LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
Data File : BG029351.D
Acq On : 19 Oct 2017 3:48
Operator : SJ/JU
Sample : I5901-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-3-20170690

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-BG101617.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	5.241	326	332	339	rBV	174411	260043	6.25%	1.171%
2	5.717	404	413	421	rBV	967024	1511889	36.35%	6.811%
3	7.321	678	686	701	rVB	948304	1714718	41.23%	7.725%
4	7.697	741	750	757	rBV	947476	1604508	38.58%	7.228%
5	8.167	822	830	838	rBV	201725	339175	8.16%	1.528%
6	8.491	877	885	893	rBV	629415	1111382	26.72%	5.007%
7	9.331	1020	1028	1039	rBV	544967	963718	23.17%	4.341%
8	10.982	1302	1309	1316	rBV	281976	509998	12.26%	2.298%
9	13.408	1715	1722	1729	rBV	1437028	2227387	53.56%	10.034%
10	14.225	1855	1861	1867	rBV	40924	56858	1.37%	0.256%
11	14.783	1949	1956	1964	rVB2	478152	781505	18.79%	3.521%
12	16.264	2200	2208	2220	rBV	1508007	2259457	54.33%	10.179%
13	17.521	2415	2422	2429	rBV2	710984	1085135	26.09%	4.888%
14	18.391	2563	2570	2580	rBV2	172557	266115	6.40%	1.199%
15	19.648	2780	2784	2793	rBV2	52552	89265	2.15%	0.402%
16	20.112	2857	2863	2869	rBV	3220604	4158769	100.00%	18.735%
17	21.411	3079	3084	3099	rBV	227057	379391	9.12%	1.709%
18	21.793	3142	3149	3159	rVB2	822319	1398952	33.64%	6.302%
19	22.627	3284	3291	3301	rVB2	22014	65451	1.57%	0.295%
20	23.673	3464	3469	3477	rVB2	17916	41687	1.00%	0.188%
21	25.095	3701	3711	3723	rVB3	466623	1372494	33.00%	6.183%

Sum of corrected areas: 22197897

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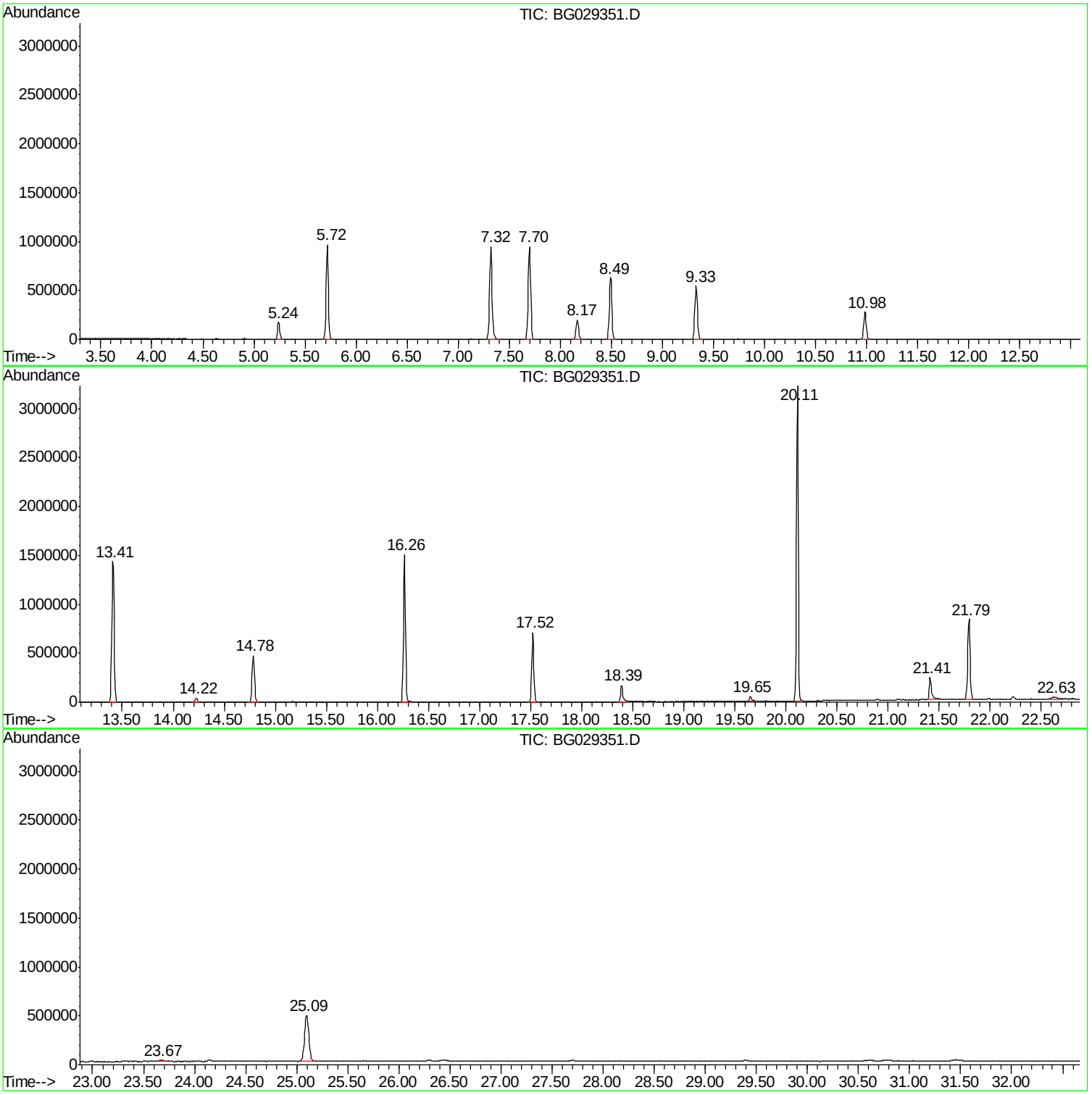
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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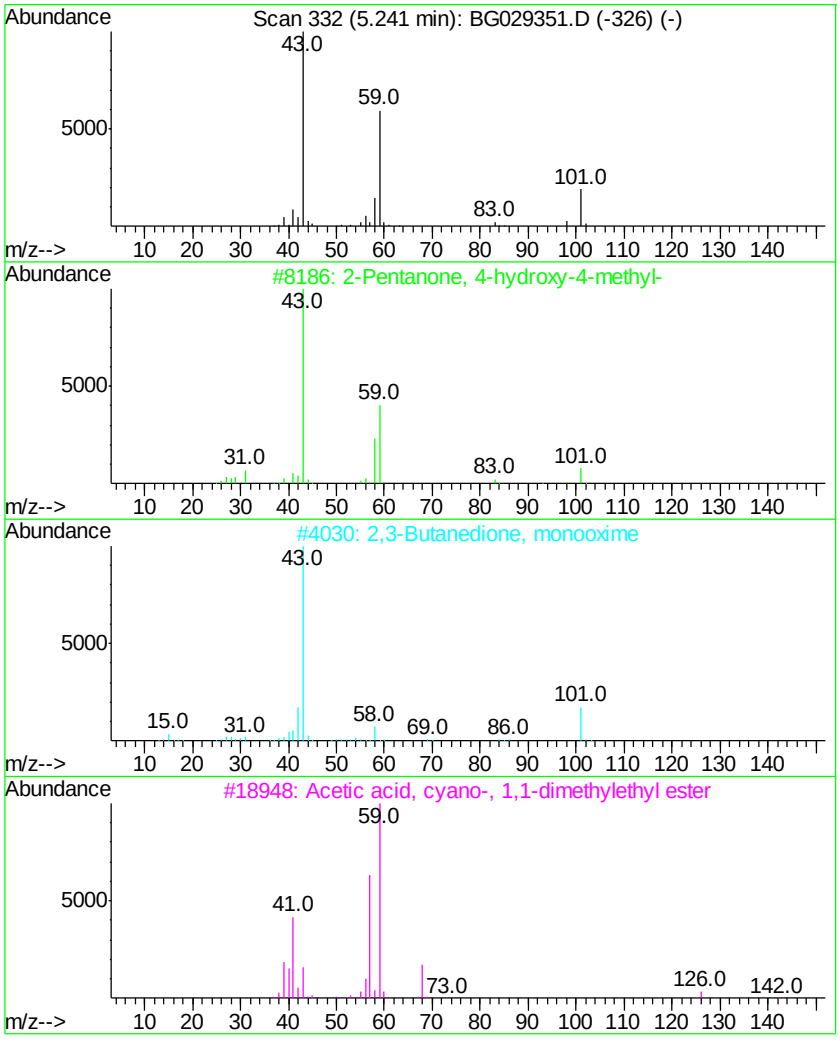
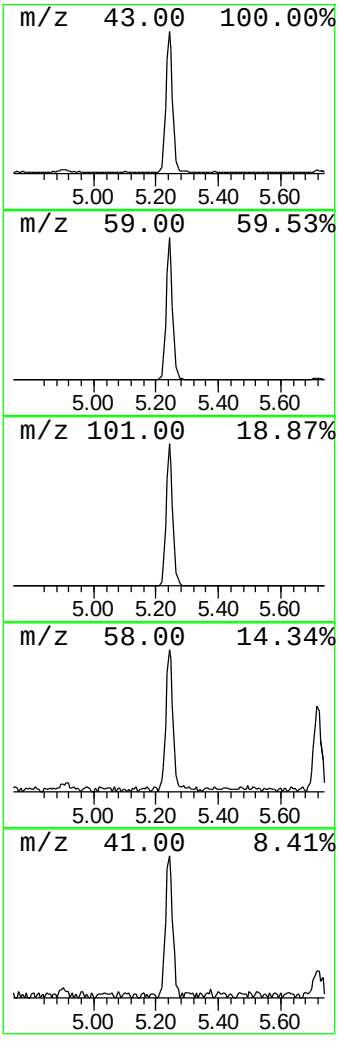
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	15.33 ng	260043	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Library Search Compound Report

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ClientSampleId : S-3-20170690

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
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TIC Library : C:\Database\NIST11.L
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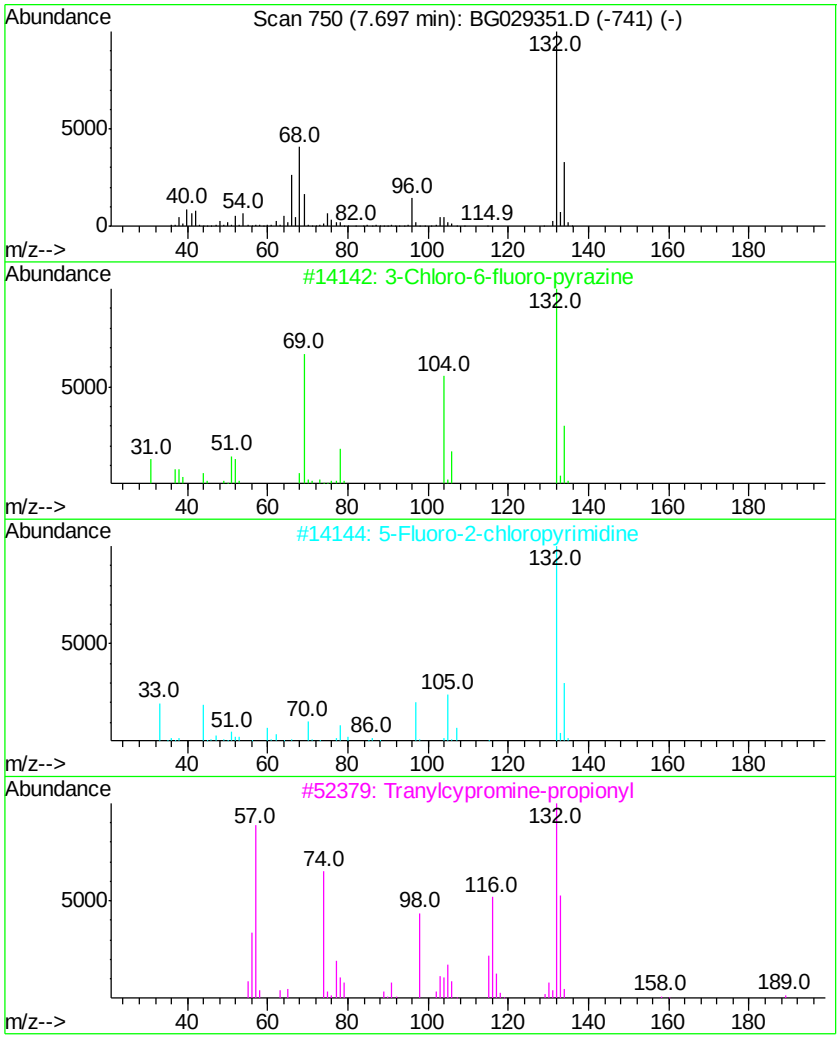
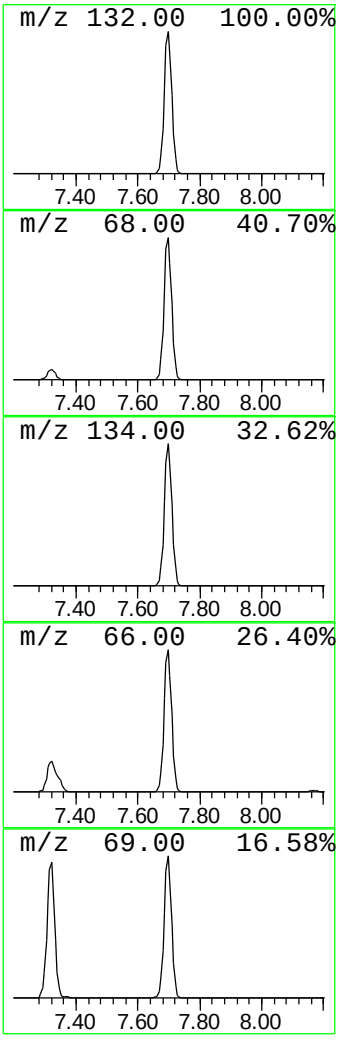
Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	94.61 ng	1604510	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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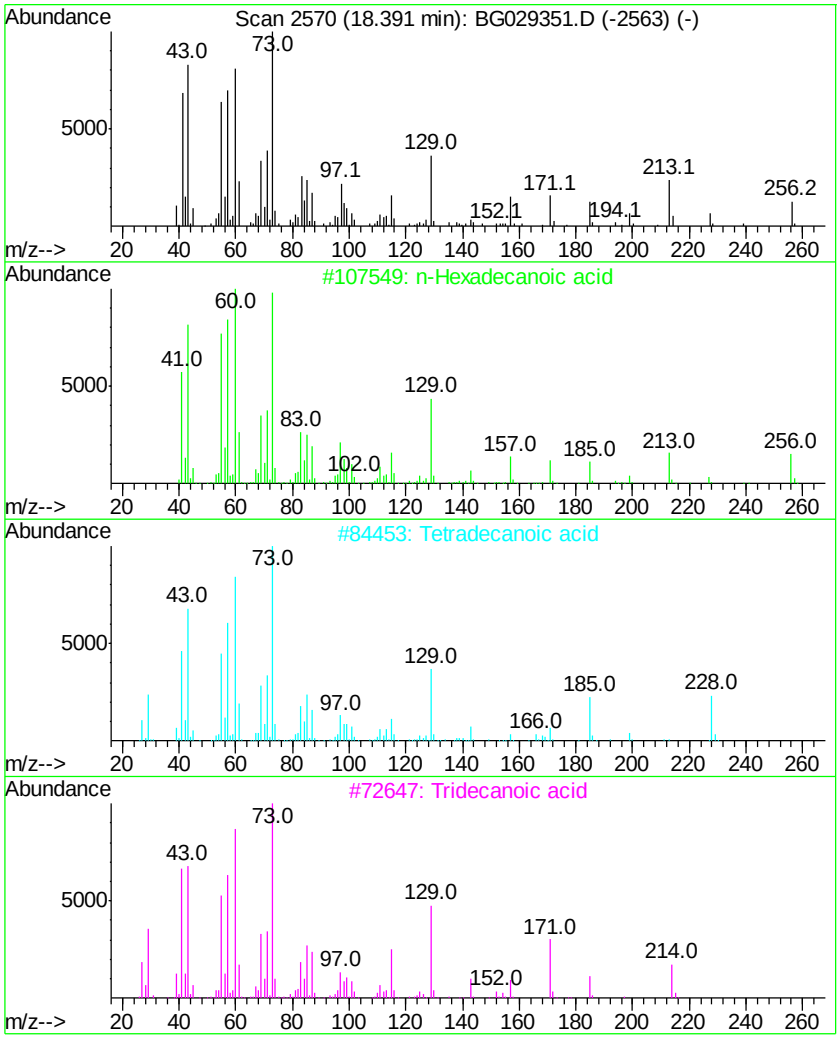
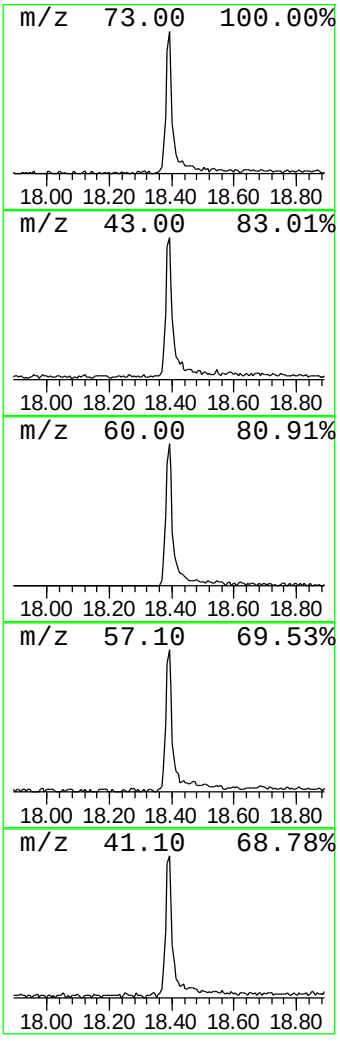
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	4.90 ng	266115	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





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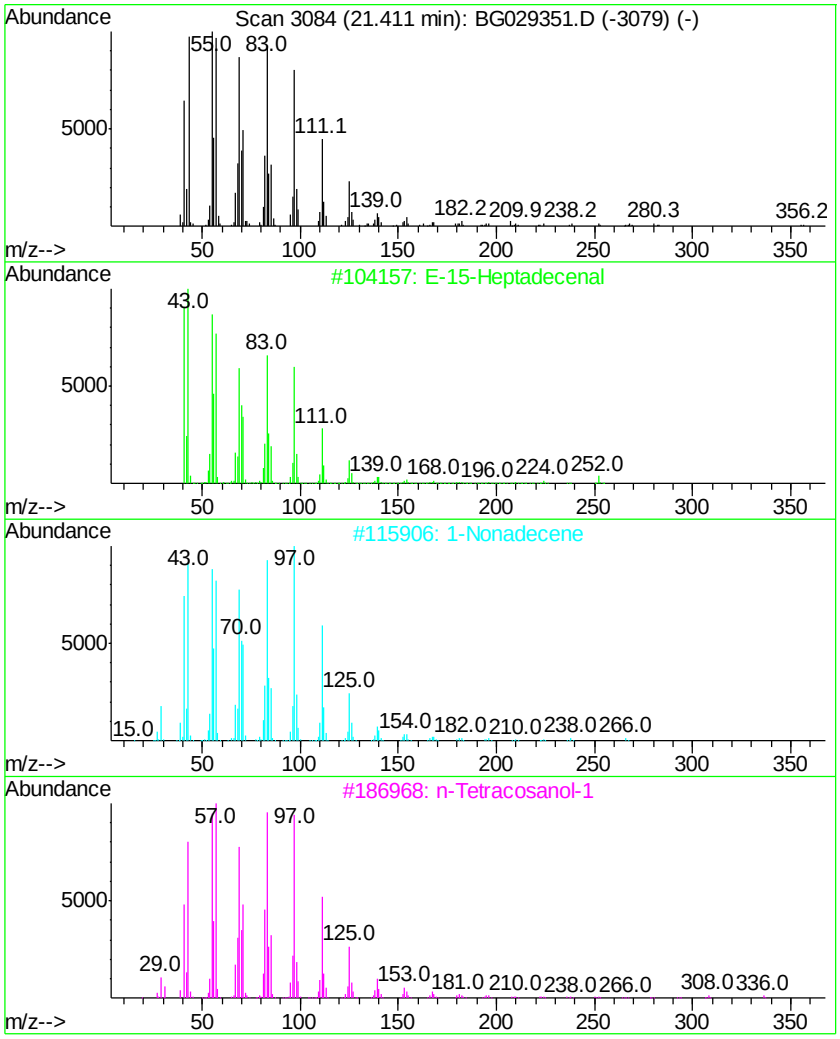
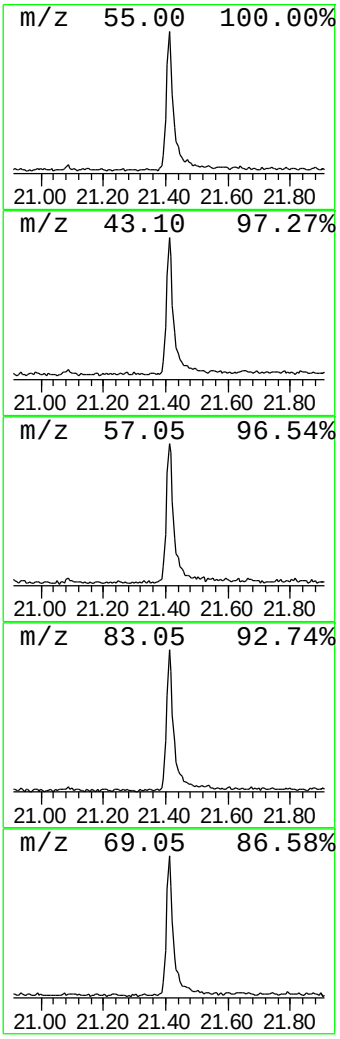
Peak Number 5 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	5.42 ng	379391	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	99
2	1-Nonadecene	266	C19H38	018435-45-5	98
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Cycloeicosane	280	C20H40	000296-56-0	93





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	15.3	ng	260043	1	8.17	339175	20.0
unknown7.70	7.70	94.6	ng	1604510	1	8.17	339175	20.0
n-Hexadecanoic acid	18.39	4.9	ng	266115	4	17.52	1085140	20.0
E-15-Heptadecenal	21.41	5.4	ng	379391	5	21.79	1398950	20.0