

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
 Data File : BM016249.D
 Acq On : 08 Aug 2018 14:37
 Operator : SJ/JU
 Sample : J4313-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C-7

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BM072318.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	5.187	317	323	333	rBV	132219	199729	10.45%	1.357%
2	5.663	398	404	420	rBV	754756	1142073	59.73%	7.760%
3	7.304	676	683	697	rBV	703765	1159193	60.62%	7.877%
4	7.663	738	744	758	rBV	831954	1303875	68.19%	8.860%
5	8.134	819	824	835	rBB	184928	299418	15.66%	2.035%
6	8.457	872	879	889	rBV	641355	1013159	52.98%	6.884%
7	9.322	1020	1026	1046	rBV	436235	734000	38.39%	4.987%
8	10.951	1297	1303	1311	rBV	199680	338240	17.69%	2.298%
9	13.392	1711	1718	1728	rBV	973124	1407972	73.63%	9.567%
10	14.222	1854	1859	1866	rBB	53063	73124	3.82%	0.497%
11	14.769	1946	1952	1960	rBB2	241768	362128	18.94%	2.461%
12	16.257	2199	2205	2215	rBV	773229	1069164	55.91%	7.265%
13	17.504	2412	2417	2421	rBV	301070	412280	21.56%	2.801%
14	17.545	2421	2424	2430	rVB	101779	143038	7.48%	0.972%
15	17.639	2436	2440	2445	rBV2	18279	26745	1.40%	0.182%
16	18.357	2557	2562	2569	rBV2	149731	219009	11.45%	1.488%
17	18.421	2569	2573	2579	rVB2	23115	36344	1.90%	0.247%
18	18.568	2592	2598	2602	rBV4	19420	39933	2.09%	0.271%
19	19.539	2758	2763	2770	rVB	189005	259845	13.59%	1.766%
20	19.615	2771	2776	2780	rBV2	52053	74197	3.88%	0.504%
21	19.862	2814	2818	2821	rBV3	27345	41271	2.16%	0.280%
22	19.898	2821	2824	2831	rVB	162723	222104	11.62%	1.509%
23	20.086	2850	2856	2861	rBV	1622683	1912197	100.00%	12.993%
24	20.233	2875	2881	2885	rVB6	12670	25294	1.32%	0.172%
25	20.357	2896	2902	2904	rBV7	16141	29327	1.53%	0.199%
26	20.386	2904	2907	2913	rVB2	23670	33703	1.76%	0.229%
27	20.486	2921	2924	2928	rBV4	16819	21426	1.12%	0.146%
28	20.545	2928	2934	2938	rVV4	16143	29036	1.52%	0.197%
29	21.127	3030	3033	3038	rBV3	23370	41424	2.17%	0.281%
30	21.309	3058	3064	3070	rVB3	93095	173919	9.10%	1.182%
31	21.509	3095	3098	3103	rBV	60674	62796	3.28%	0.427%
32	21.633	3113	3119	3123	rBV2	429987	687005	35.93%	4.668%
33	21.674	3123	3126	3134	rVB	103875	135632	7.09%	0.922%
34	22.203	3214	3216	3222	rVB4	58238	79068	4.13%	0.537%

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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

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35	22.903	3331	3335	3339	rVB4	78104	112651	5.89%	0.765%
36	23.239	3388	3392	3394	rBV3	105597	161983	8.47%	1.101%
37	23.874	3496	3500	3508	rVB	75208	140163	7.33%	0.952%
38	23.974	3511	3517	3523	rBV	260259	494558	25.86%	3.360%

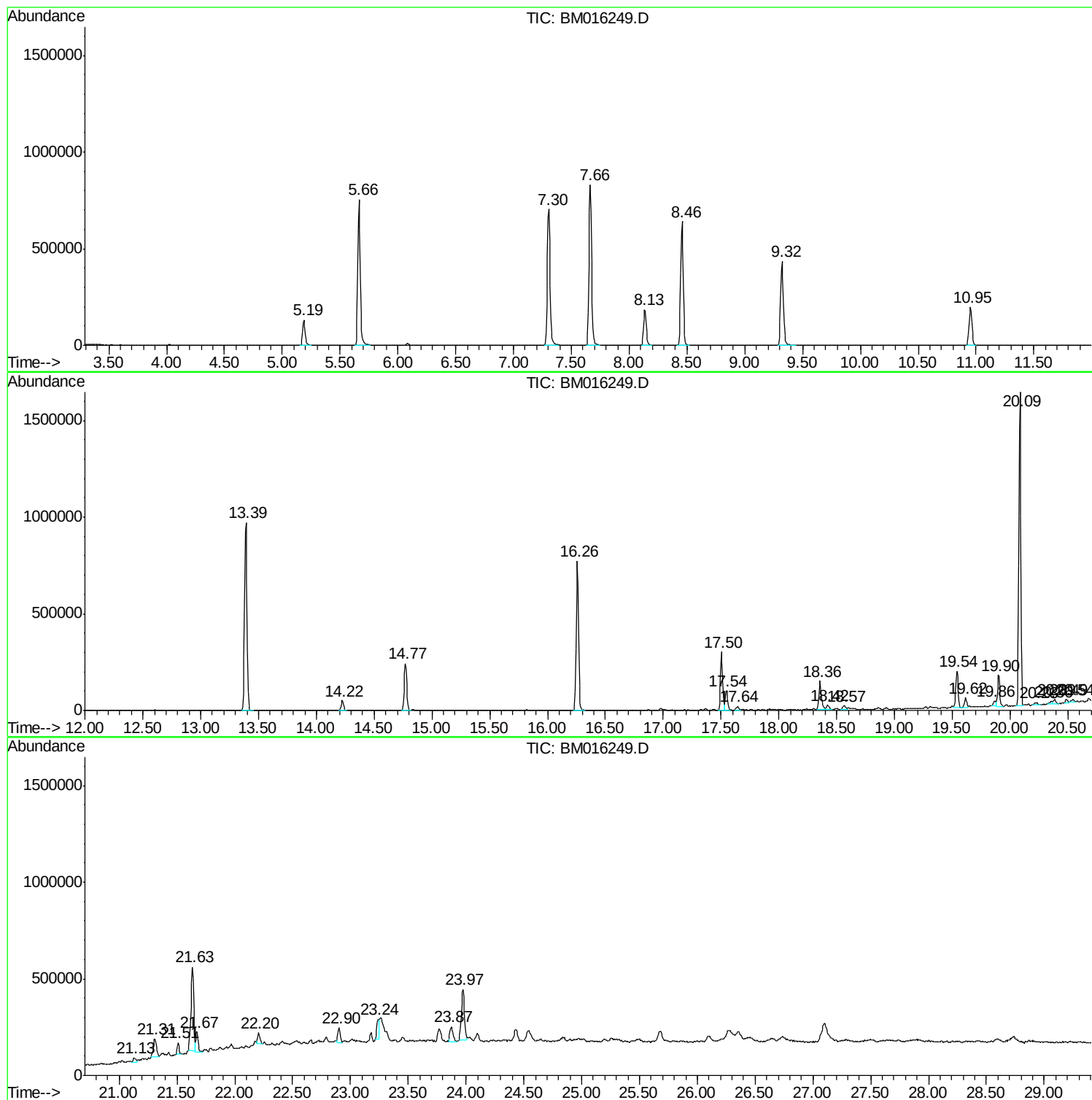
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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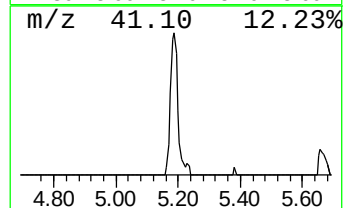
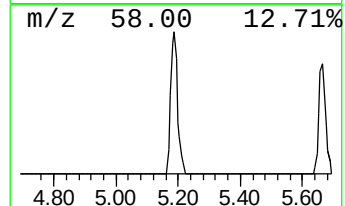
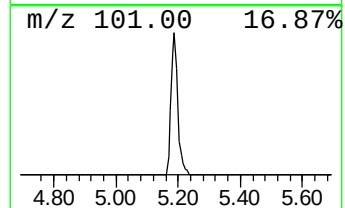
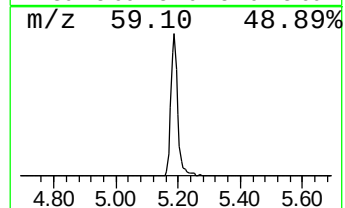
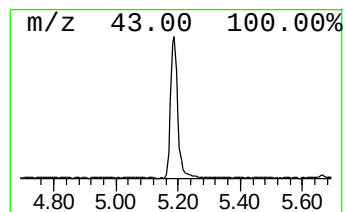
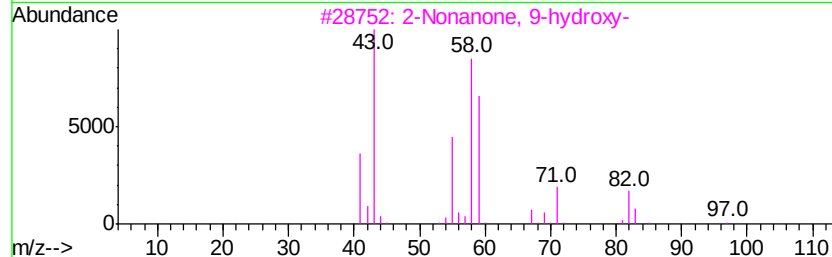
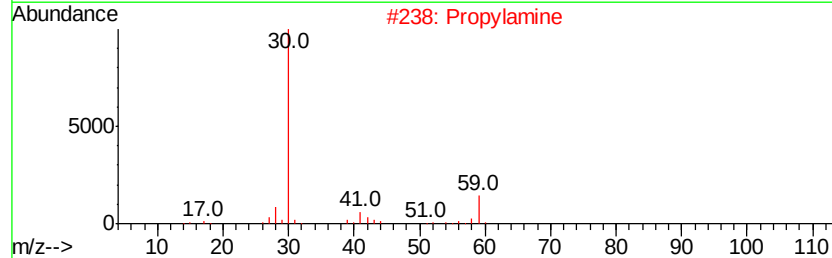
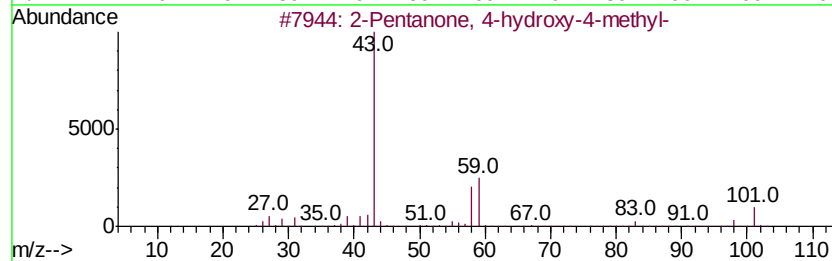
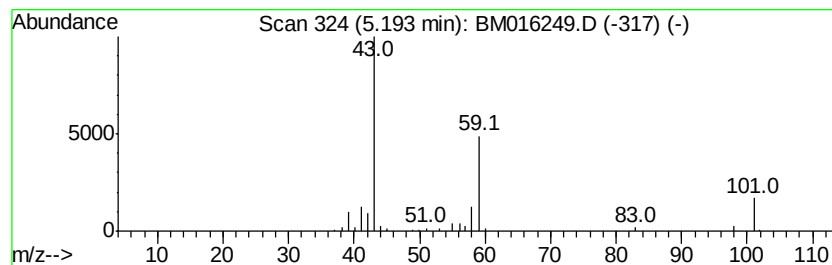
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	13.34 ng	199729	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propylamine	59	C3H9N	000107-10-8	40
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
5			Butane	58	C4H10	000106-97-8	27



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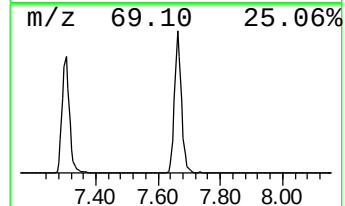
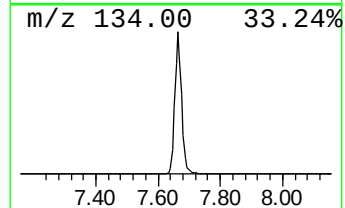
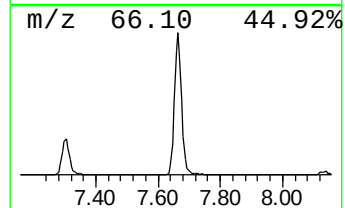
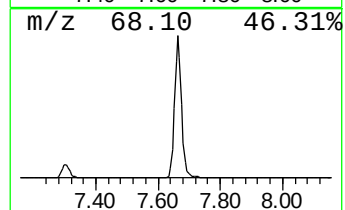
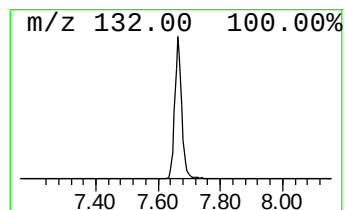
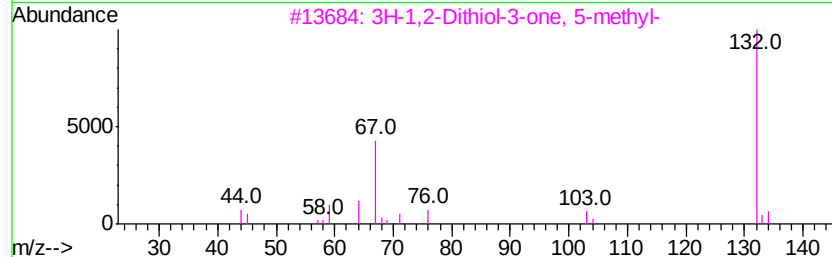
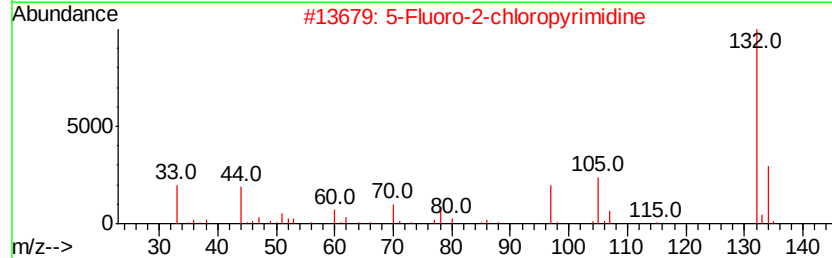
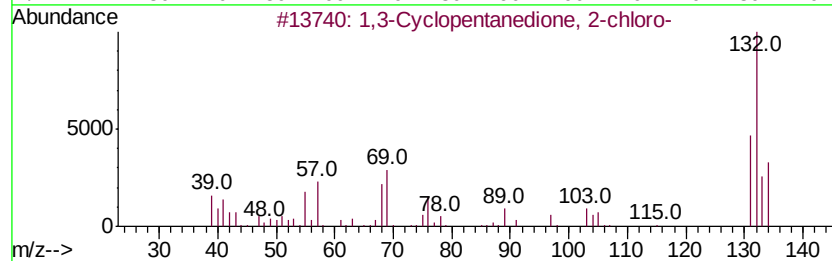
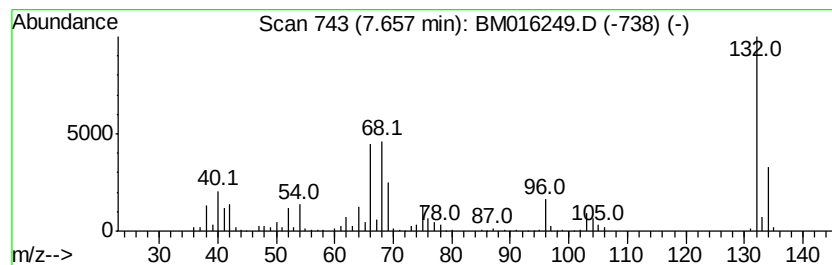
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	87.09 ng	1303880	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10



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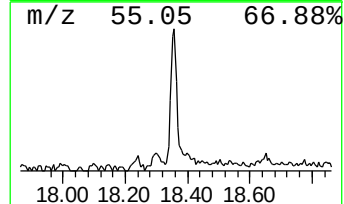
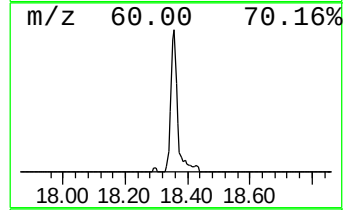
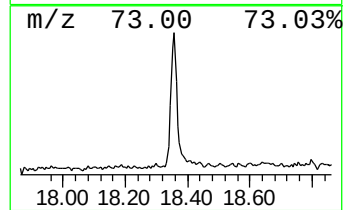
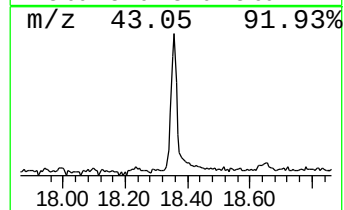
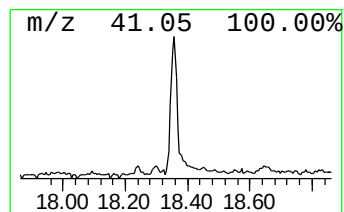
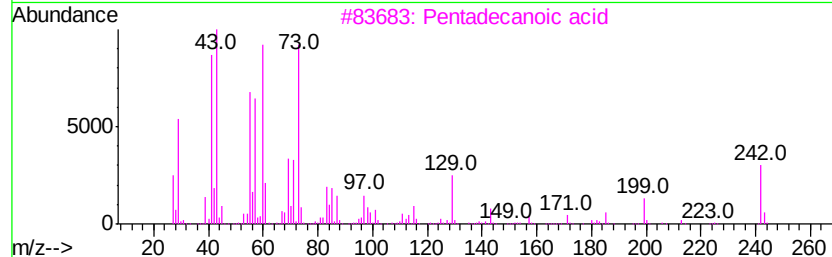
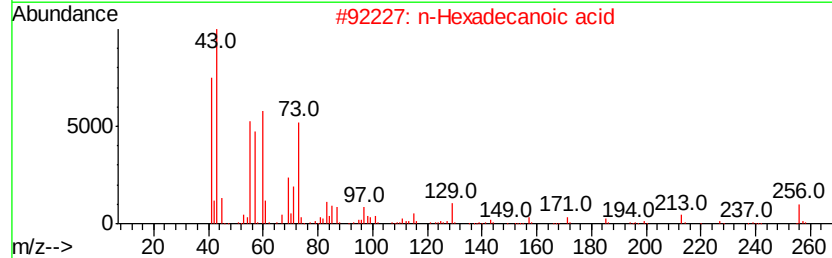
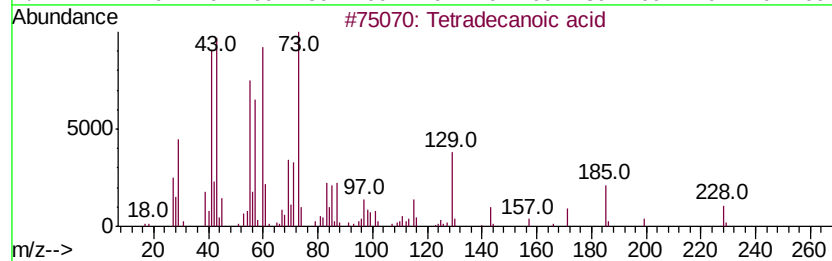
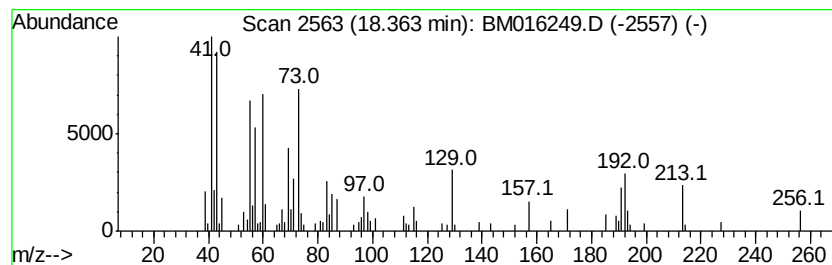
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	10.62 ng	219009	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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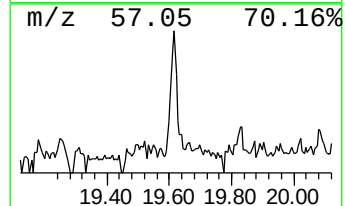
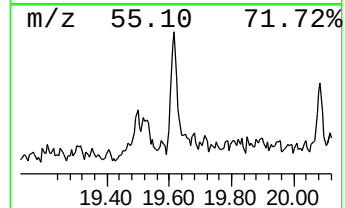
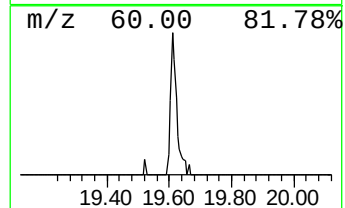
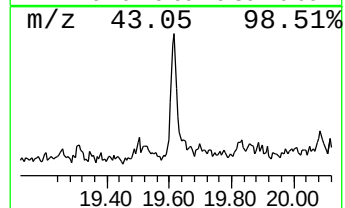
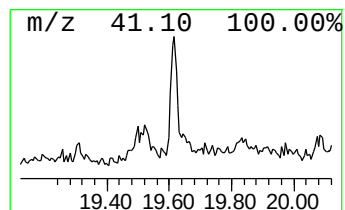
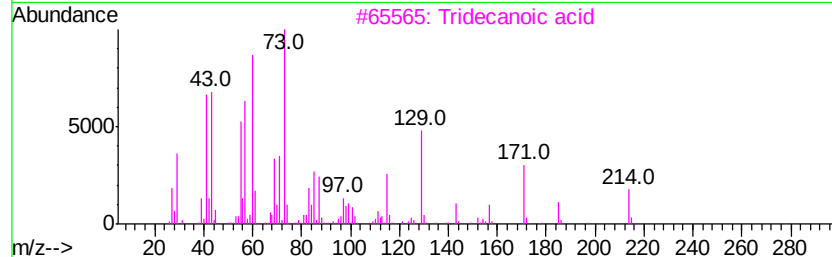
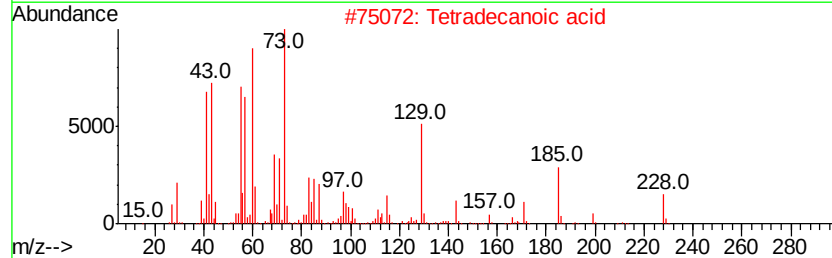
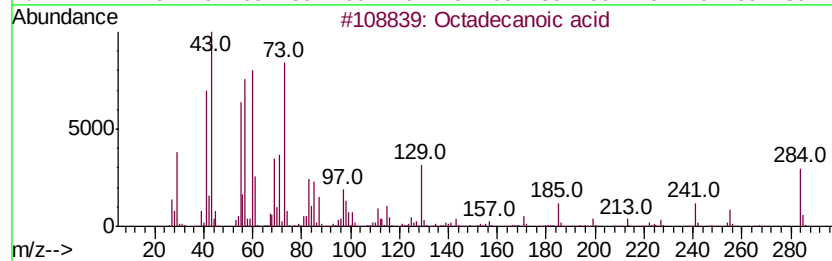
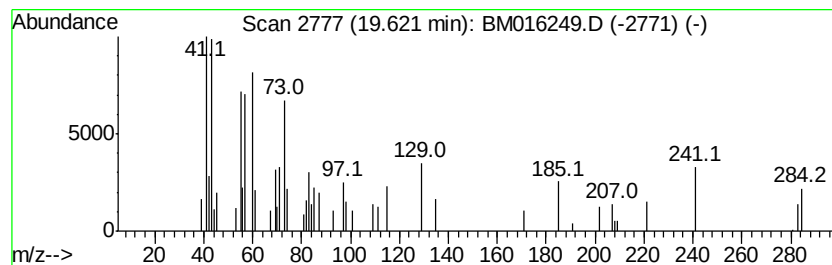
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.16 ng	74197	Chrysene-d12	21.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	55
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	46
3		Tridecanoic acid	214	C13H26O2	000638-53-9	43
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	38
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35



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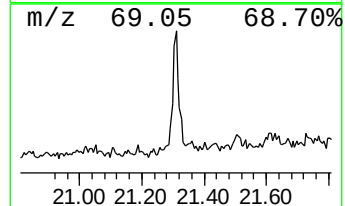
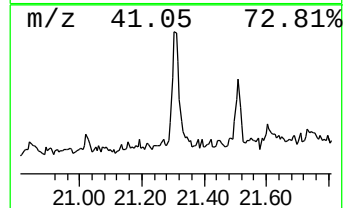
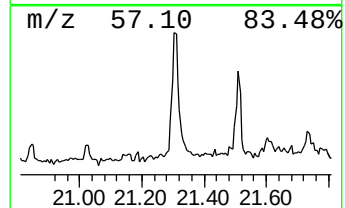
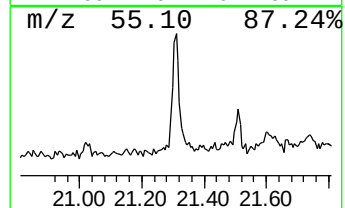
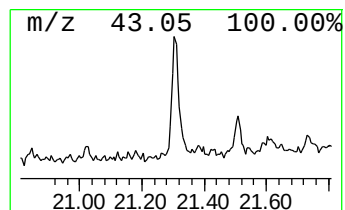
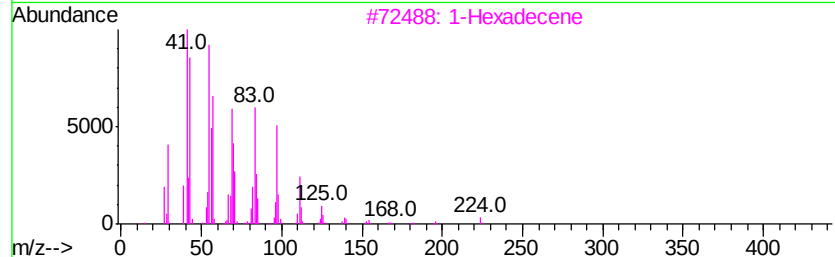
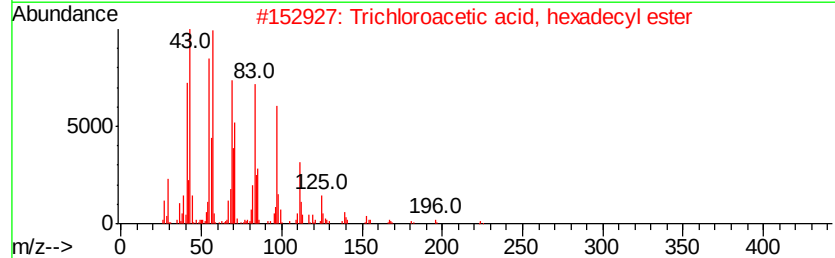
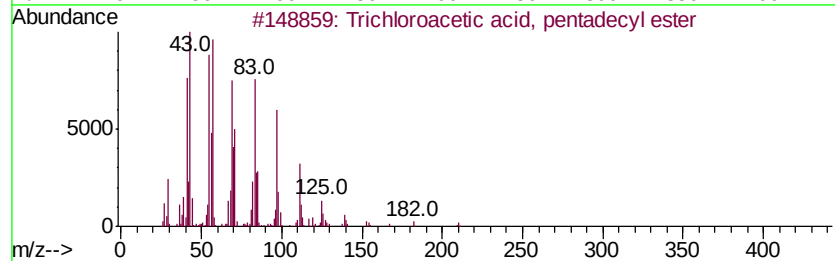
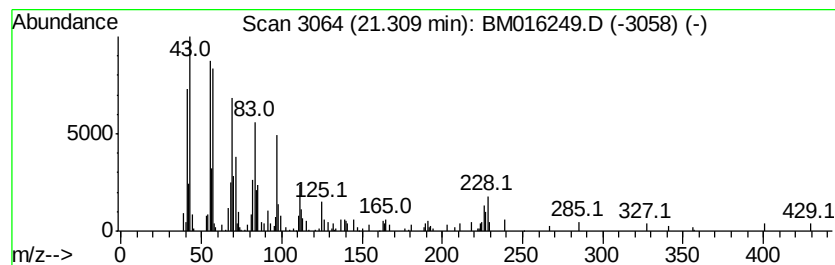
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.06 ng	173919	Chrysene-d12	21.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			1-Hexadecene	224	C16H32	000629-73-2	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81
5			1-Nonadecanol	284	C19H40O	001454-84-8	81



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Operator : SJ/JU
Sample : J4313-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C-7

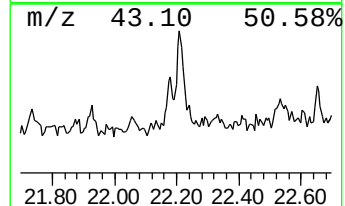
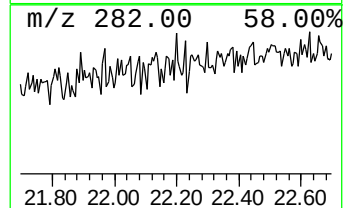
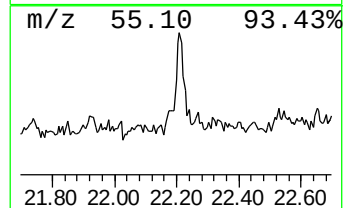
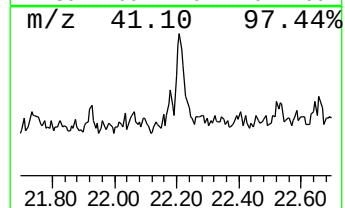
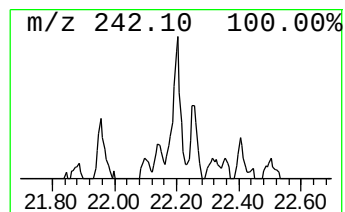
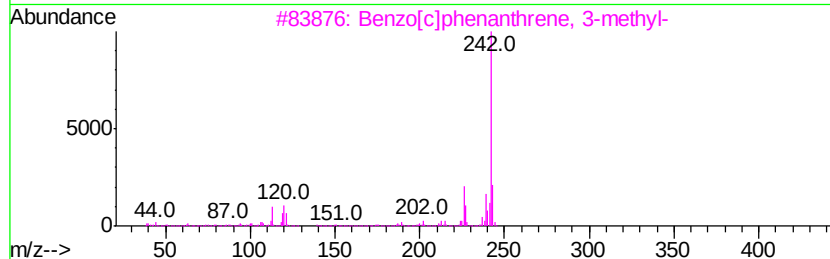
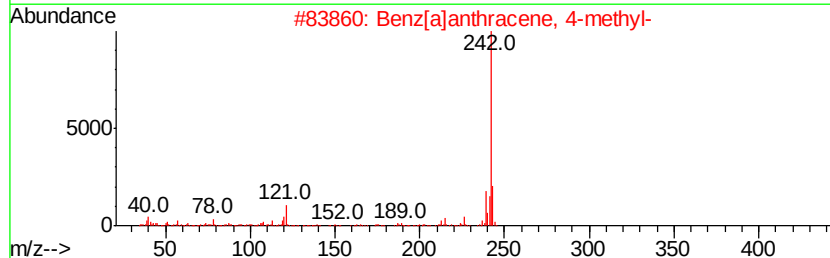
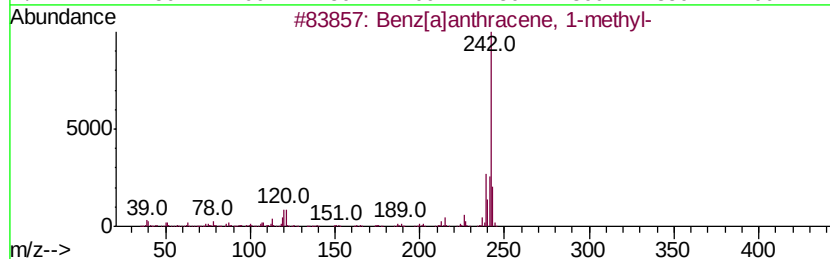
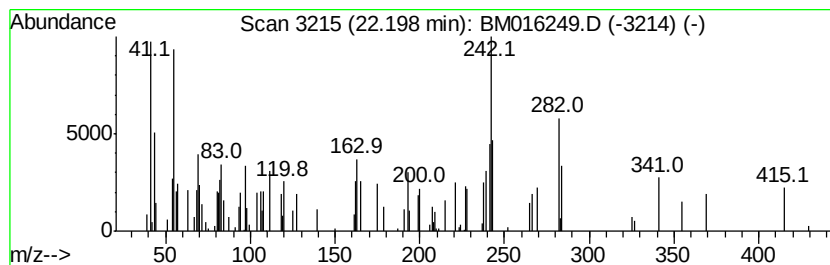
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown22.20 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.20	2.30 ng	79068	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	25
2		Benz[a]anthracene, 4-methyl-	242	C19H14	000316-49-4	22
3		Benzo[c]phenanthrene, 3-methyl-	242	C19H14	002381-19-3	22
4		Benz[a]anthracene, 3-methyl-	242	C19H14	002498-75-1	22
5		Benz[a]anthracene, 2-methyl-	242	C19H14	002498-76-2	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016249.D
Acq On : 08 Aug 2018 14:37
Operator : SJ/JU
Sample : J4313-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

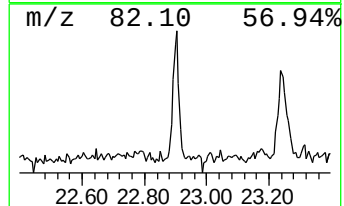
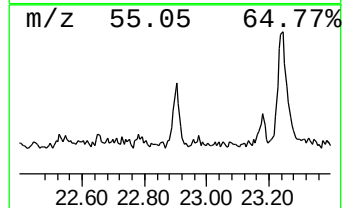
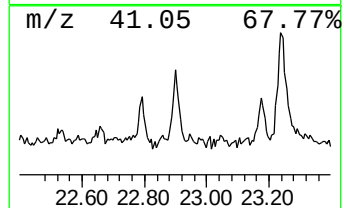
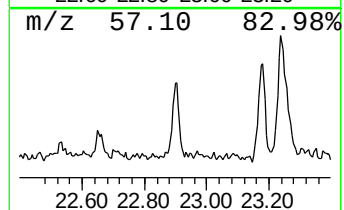
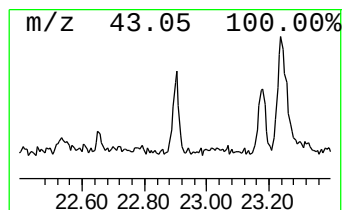
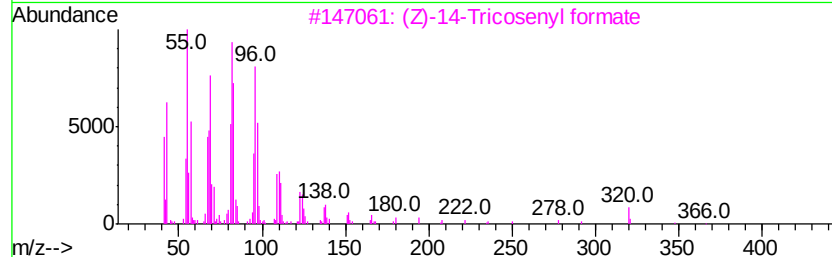
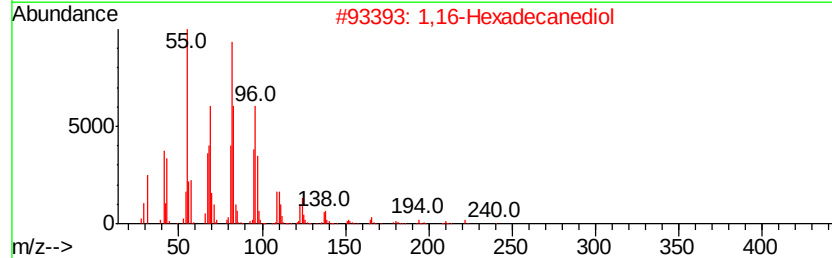
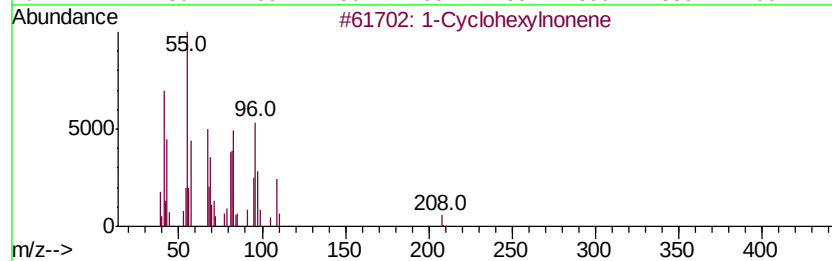
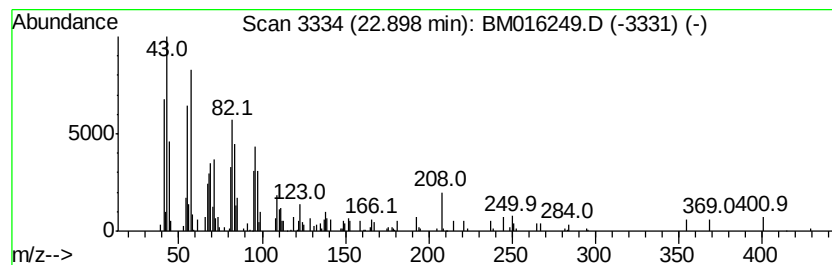
Instrument :
BNA_M
ClientSampled :
C-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Cyclohexylnonene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.90	4.56 ng	112651	Perylene-d12	23.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexyl-nonene	208	C15H28	114614-84-5	53
2	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	49
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	47
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	46
5	Pentadecanal-	226	C15H30O	002765-11-9	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080818\
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Sample : J4313-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	13.3	ng	199729	1	8.13	299418	20.0
unknown7.66	7.66	87.1	ng	1303880	1	8.13	299418	20.0
Tetradecanoic acid	18.36	10.6	ng	219009	4	17.50	412280	20.0
Octadecanoic acid	19.62	2.2	ng	74197	5	21.63	687005	20.0
Trichloroacetic a...	21.31	5.1	ng	173919	5	21.63	687005	20.0
unknown22.20	22.20	2.3	ng	79068	5	21.63	687005	20.0
1-Cyclohexylnonene	22.90	4.6	ng	112651	6	23.97	494558	20.0