

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050617\
 Data File : BM009965.D
 Acq On : 07 May 2017 05:51
 Operator : SJ/MA
 Sample : I2997-06
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OWL-C8-GW

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_M\METHODS\8270-BM050517.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	4.905	304	309	319	rVB	121454	181549	2.33%	0.497%
2	5.358	379	386	397	rBV	1162337	1729572	22.21%	4.730%
3	6.952	650	657	669	rBV	767516	1277780	16.41%	3.495%
4	7.305	709	717	729	rBV	1932554	3042919	39.07%	8.323%
5	7.769	788	796	803	rBV	389845	621719	7.98%	1.700%
6	8.087	843	850	859	rBV	1528264	2468693	31.70%	6.752%
7	8.940	988	995	1008	rBV	1506716	2553405	32.78%	6.984%
8	10.563	1264	1271	1283	rVB2	489432	846315	10.87%	2.315%
9	13.034	1684	1691	1701	rBV	3409942	4903547	62.96%	13.411%
10	14.422	1919	1927	1934	rBV2	729358	1159910	14.89%	3.172%
11	15.792	2155	2160	2170	rBV6	58137	133402	1.71%	0.365%
12	15.928	2176	2183	2194	rBV	3243275	4671944	59.98%	12.778%
13	17.180	2390	2396	2402	rBV	1055737	1504323	19.31%	4.114%
14	18.057	2541	2545	2552	rBV3	109333	169811	2.18%	0.464%
15	19.339	2759	2763	2767	rBV5	66364	83536	1.07%	0.228%
16	19.804	2836	2842	2847	rBV	6563609	7788577	100.00%	21.302%
17	21.051	3051	3054	3059	rVB4	146636	168369	2.16%	0.460%
18	21.368	3103	3108	3115	rBV	1513196	1860395	23.89%	5.088%
19	23.668	3493	3499	3506	rVB	704477	1396744	17.93%	3.820%

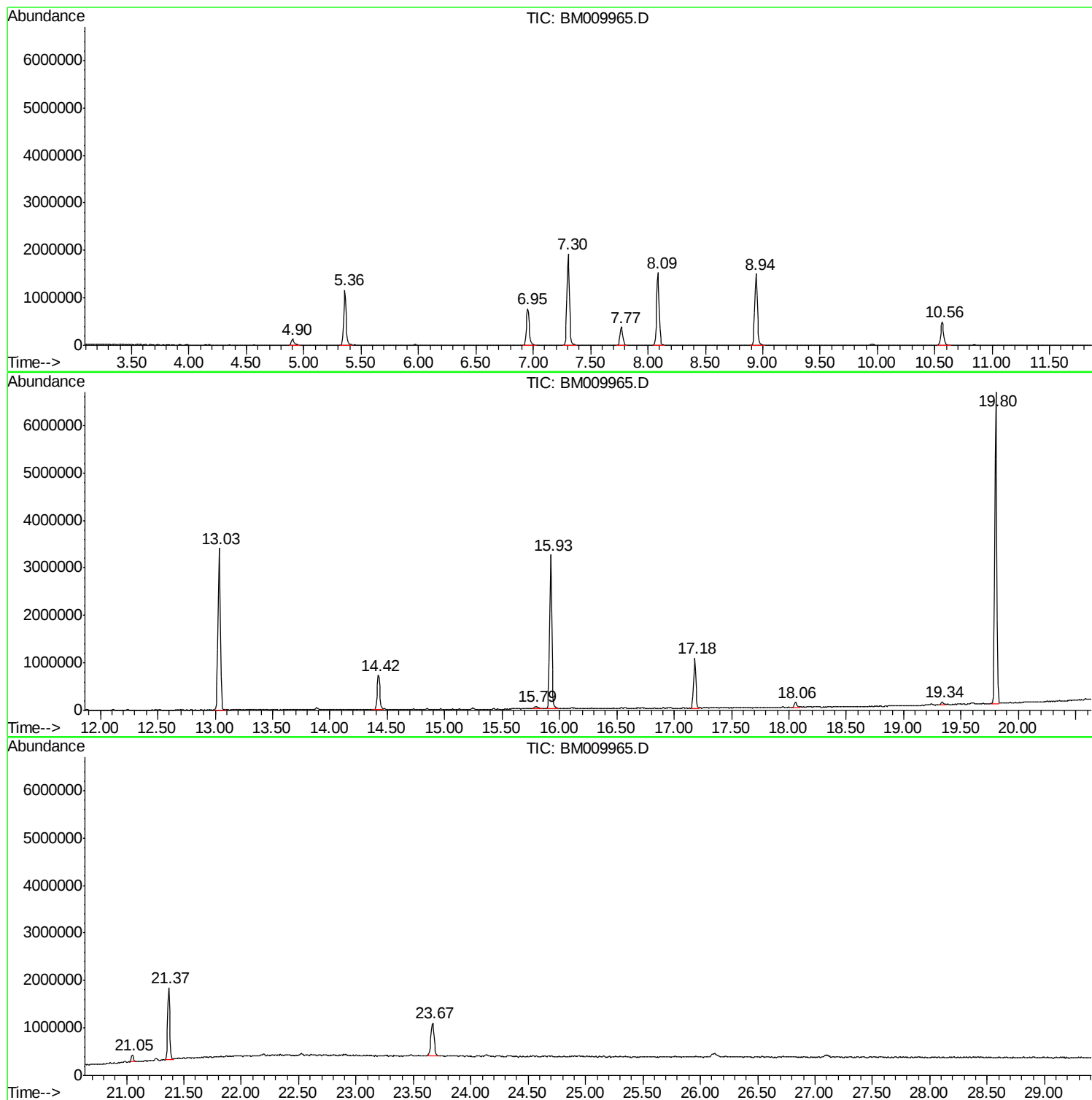
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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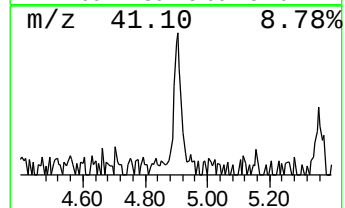
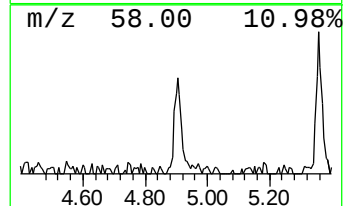
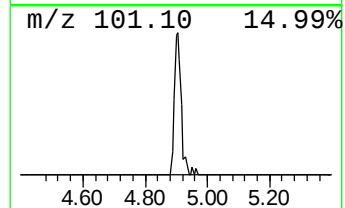
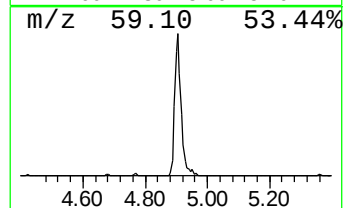
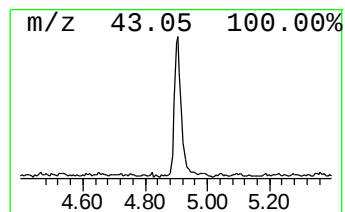
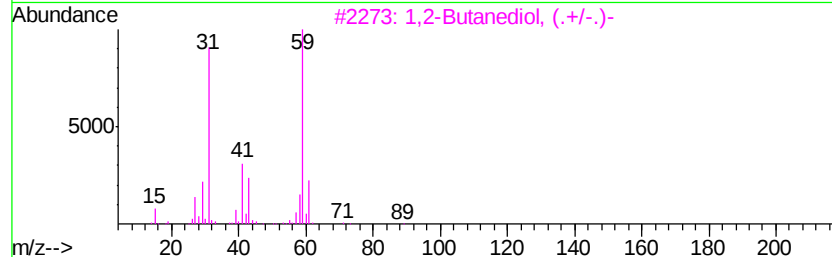
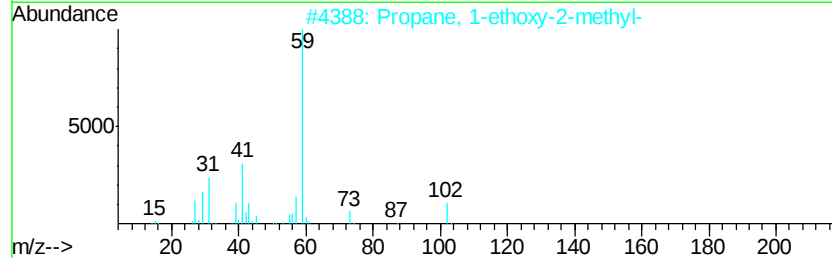
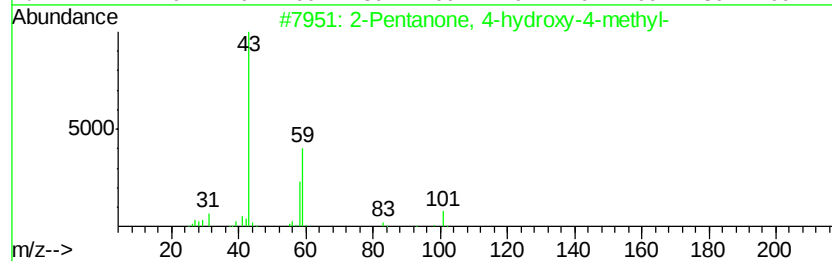
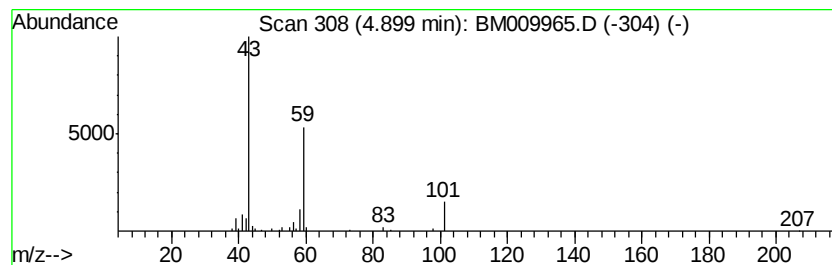
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	5.84 ng	181549	1,4-Dichlorobenzene-d4	7.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38	
3	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	38	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	3-Octanol	130	C8H18O	000589-98-0	33	



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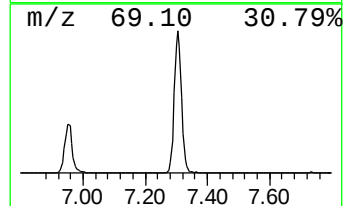
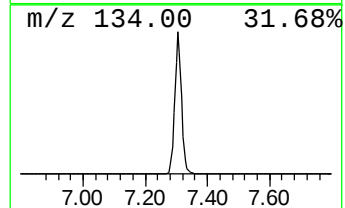
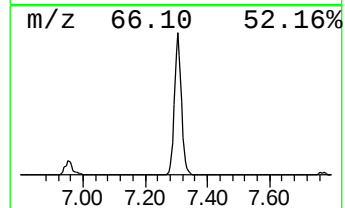
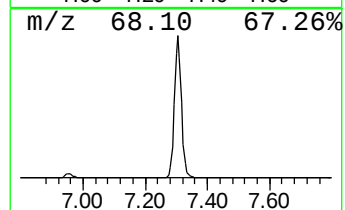
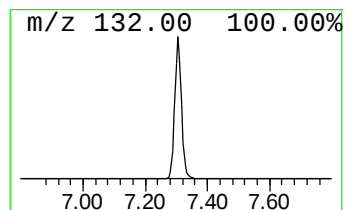
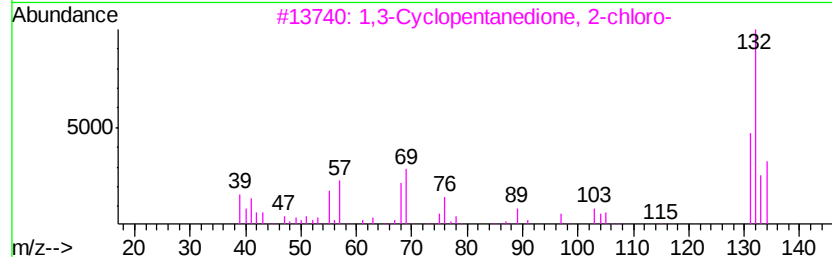
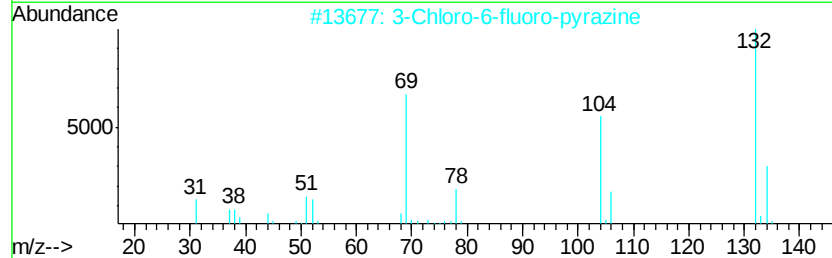
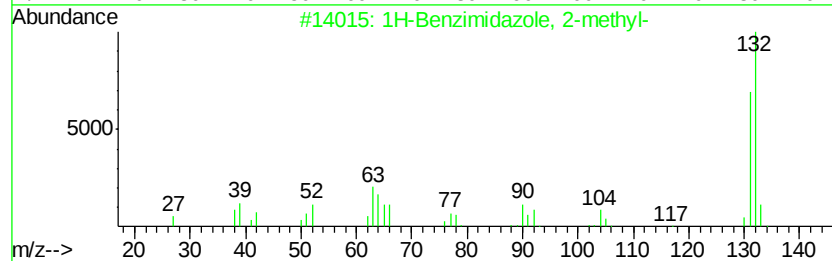
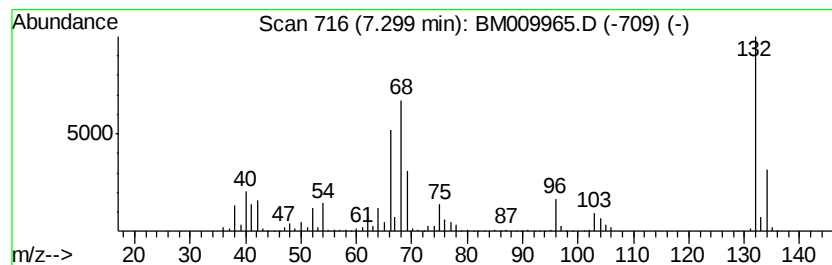
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Peak Number 2 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	97.89 ng	3042920	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10



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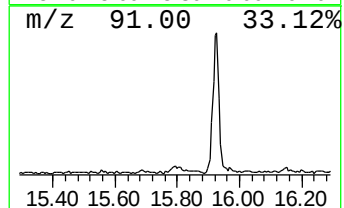
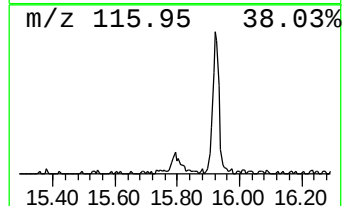
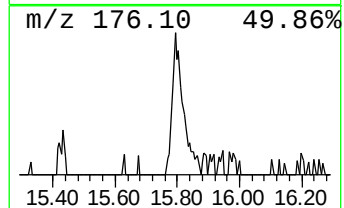
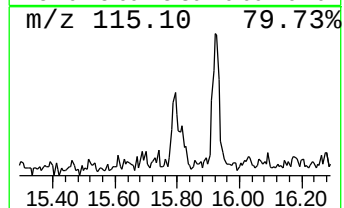
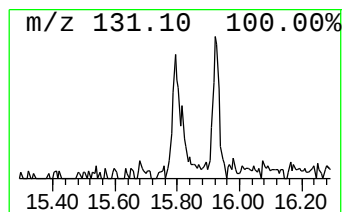
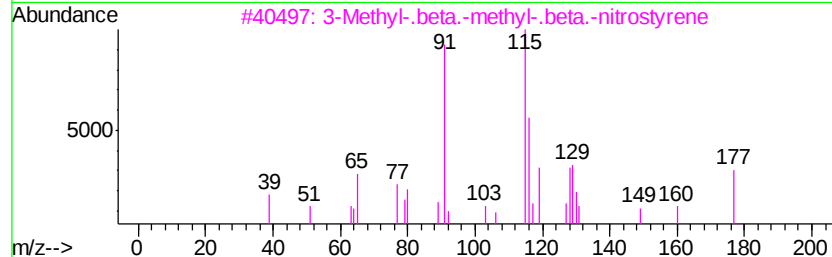
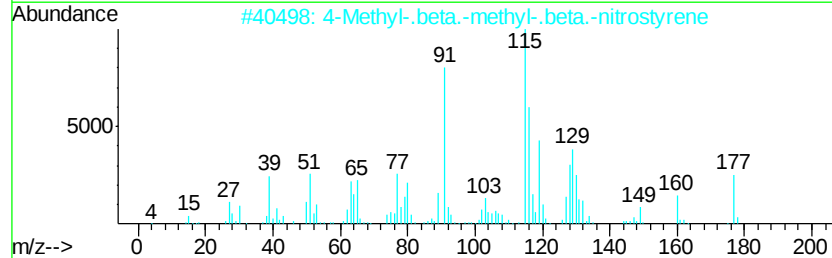
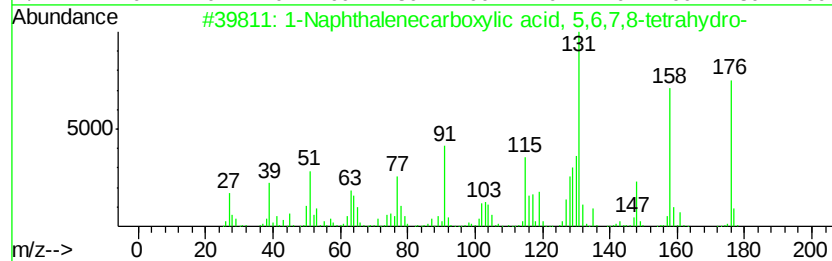
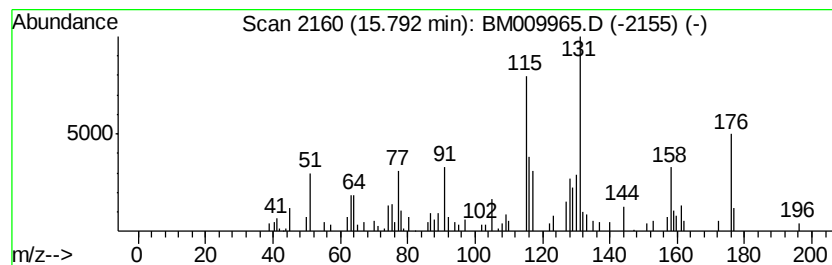
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Peak Number 4 1-Naphthalenecarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.79	2.30 ng	133402	Acenaphthene-d10	14.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	62
2		4-Methyl-.beta.-methyl-.beta.-ni...	177	C10H11NO2	052287-56-6	41
3		3-Methyl-.beta.-methyl-.beta.-ni...	177	C10H11NO2	086969-37-1	38
4		cis-4-Methyl-.beta.-methyl-.beta...	177	C10H11NO2	1000122-76-8	38
5		Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	27



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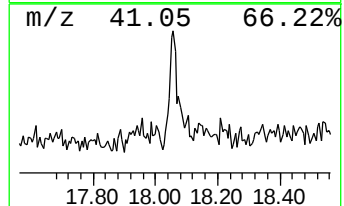
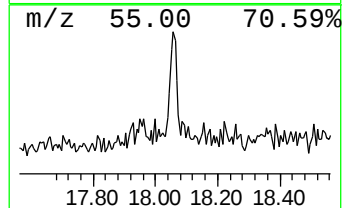
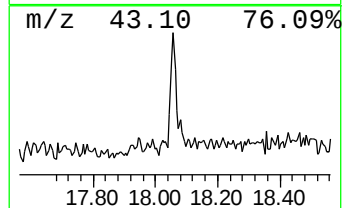
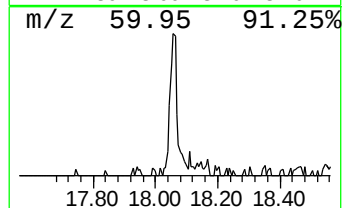
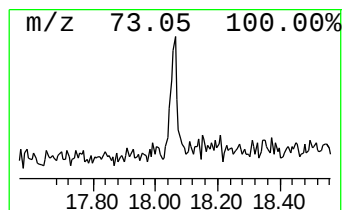
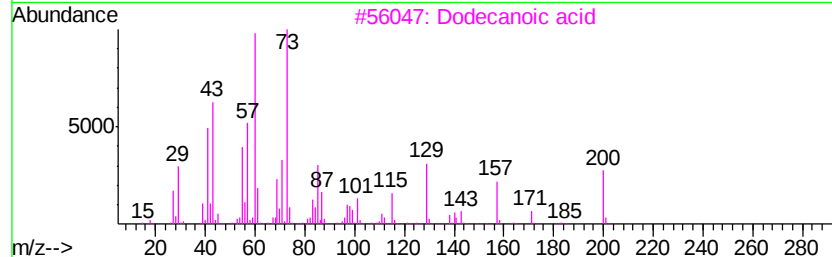
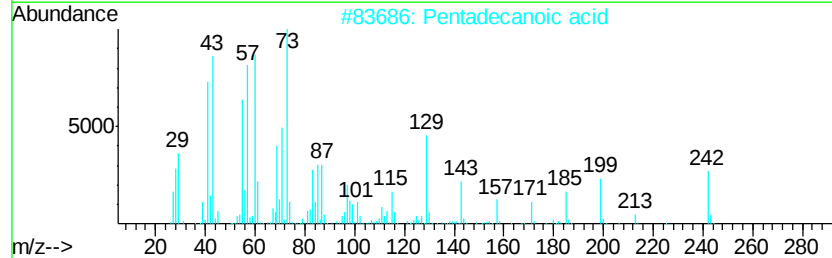
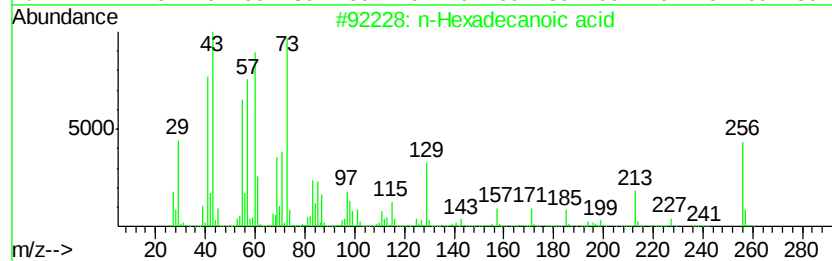
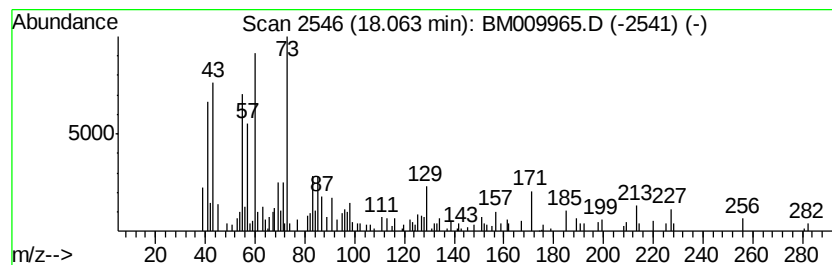
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	2.26 ng	169811	Phenanthrene-d10	17.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Dodecanoic acid	200	C12H24O2	000143-07-7	53
4		Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	49
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	5.8	ng	181549	1	7.77	621719	20.0
unknown7.30	7.30	97.9	ng	3042920	1	7.77	621719	20.0
1-Naphthalenecarb...	15.79	2.3	ng	133402	3	14.42	1159910	20.0
n-Hexadecanoic acid	18.06	2.3	ng	169811	4	17.18	1504320	20.0