

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061518\
 Data File : BG035188.D
 Acq On : 16 Jun 2018 1:32
 Operator : SJ/JU
 Sample : J3518-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-106-7(60-62)

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-BG060718.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	5.170	315	320	328	rBV	63573	103576	2.41%	0.472%
2	5.634	392	399	414	rVB	956023	1542757	35.96%	7.026%
3	7.220	660	669	682	rBV	1045533	1817993	42.37%	8.279%
4	7.596	724	733	745	rBV	954919	1654904	38.57%	7.537%
5	8.060	805	812	819	rBV	162262	284986	6.64%	1.298%
6	8.383	859	867	876	rBV	656761	1159905	27.04%	5.282%
7	9.223	1003	1010	1022	rBV	618740	1090201	25.41%	4.965%
8	10.868	1282	1290	1297	rBV	220550	399604	9.31%	1.820%
9	13.312	1698	1706	1716	rBV	1643098	2590795	60.39%	11.799%
10	14.128	1839	1845	1854	rBV	179412	271720	6.33%	1.237%
11	14.680	1929	1939	1949	rBV2	408528	674075	15.71%	3.070%
12	16.167	2184	2192	2203	rBV	1671308	2600564	60.61%	11.843%
13	17.424	2399	2406	2414	rBV2	608533	931399	21.71%	4.242%
14	18.305	2551	2556	2563	rBV2	100770	149639	3.49%	0.681%
15	19.574	2768	2772	2782	rBV4	28417	45975	1.07%	0.209%
16	20.032	2844	2850	2860	rBV	3193384	4290346	100.00%	19.539%
17	21.342	3068	3073	3084	rBV6	38300	101349	2.36%	0.462%
18	21.694	3126	3133	3142	rBV	656803	1107119	25.80%	5.042%
19	23.386	3415	3421	3429	rVB2	68648	136357	3.18%	0.621%
20	24.919	3670	3682	3698	rBV	330594	1004947	23.42%	4.577%

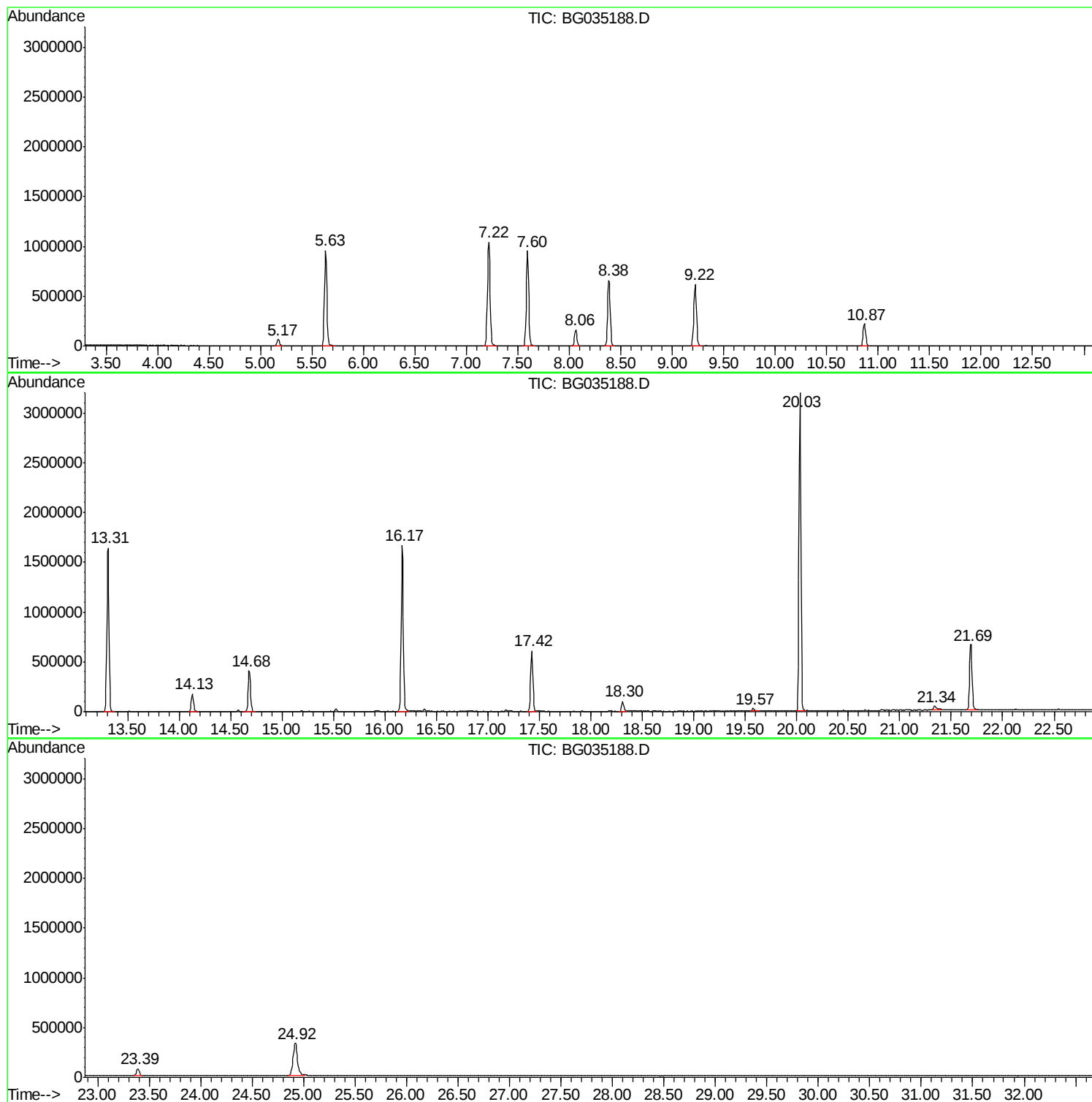
Sum of corrected areas: 21958211

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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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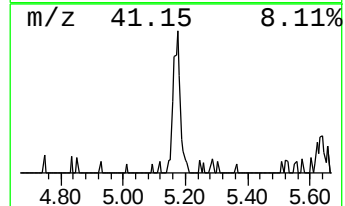
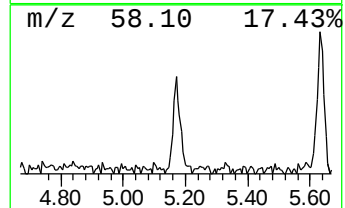
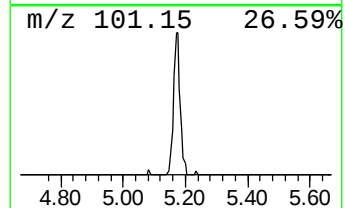
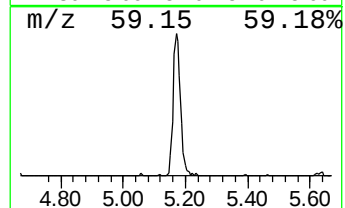
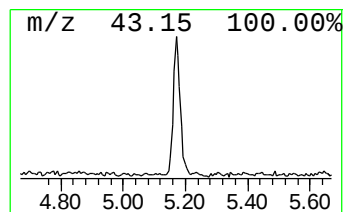
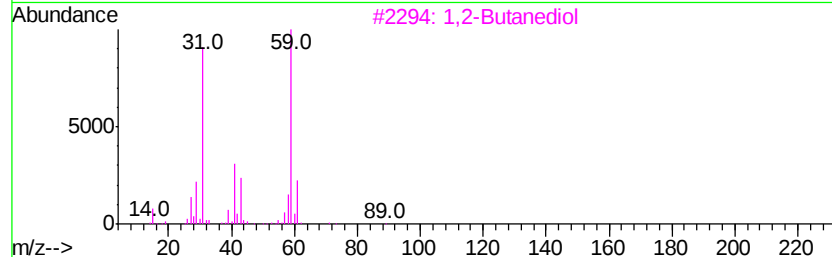
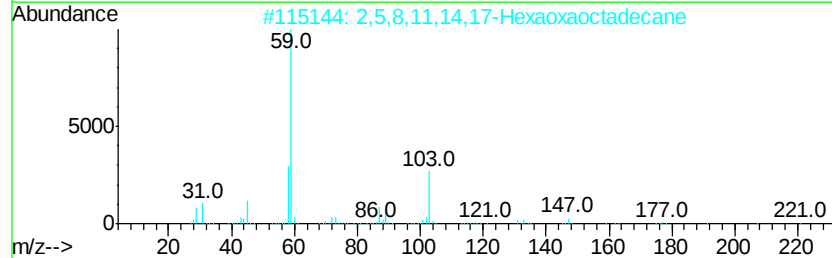
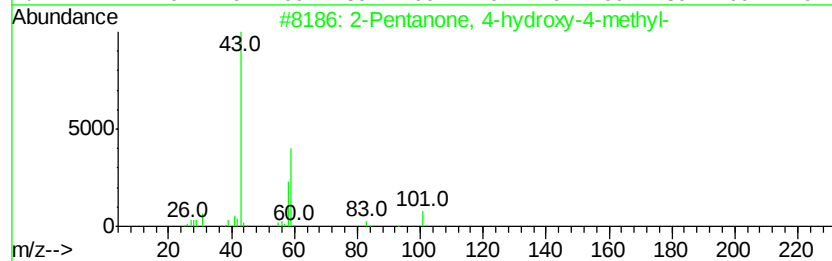
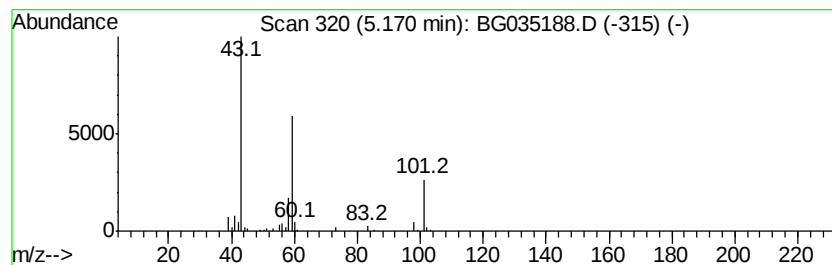
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	7.27 ng	103576	1,4-Dichlorobenzene-d4	8.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	25
3			1,2-Butanediol	90	C4H10O2	000584-03-2	23
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17



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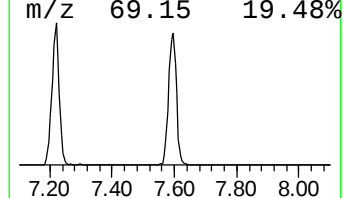
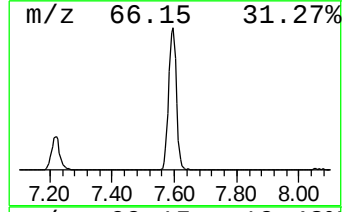
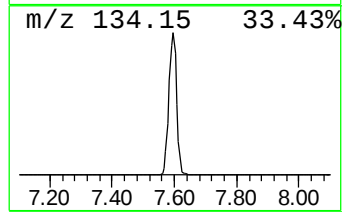
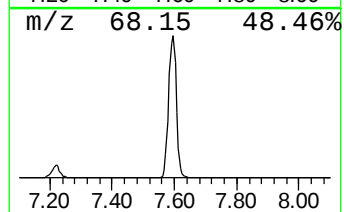
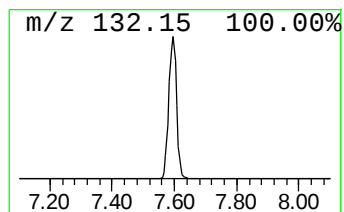
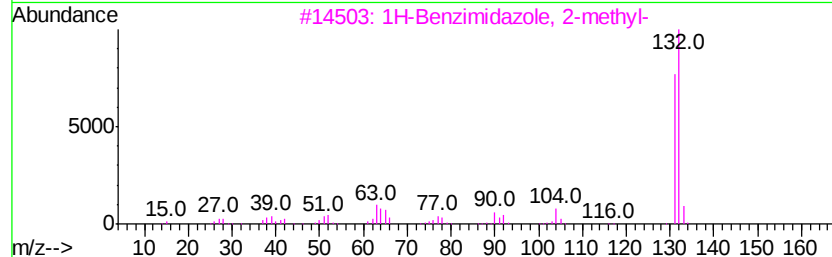
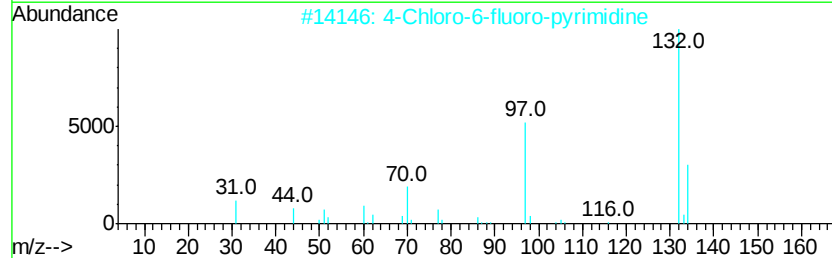
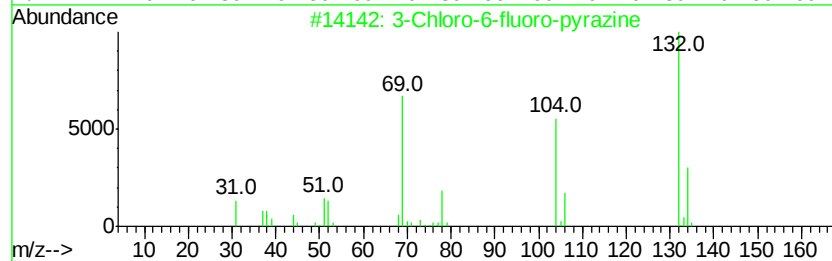
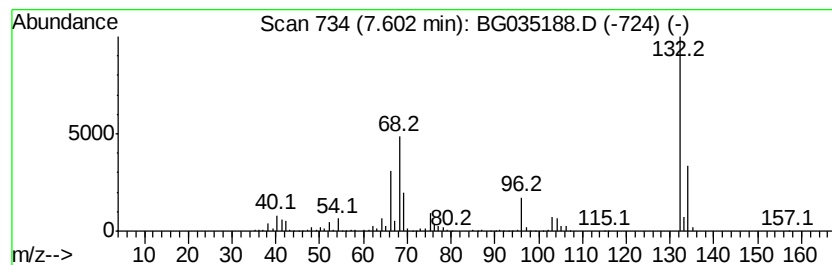
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Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	116.14 ng	1654900	1,4-Dichlorobenzene-d4	8.07

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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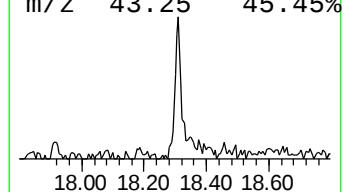
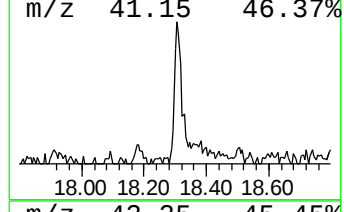
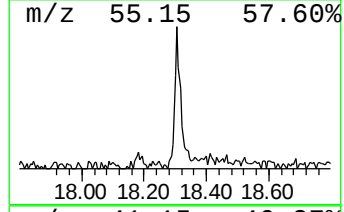
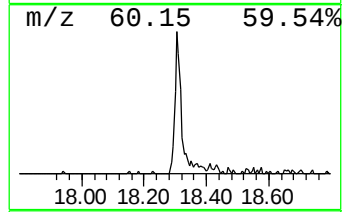
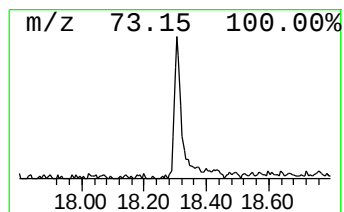
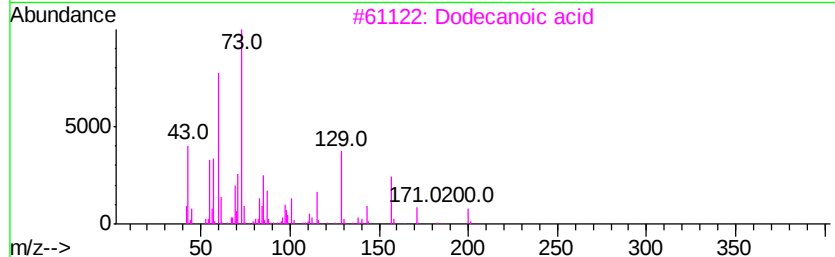
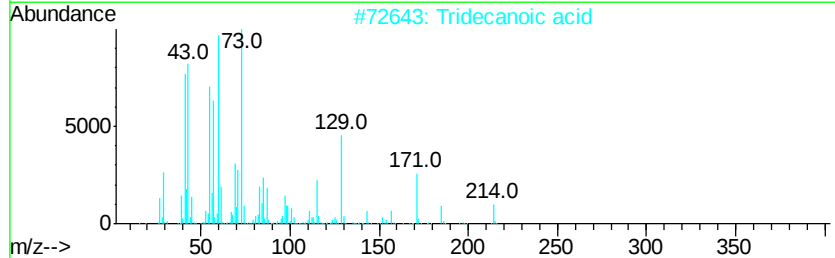
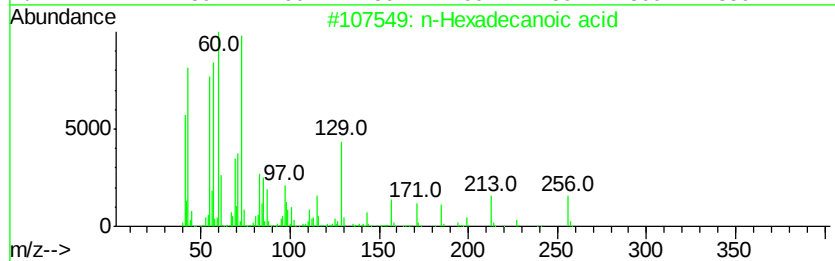
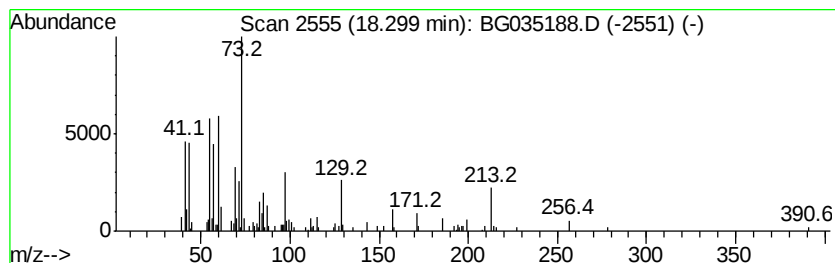
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.30	3.21 ng	149639	Phenanthrene-d10	17.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Dodecanoic acid	200	C12H24O2	000143-07-7	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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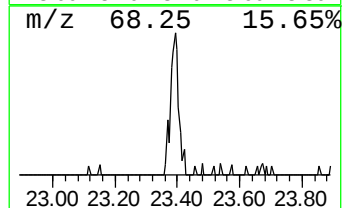
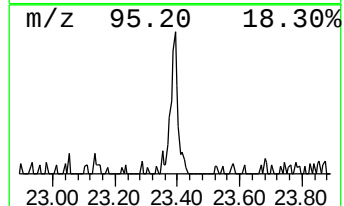
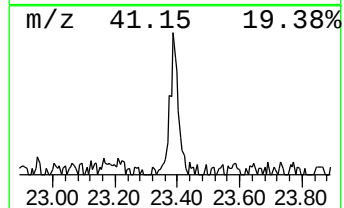
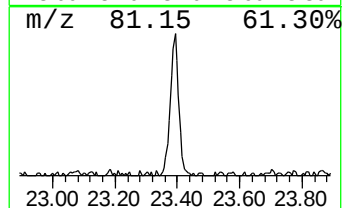
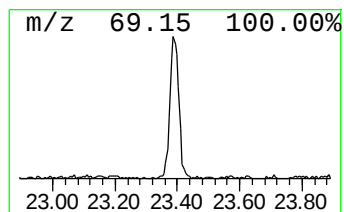
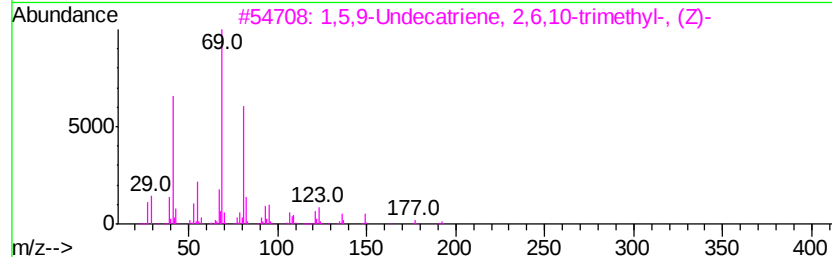
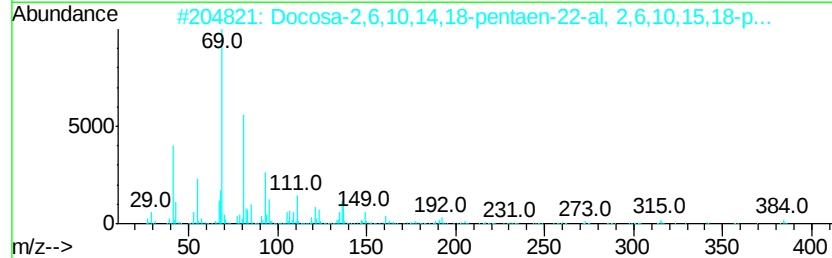
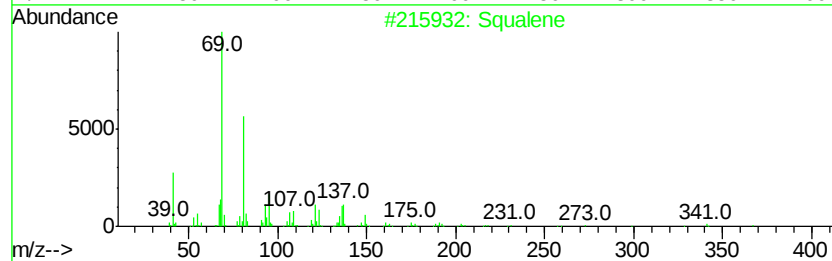
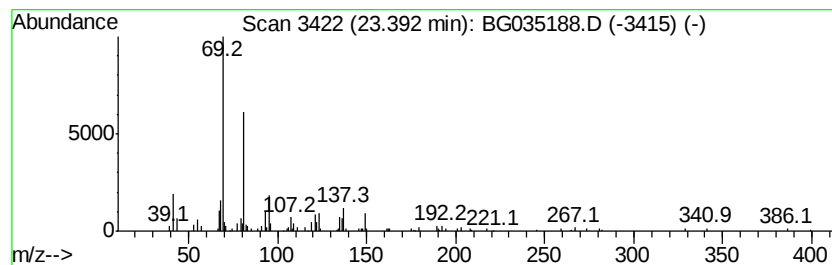
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
23.39	2.71 ng	136357	Perylene-d12		24.92		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	83
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	72
5			Oxirane, 2,2-dimethyl-3-(3,7,12,...	426	C30H50O	007200-26-2	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	7.3	ng	103576	1	8.07	284986	20.0
unknown7.60	7.60	116.1	ng	1654900	1	8.07	284986	20.0
n-Hexadecanoic acid	18.30	3.2	ng	149639	4	17.42	931399	20.0
Squalene	23.39	2.7	ng	136357	6	24.92	1004950	20.0