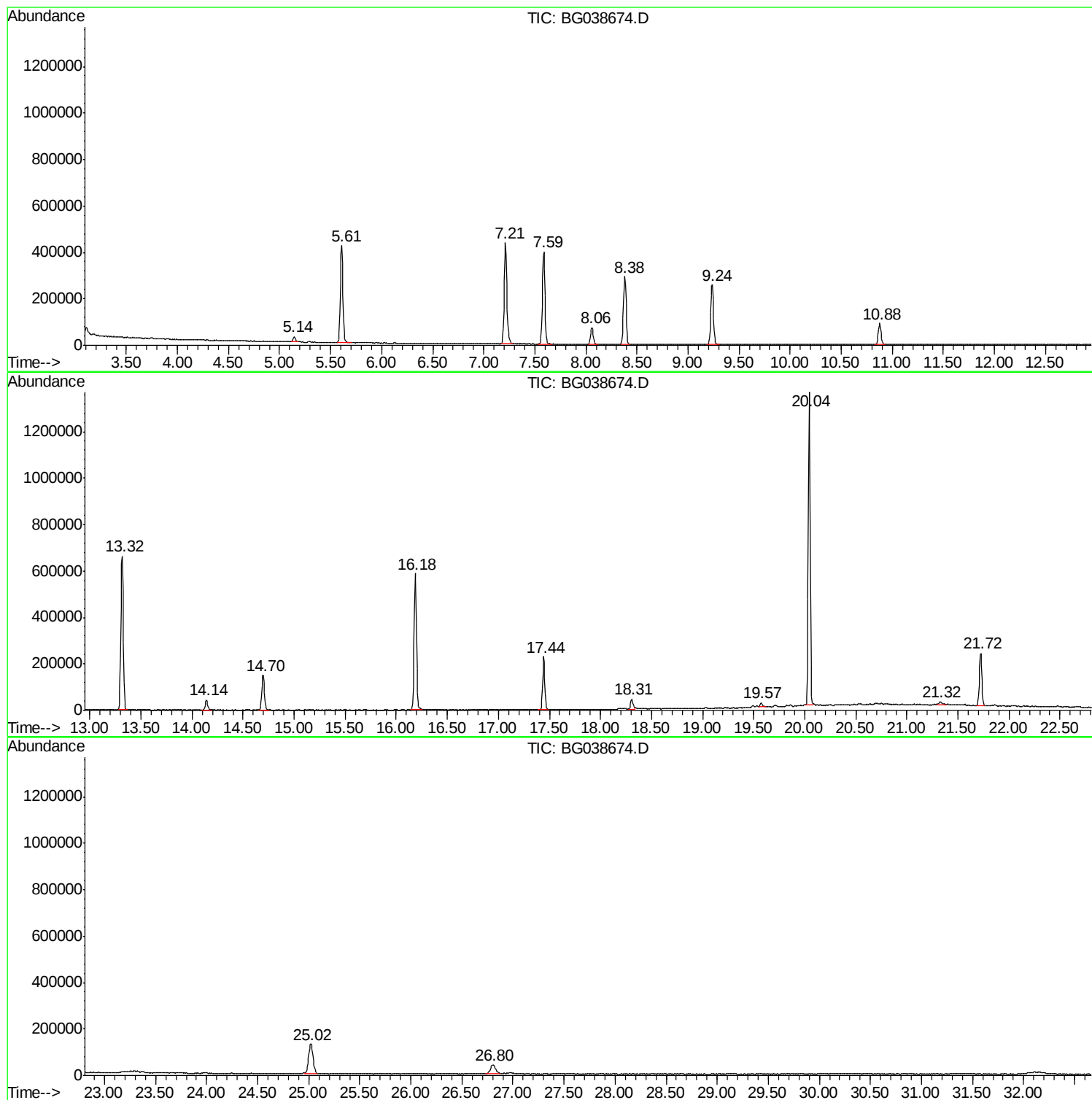
Sum of corrected areas: 9036652

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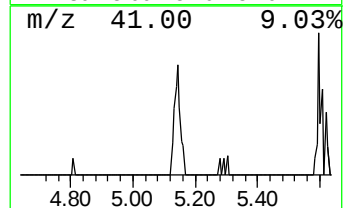
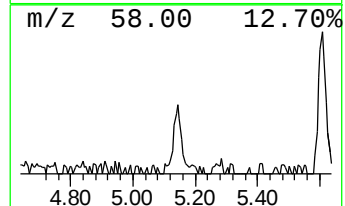
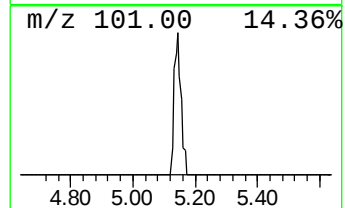
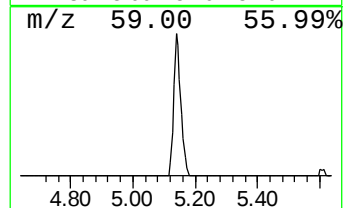
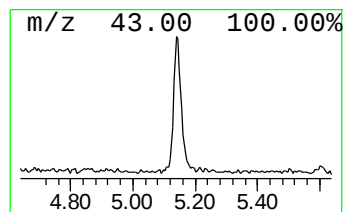
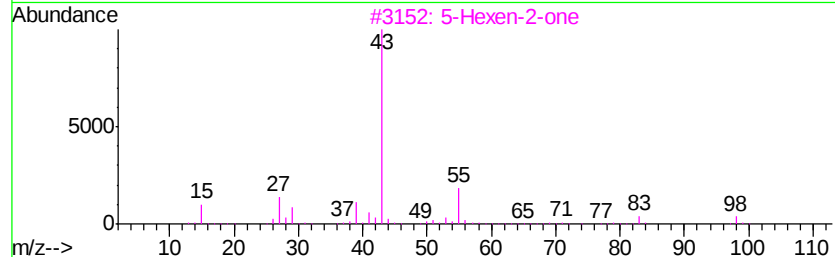
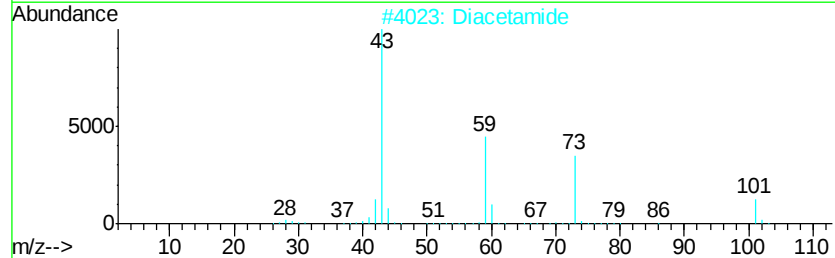
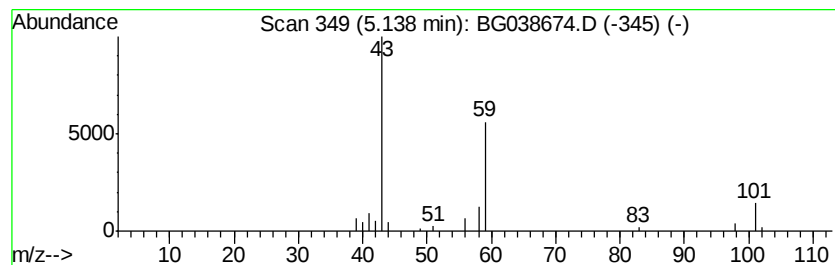
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.62 ng	35304	1,4-Dichlorobenzene-d4	8.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Diacetamide	101	C4H7NO2	000625-77-4	9	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	9	



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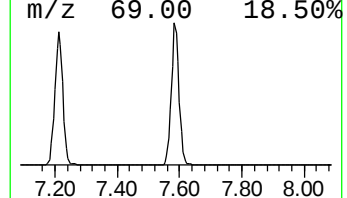
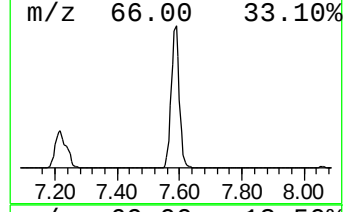
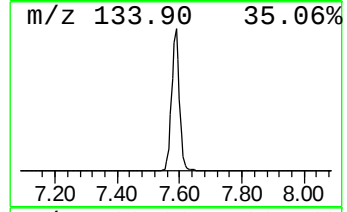
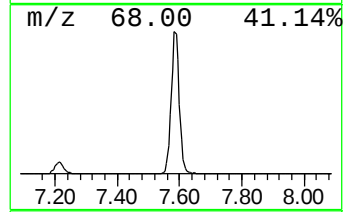
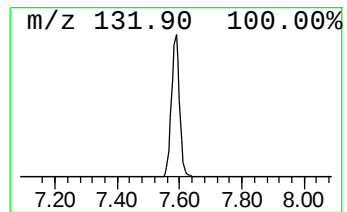
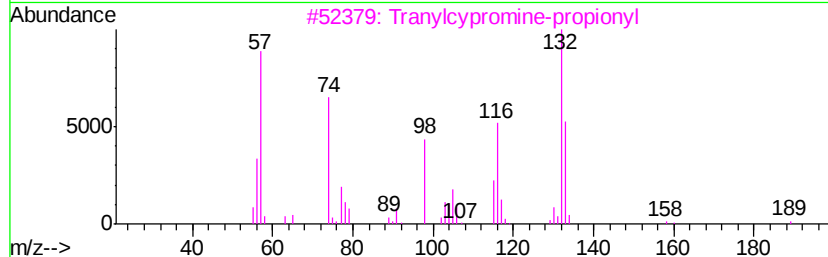
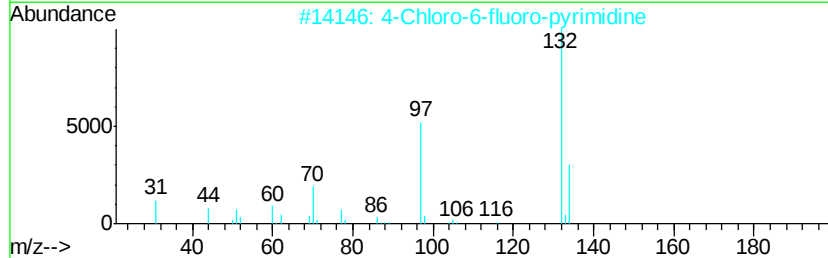
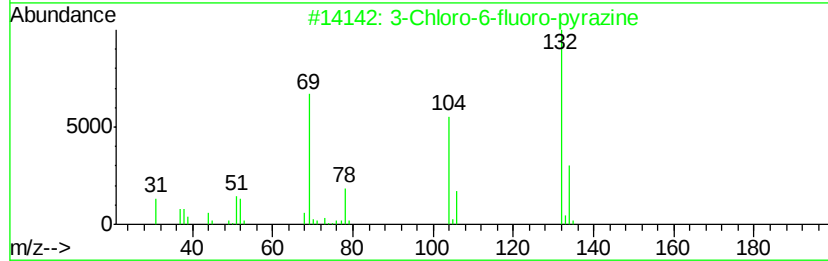
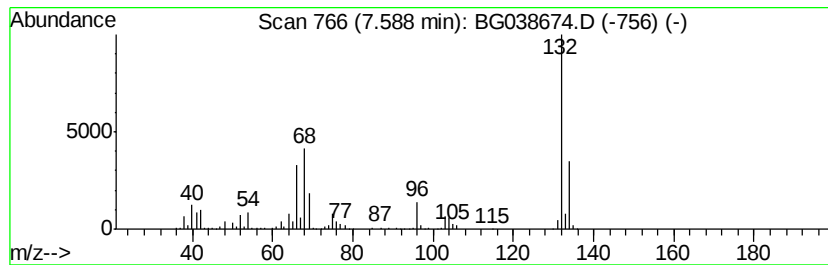
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	113.99 ng	715414	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12



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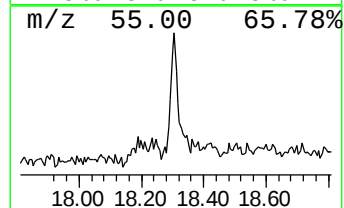
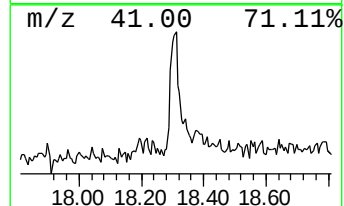
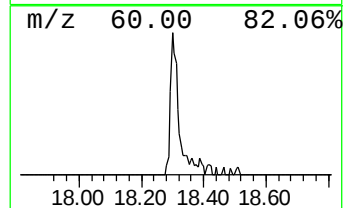
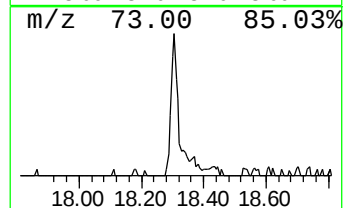
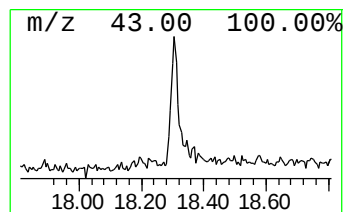
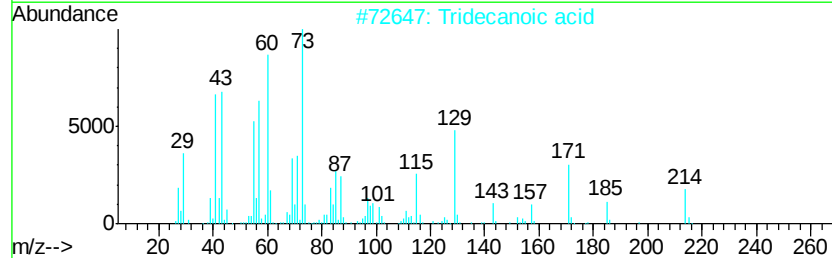
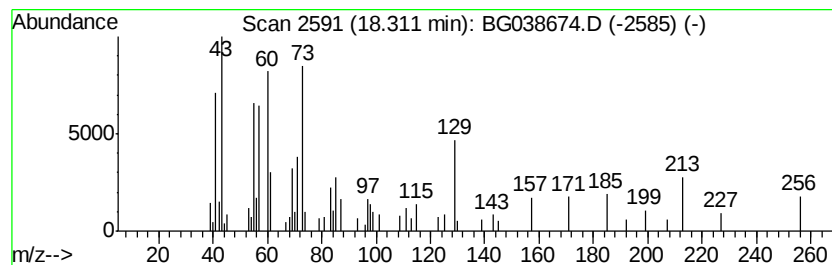
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	3.98 ng	70136	Phenanthrene-d10	17.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	35



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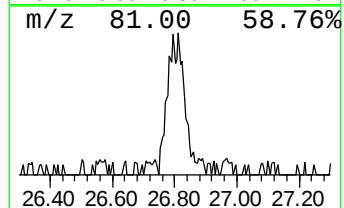
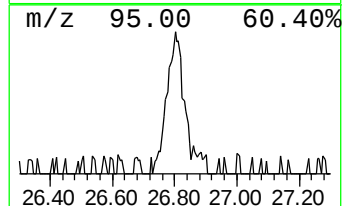
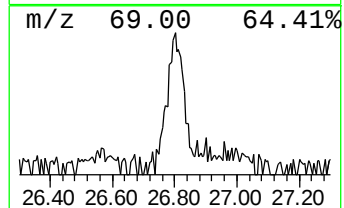
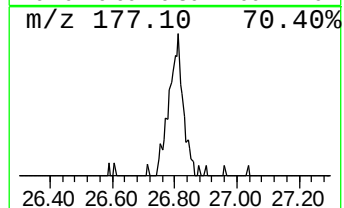
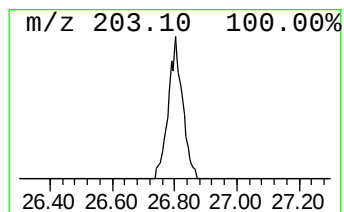
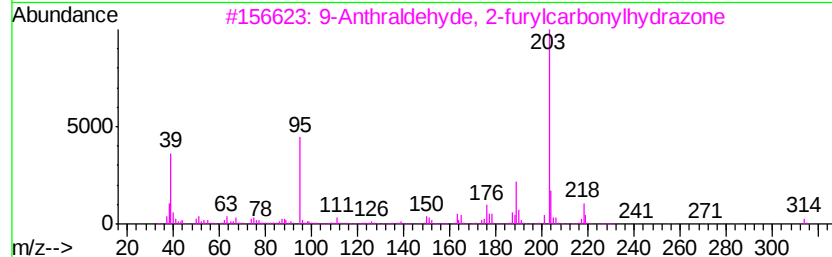
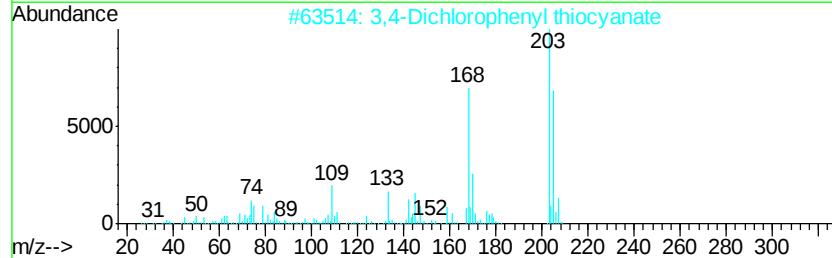
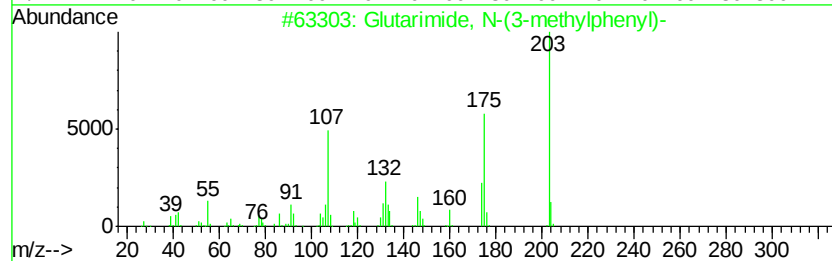
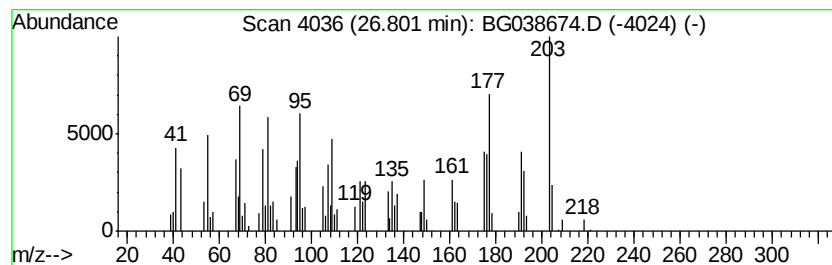
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Peak Number 5 unknown26.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.80	7.60 ng	141700	Perylene-d12	25.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Glutarimide, N-(3-methylphenyl)-	203	C12H13NO2	1000360-92-6	25
2		3,4-Dichlorophenyl thiocyanate	203	C7H3Cl2NS	003313-77-7	18
3		9-Anthraldehyde, 2-furylcarbonyl...	314	C20H14N2O2	292180-87-1	16
4		.beta.-Bisabolene	204	C15H24	000495-61-4	11
5		2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	035044-68-9	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	5.6	ng	35304	1	8.06	125526	20.0
unknown7.59	7.59	114.0	ng	715414	1	8.06	125526	20.0
n-Hexadecanoic acid	18.31	4.0	ng	70136	4	17.44	352032	20.0
unknown26.80	26.80	7.6	ng	141700	6	25.02	373011	20.0