

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
 Data File : BF081651.D
 Acq On : 16 Sep 2015 16:10
 Operator : UM/IZ
 Sample : G3647-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S12

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-BF090115.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	1.440	8	9	15	rBV	196765	516493	15.38%	2.823%
2	1.531	15	17	61	rVB	970717	3357764	100.00%	18.355%
3	4.469	270	274	294	rBV	292176	859739	25.60%	4.700%
4	5.337	347	350	366	rBV	701317	1468003	43.72%	8.025%
5	7.612	544	549	553	rBV	826111	1551755	46.21%	8.482%
6	7.703	553	557	565	rVB	895456	1548680	46.12%	8.466%
7	8.183	596	599	606	rBB	196112	303963	9.05%	1.662%
8	8.515	624	628	631	rBV	656809	1110938	33.09%	6.073%
9	9.486	708	713	716	rBV	551081	992464	29.56%	5.425%
10	11.086	849	853	857	rBV	224166	396591	11.81%	2.168%
11	13.727	1079	1084	1087	rBV	860765	1619859	48.24%	8.855%
12	14.778	1173	1176	1186	rBB	121918	206669	6.15%	1.130%
13	15.212	1210	1214	1220	rBB2	246700	426939	12.71%	2.334%
14	17.121	1376	1381	1390	rBB	578849	1066437	31.76%	5.829%
15	18.721	1517	1521	1528	rBV	247613	454667	13.54%	2.485%
16	20.470	1671	1674	1685	rVB	24594	54521	1.62%	0.298%
17	22.082	1812	1815	1818	rBV	1119961	1554871	46.31%	8.499%
18	23.328	1921	1924	1925	rBV2	62563	88674	2.64%	0.485%
19	23.350	1925	1926	1929	rVB	328203	407421	12.13%	2.227%
20	24.791	2049	2052	2055	rBV	303114	307479	9.16%	1.681%

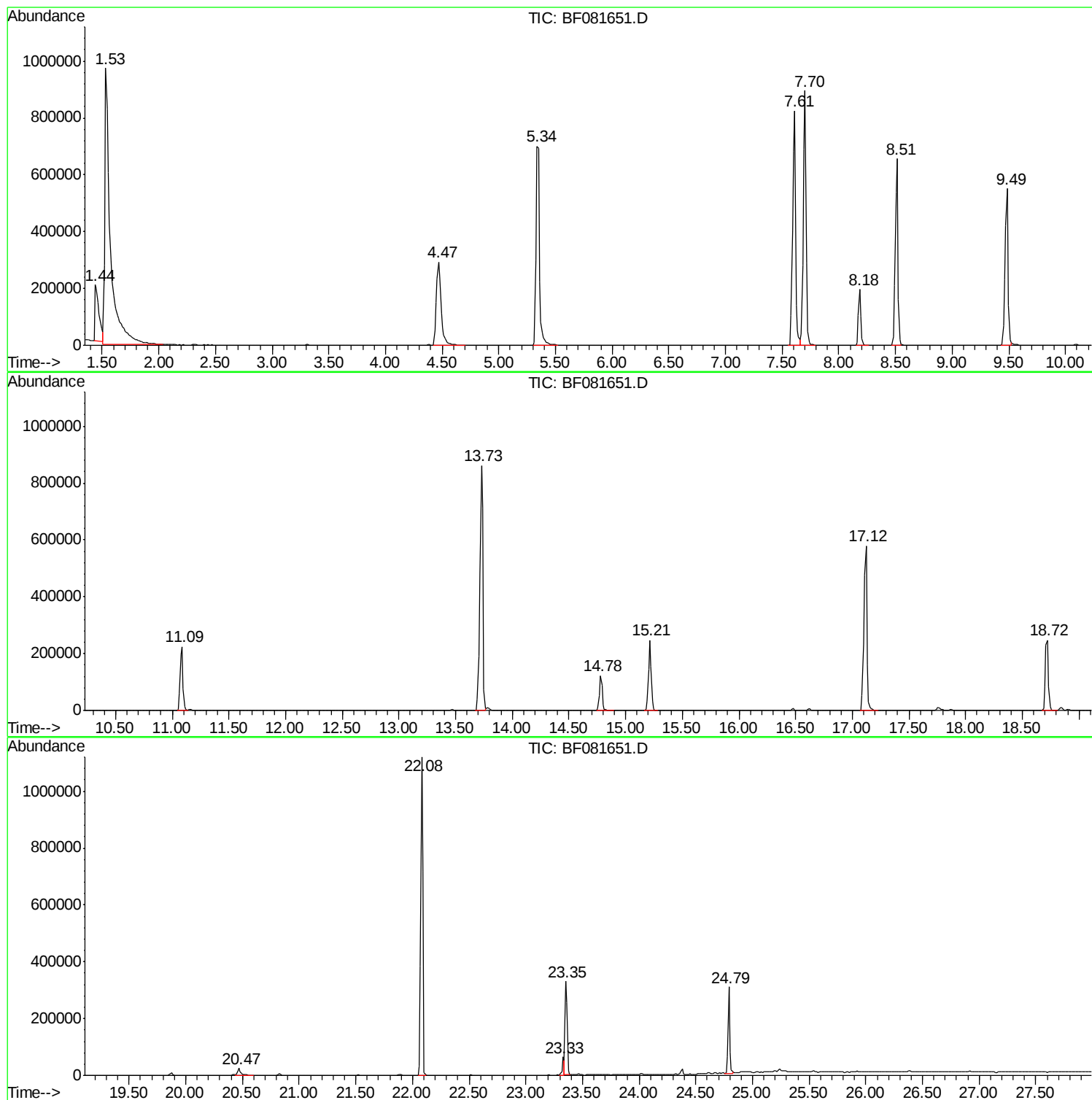
Sum of corrected areas: 18293927

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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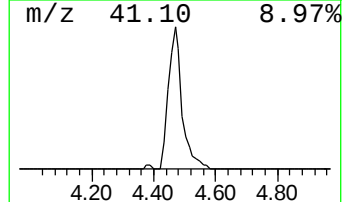
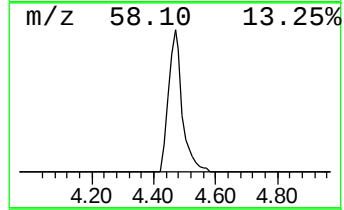
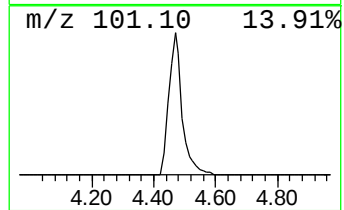
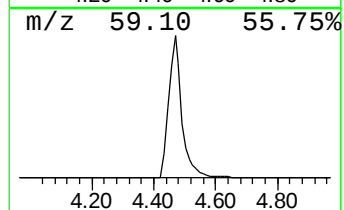
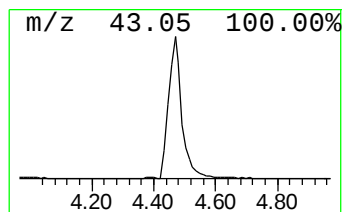
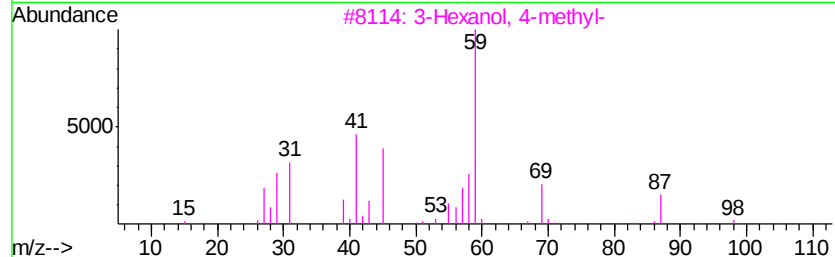
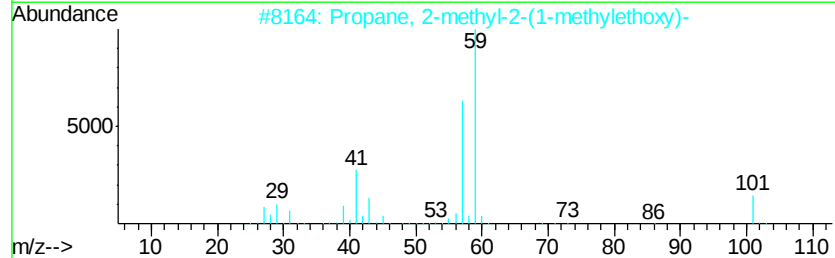
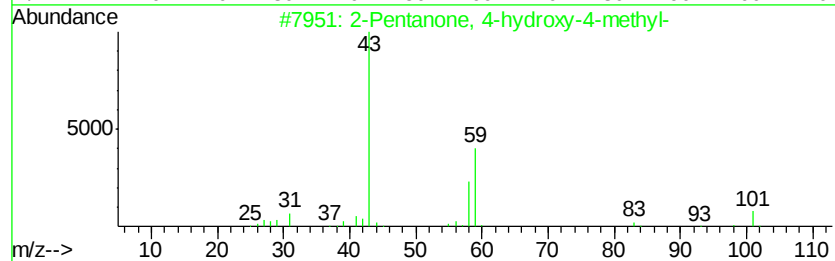
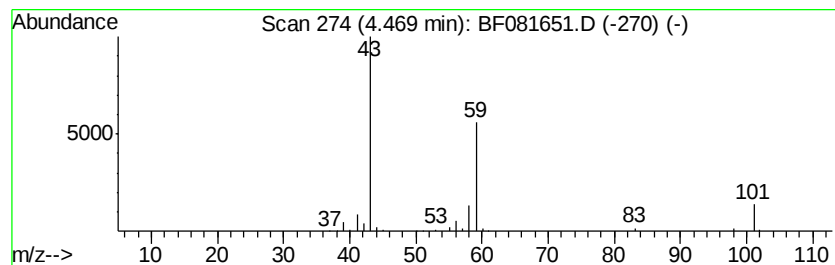
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	56.57 ng	859739	1,4-Dichlorobenzene-d4	8.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	



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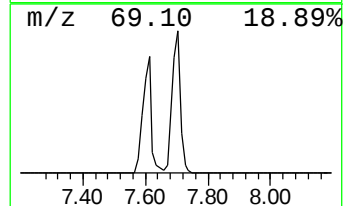
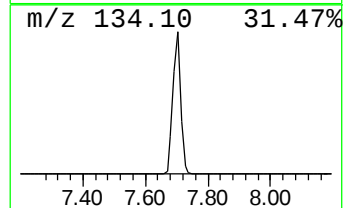
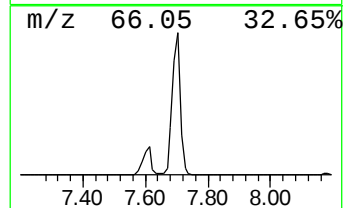
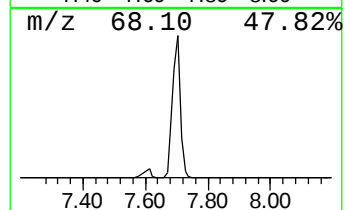
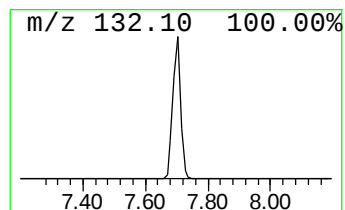
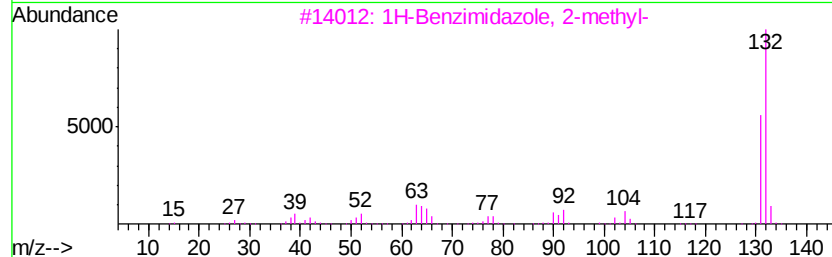
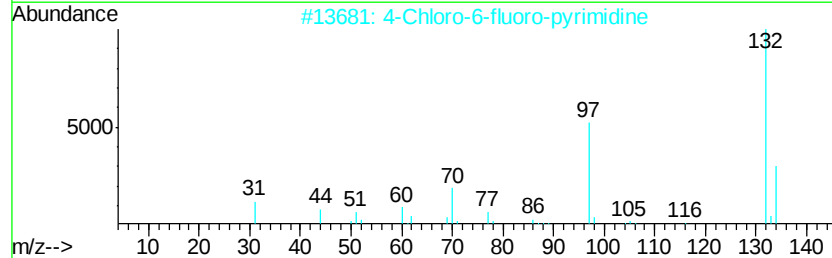
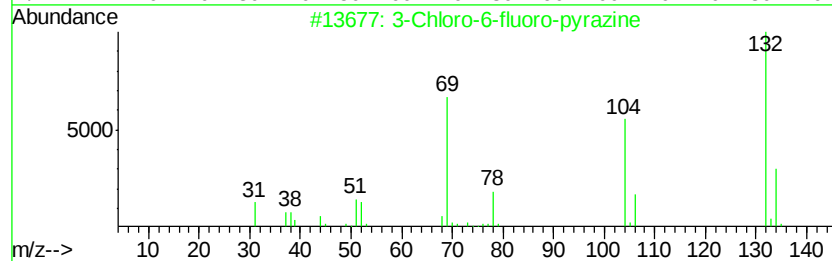
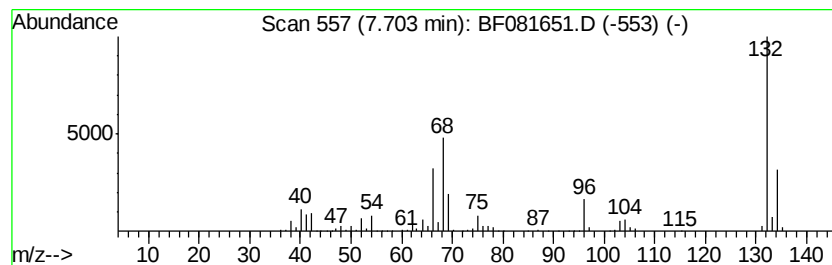
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Peak Number 4 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	101.90 ng	1548680	1,4-Dichlorobenzene-d4	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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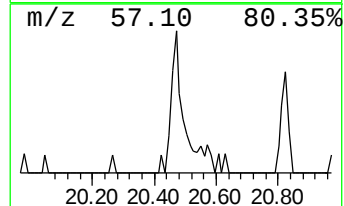
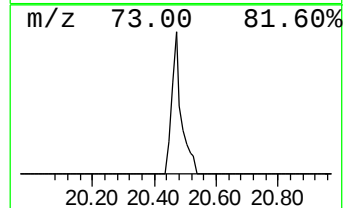
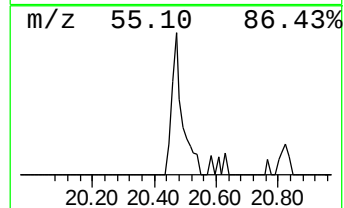
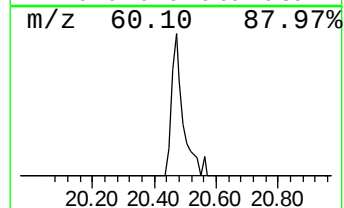
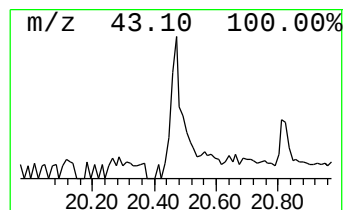
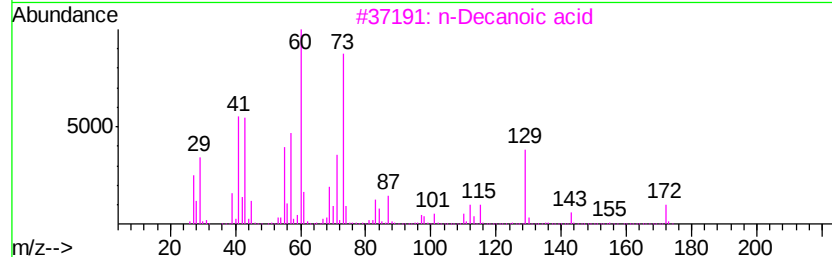
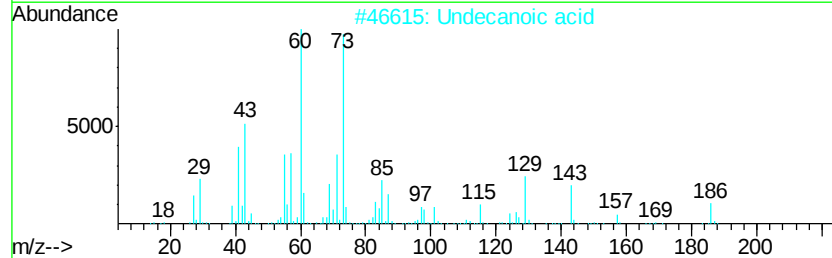
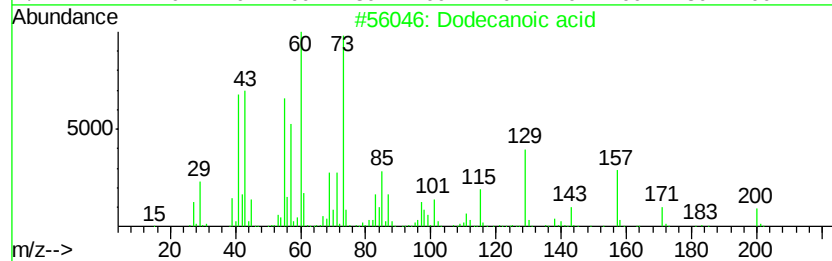
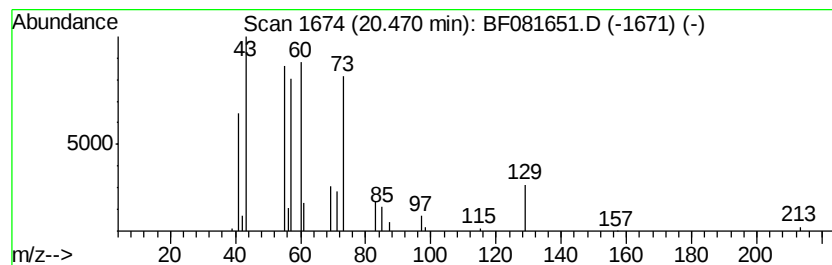
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Peak Number 6 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	2.40 ng	54521	Phenanthrene-d10	18.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	72
2		Undecanoic acid	186	C11H22O2	000112-37-8	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47
5		Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.47	56.6	ng	859739	1	8.18	303963	20.0
unknown7.70	7.70	101.9	ng	1548680	1	8.18	303963	20.0
Dodecanoic acid	20.47	2.4	ng	54521	4	18.72	454667	20.0