

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
 Data File : BM016586.D
 Acq On : 24 Aug 2018 13:51
 Operator : SJ/JU
 Sample : J4523-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-1

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_M\METHODS\8270-BM082118.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	5.551	380	385	395	rBV	531245	971190	8.53%	1.893%
2	7.187	658	663	681	rBV2	320718	679452	5.97%	1.325%
3	7.534	716	722	740	rBV	1538521	2676983	23.51%	5.218%
4	8.010	796	803	812	rBV	430033	763566	6.71%	1.488%
5	8.281	840	849	851	rBV3	67345	143135	1.26%	0.279%
6	8.322	851	856	873	rVB	1753461	3035632	26.66%	5.918%
7	9.192	997	1004	1022	rBV	1116548	2041681	17.93%	3.980%
8	10.816	1274	1280	1294	rVB2	520573	942843	8.28%	1.838%
9	13.263	1688	1696	1708	rBV	5290933	7169509	62.97%	13.976%
10	14.110	1835	1840	1848	rBV	449701	649893	5.71%	1.267%
11	14.651	1924	1932	1942	rVB2	920411	1487727	13.07%	2.900%
12	16.145	2177	2186	2202	rBV	6103679	8812187	77.40%	17.178%
13	17.392	2392	2398	2407	rBV	1667944	2506800	22.02%	4.887%
14	18.245	2540	2543	2553	rVB3	255520	380552	3.34%	0.742%
15	19.509	2755	2758	2764	rBV5	114236	163708	1.44%	0.319%
16	19.980	2832	2838	2845	rBV	9943387	11385666	100.00%	22.195%
17	21.533	3098	3102	3112	rBV	2891491	3796320	33.34%	7.400%
18	23.815	3484	3490	3500	rBV	1868746	3691791	32.42%	7.197%

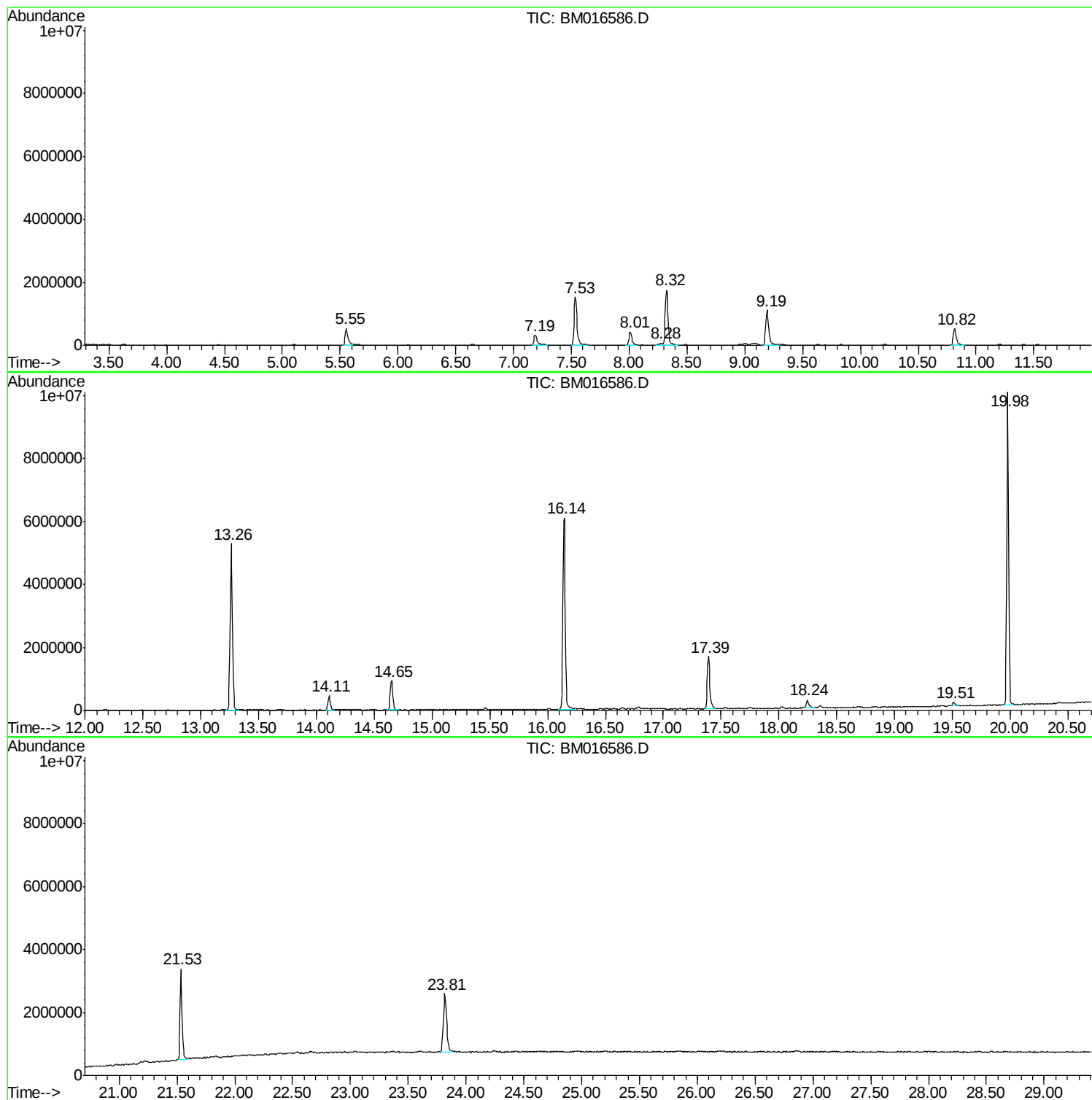
Sum of corrected areas: 51298635

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.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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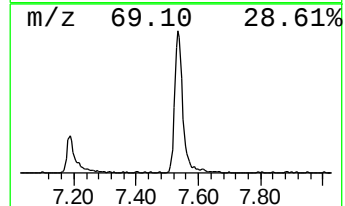
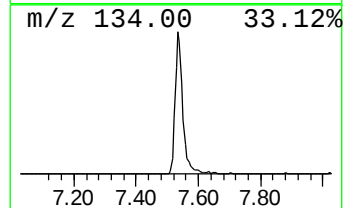
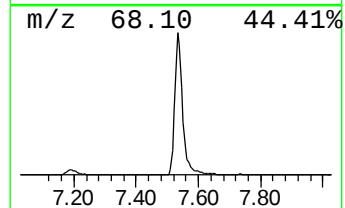
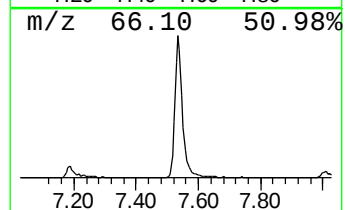
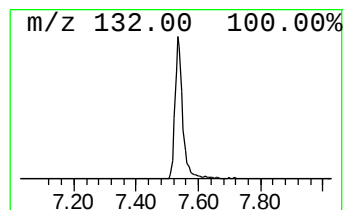
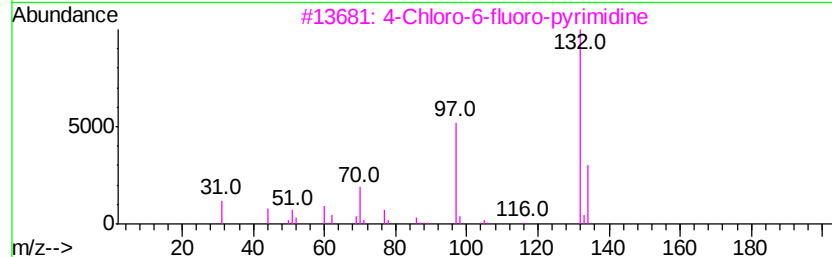
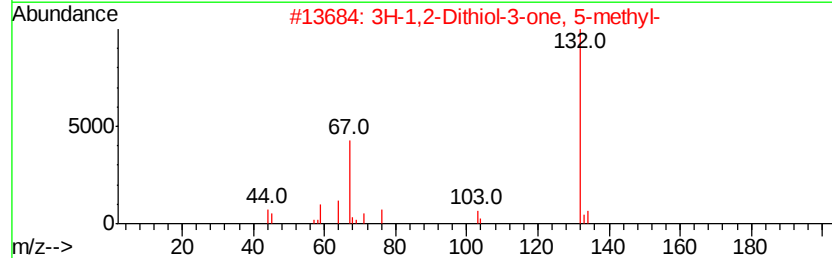
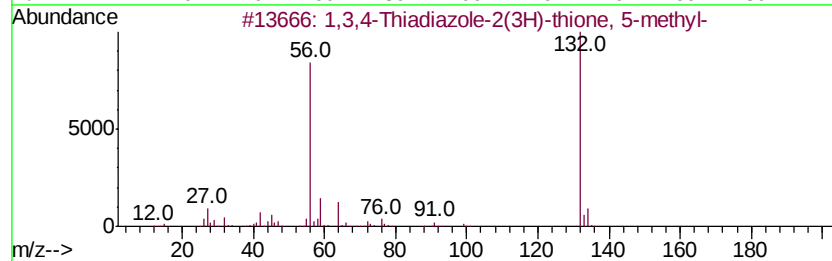
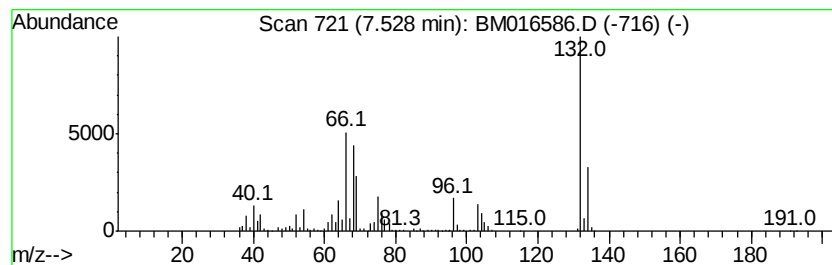
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	70.12 ng	2676980	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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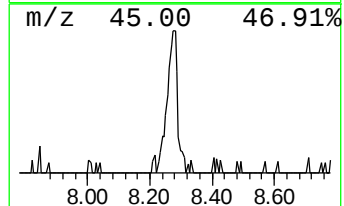
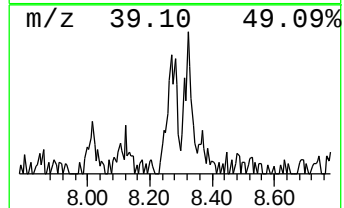
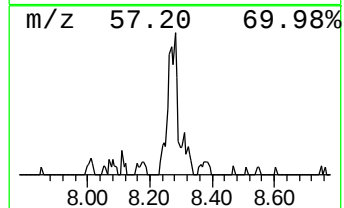
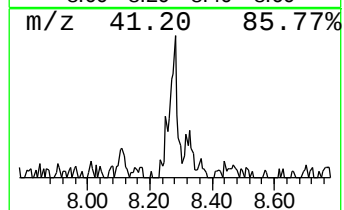
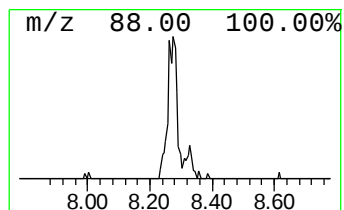
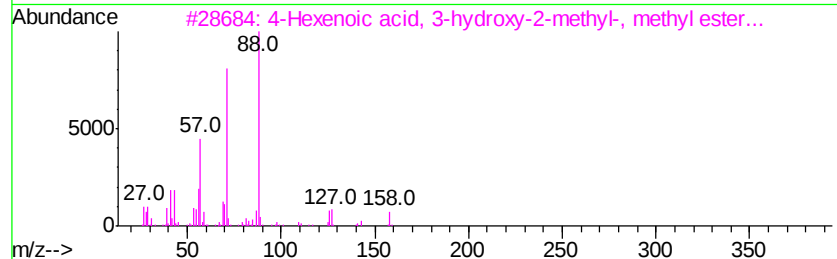
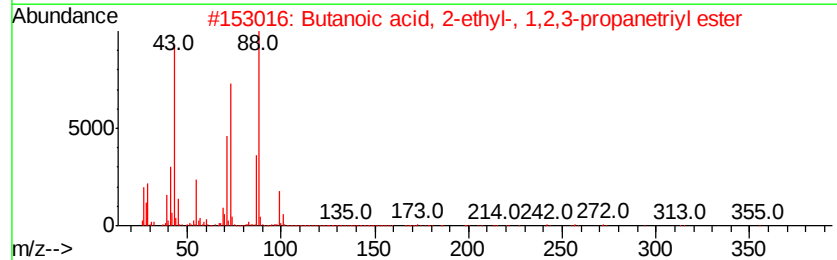
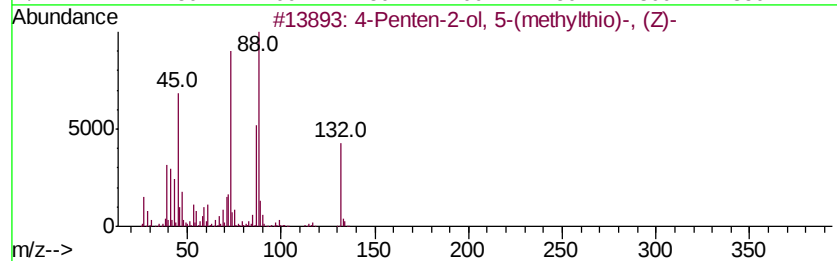
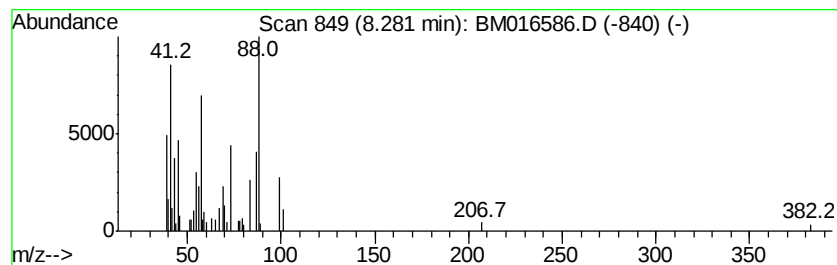
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Peak Number 2 unknown8.28 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	3.75 ng	143135	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-ol, 5-(methylthio)-, ...	132	C6H12OS	097369-79-4	40
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
3		4-Hexenoic acid, 3-hydroxy-2-met...	158	C8H14O3	067498-09-3	25
4		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	22
5		Urea, N,N'-dimethyl-	88	C3H8N2O	000096-31-1	16



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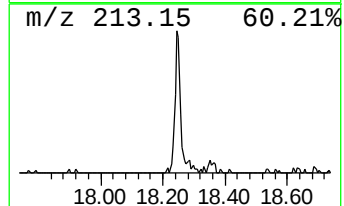
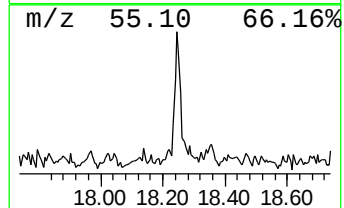
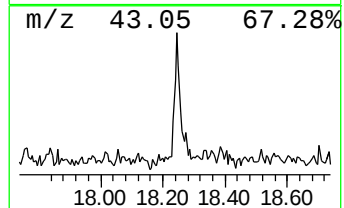
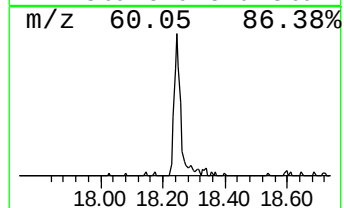
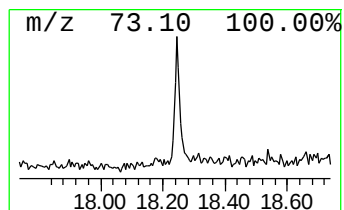
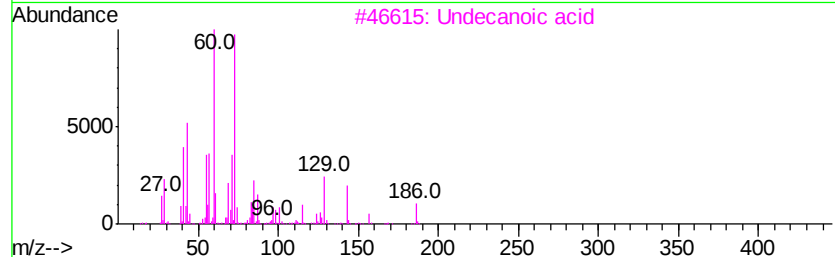
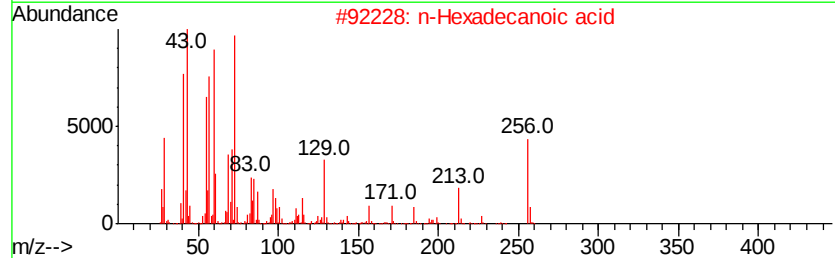
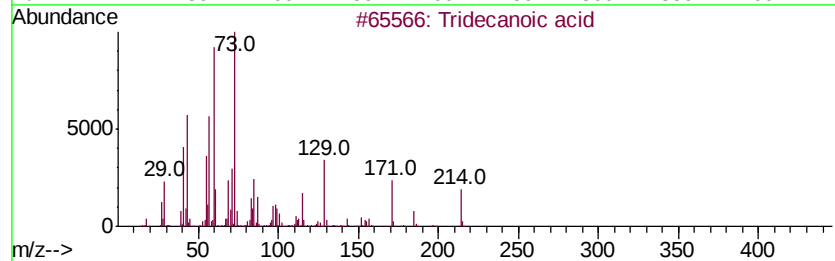
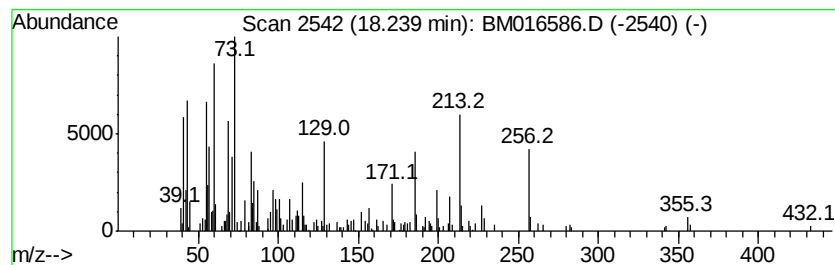
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Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	3.04 ng	380552	Phenanthrene-d10	17.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
3		Undecanoic acid	186	C11H22O2	000112-37-8	42
4		.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	27
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.53	7.53	70.1	ng	2676980	1	8.01	763566	20.0
unknown8.28	8.28	3.8	ng	143135	1	8.01	763566	20.0
Tridecanoic acid	18.24	3.0	ng	380552	4	17.39	2506800	20.0