

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
 Data File : BG031692.D
 Acq On : 22 Dec 2017 2:51
 Operator : SJ/JU
 Sample : I7002-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-106-3DS(55-57)

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_G\METHODS\8270-BG122117.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	3.450	21	27	35	rBV	41763	84297	2.35%	0.467%
2	5.735	410	416	424	rBV	35974	62084	1.73%	0.344%
3	6.241	495	502	514	rBB	630881	1108039	30.84%	6.135%
4	7.927	780	789	800	rBV	631520	1228206	34.18%	6.801%
5	8.338	851	859	868	rBV	679316	1250090	34.79%	6.922%
6	8.826	934	942	951	rBV	146632	266099	7.41%	1.473%
7	9.167	991	1000	1009	rBV	503427	964628	26.84%	5.341%
8	10.024	1138	1146	1154	rBV	366121	664394	18.49%	3.679%
9	11.717	1425	1434	1444	rVB	206965	391336	10.89%	2.167%
10	14.090	1830	1838	1848	rVB	1407465	2201539	61.27%	12.190%
11	14.883	1966	1973	1980	rBV	85492	130483	3.63%	0.722%
12	15.459	2064	2071	2081	rBV2	380343	648433	18.05%	3.590%
13	16.934	2315	2322	2334	rVB	1274188	1997724	55.59%	11.061%
14	18.197	2530	2537	2544	rBV2	594521	912238	25.39%	5.051%
15	19.020	2671	2677	2686	rBV2	65225	102564	2.85%	0.568%
16	20.254	2883	2887	2898	rBV4	42482	72231	2.01%	0.400%
17	20.730	2962	2968	2977	rBV	2700068	3593394	100.00%	19.897%
18	22.110	3198	3203	3211	rBV	56341	93999	2.62%	0.520%
19	22.557	3271	3279	3287	rVB2	590303	1132382	31.51%	6.270%
20	26.341	3911	3923	3937	rVB2	356040	1156000	32.17%	6.401%

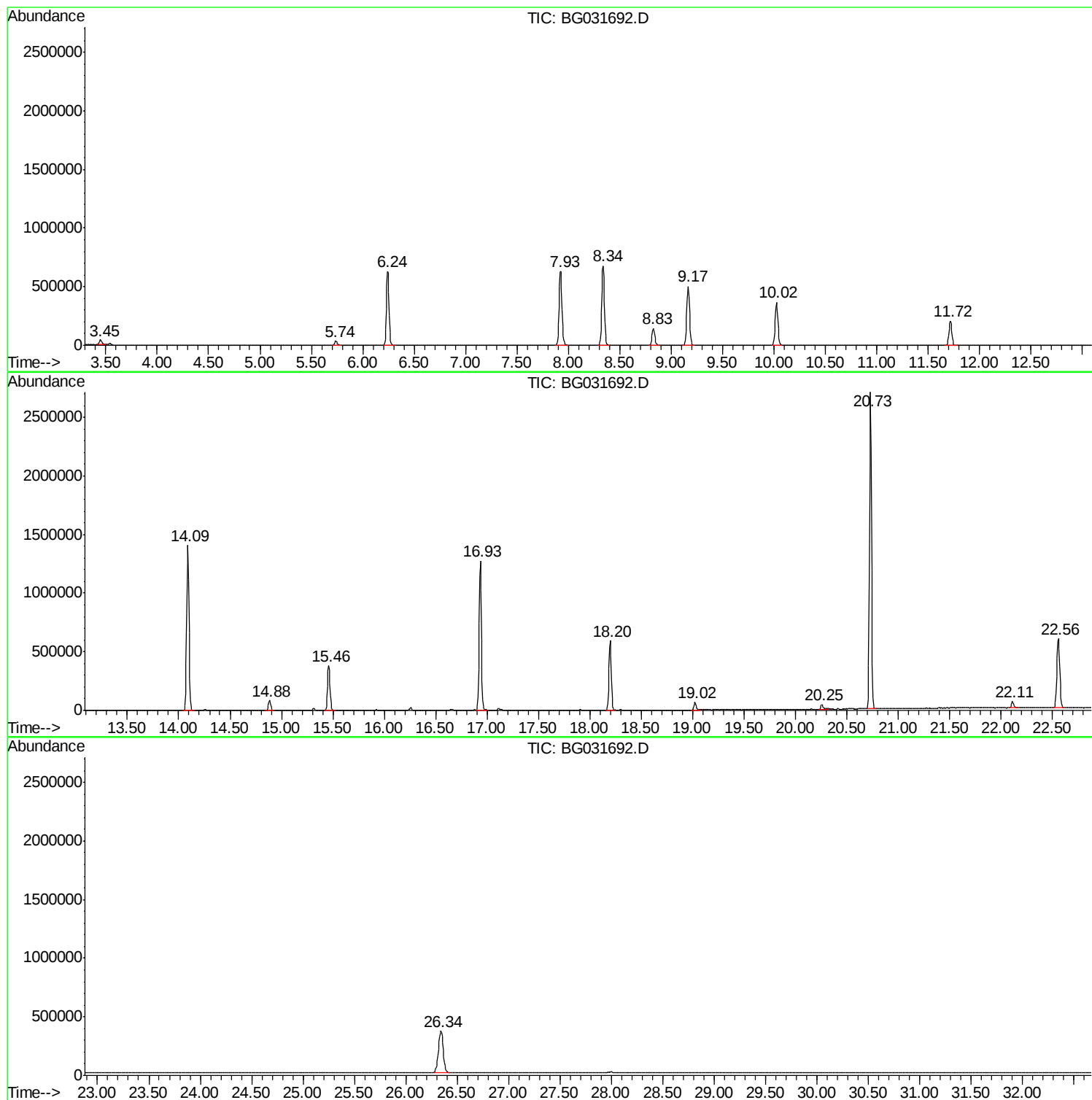
Sum of corrected areas: 18060160

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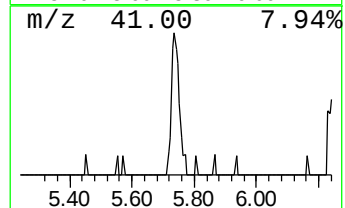
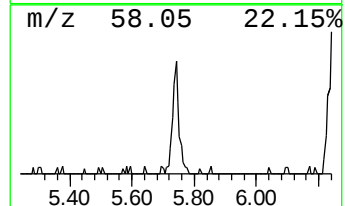
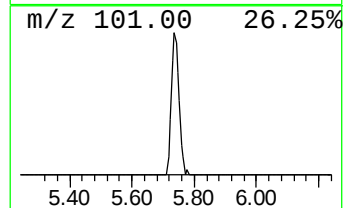
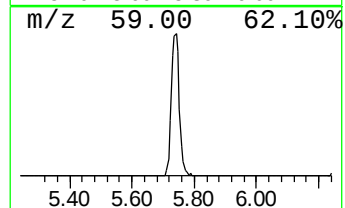
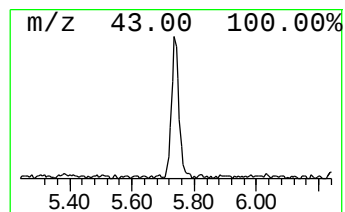
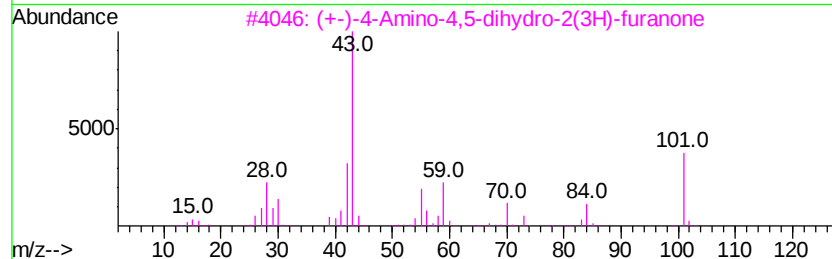
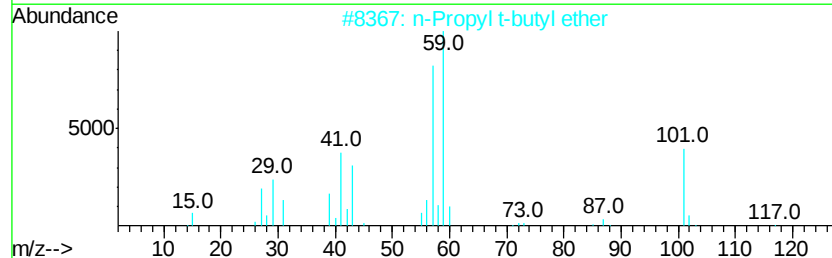
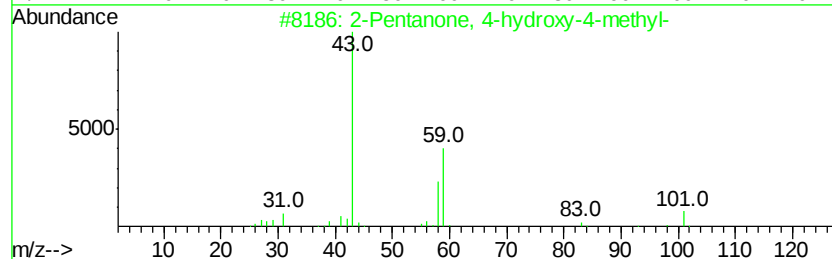
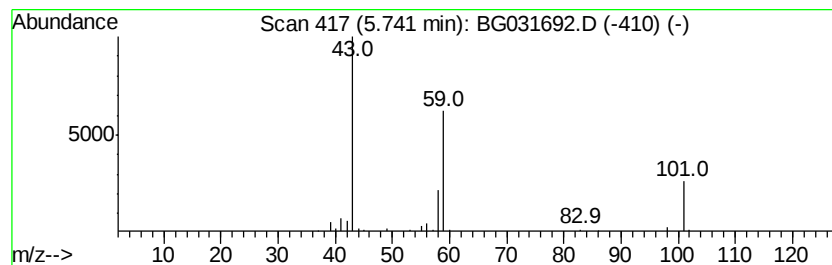
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	4.67 ng	62084	1,4-Dichlorobenzene-d4	8.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	28
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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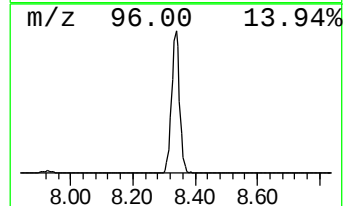
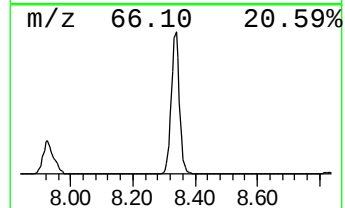
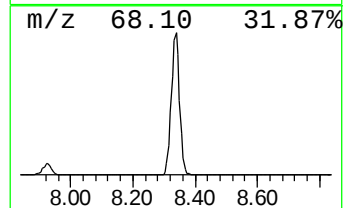
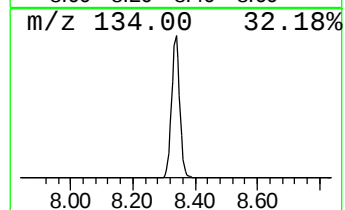
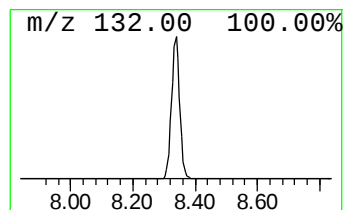
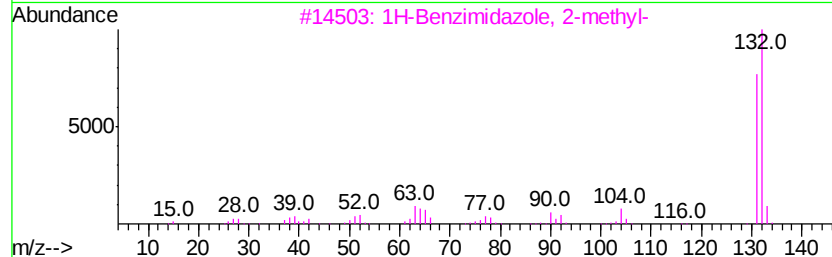
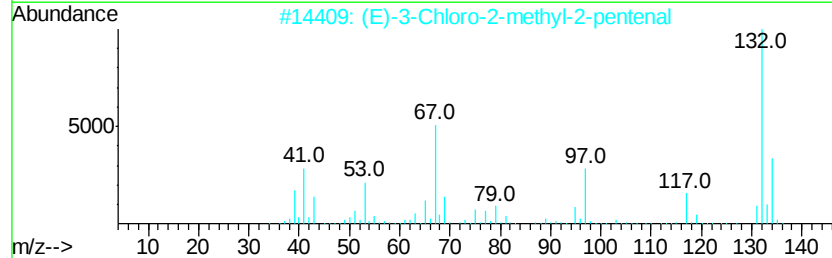
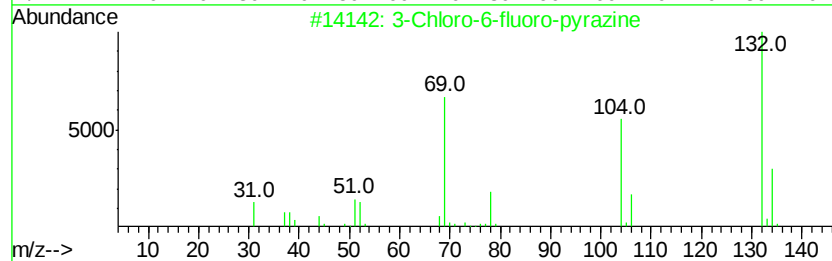
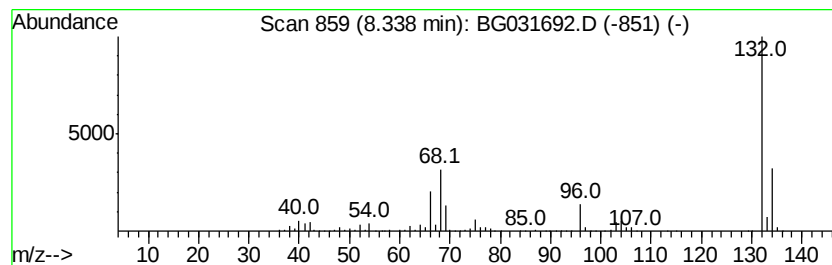
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Peak Number 3 unknown8.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	93.96 ng	1250090	1,4-Dichlorobenzene-d4	8.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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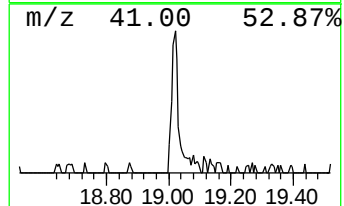
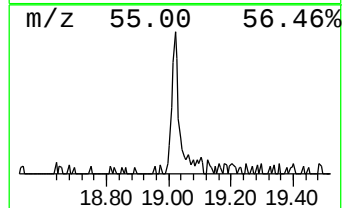
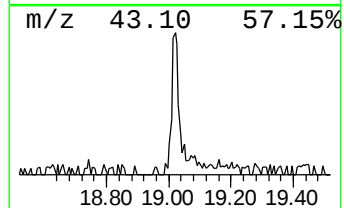
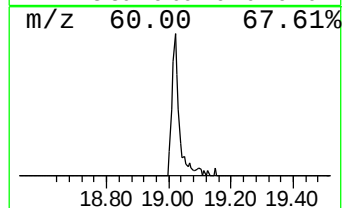
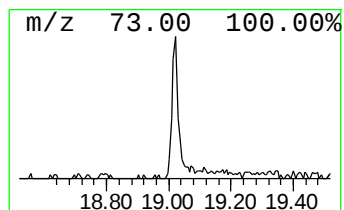
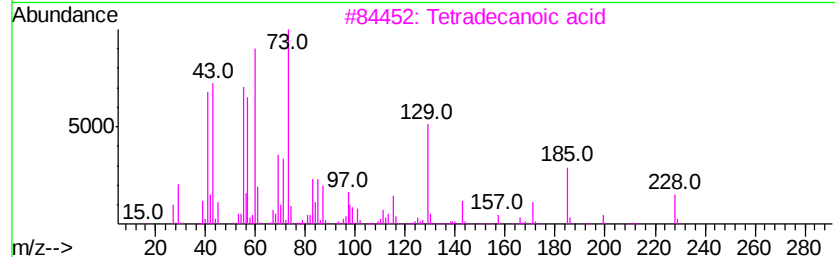
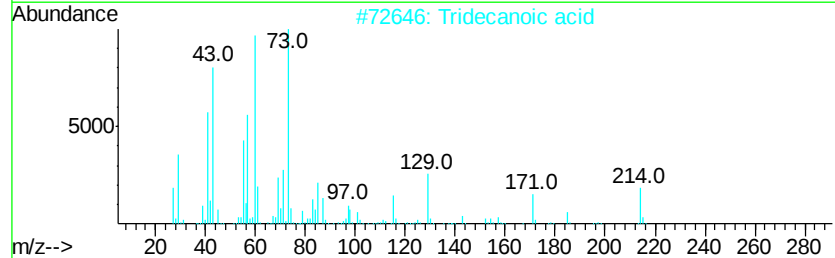
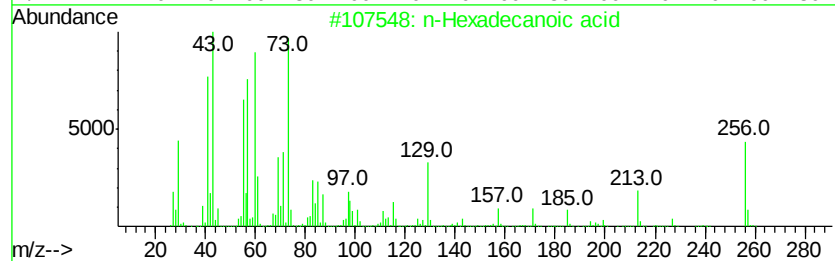
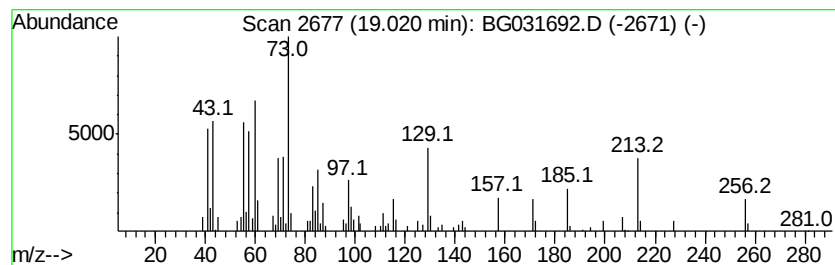
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	2.25 ng	102564	Phenanthrene-d10	18.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	55
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4		n-Decanoic acid	172	C10H20O2	000334-48-5	46
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.74	4.7	ng	62084	1	8.83	266099	20.0
unknown8.34	8.34	94.0	ng	1250090	1	8.83	266099	20.0
n-Hexadecanoic acid	19.02	2.3	ng	102564	4	18.20	912238	20.0