

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM012519\
 Data File : BM018657.D
 Acq On : 25 Jan 2019 17:57
 Operator : JU/SJ
 Sample : K1157-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-04-011519

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-BM010919.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	4.875	299	304	312	rVB	256551	364046	2.50%	0.370%
2	5.322	373	380	389	rBV	4740838	6634517	45.61%	6.748%
3	6.910	642	650	663	rBV	4601114	7296609	50.16%	7.422%
4	7.269	703	711	725	rBV	4943344	7775046	53.45%	7.908%
5	7.734	783	790	797	rBV	937386	1488404	10.23%	1.514%
6	8.051	836	844	852	rBV	3735186	5988824	41.17%	6.092%
7	8.898	980	988	999	rBV	2793869	4558961	31.34%	4.637%
8	10.522	1256	1264	1271	rBV	1179167	1960625	13.48%	1.994%
9	12.998	1677	1685	1695	rBV	6927211	10155442	69.82%	10.330%
10	13.839	1822	1828	1840	rVB	454508	637670	4.38%	0.649%
11	14.380	1911	1920	1928	rBV2	1701090	2561061	17.61%	2.605%
12	15.874	2164	2174	2184	rBV	6025110	8601471	59.14%	8.749%
13	17.133	2381	2388	2392	rBV	2164558	3059422	21.03%	3.112%
14	17.174	2392	2395	2399	rVB	245609	322586	2.22%	0.328%
15	18.021	2532	2539	2550	rBV2	1491737	2345229	16.12%	2.385%
16	19.192	2733	2738	2744	rVB	559408	740476	5.09%	0.753%
17	19.304	2752	2757	2762	rBV	508309	700232	4.81%	0.712%
18	19.557	2796	2800	2808	rVB	497818	676865	4.65%	0.688%
19	19.762	2829	2835	2840	rBV	11675569	14545437	100.00%	14.795%
20	21.021	3045	3049	3059	rVB2	1797647	2120608	14.58%	2.157%
21	21.103	3059	3063	3072	rBV	487562	613135	4.22%	0.624%
22	21.321	3094	3100	3104	rBV	3142167	4126366	28.37%	4.197%
23	21.356	3104	3106	3114	rVB	291889	353732	2.43%	0.360%
24	21.462	3121	3124	3132	rVB4	160378	219257	1.51%	0.223%
25	21.915	3195	3201	3211	rVB2	758443	1325502	9.11%	1.348%
26	22.362	3274	3277	3281	rVB	313053	373705	2.57%	0.380%
27	22.874	3360	3364	3368	rBV	603495	1007994	6.93%	1.025%
28	22.921	3369	3372	3382	rVB2	688551	1313373	9.03%	1.336%
29	23.450	3459	3462	3466	rVB	286019	334525	2.30%	0.340%
30	23.592	3480	3486	3502	rVB	1878827	3815016	26.23%	3.880%
31	24.103	3569	3573	3581	rVB	682549	1315453	9.04%	1.338%
32	24.197	3584	3589	3598	rVB	518481	981783	6.75%	0.999%

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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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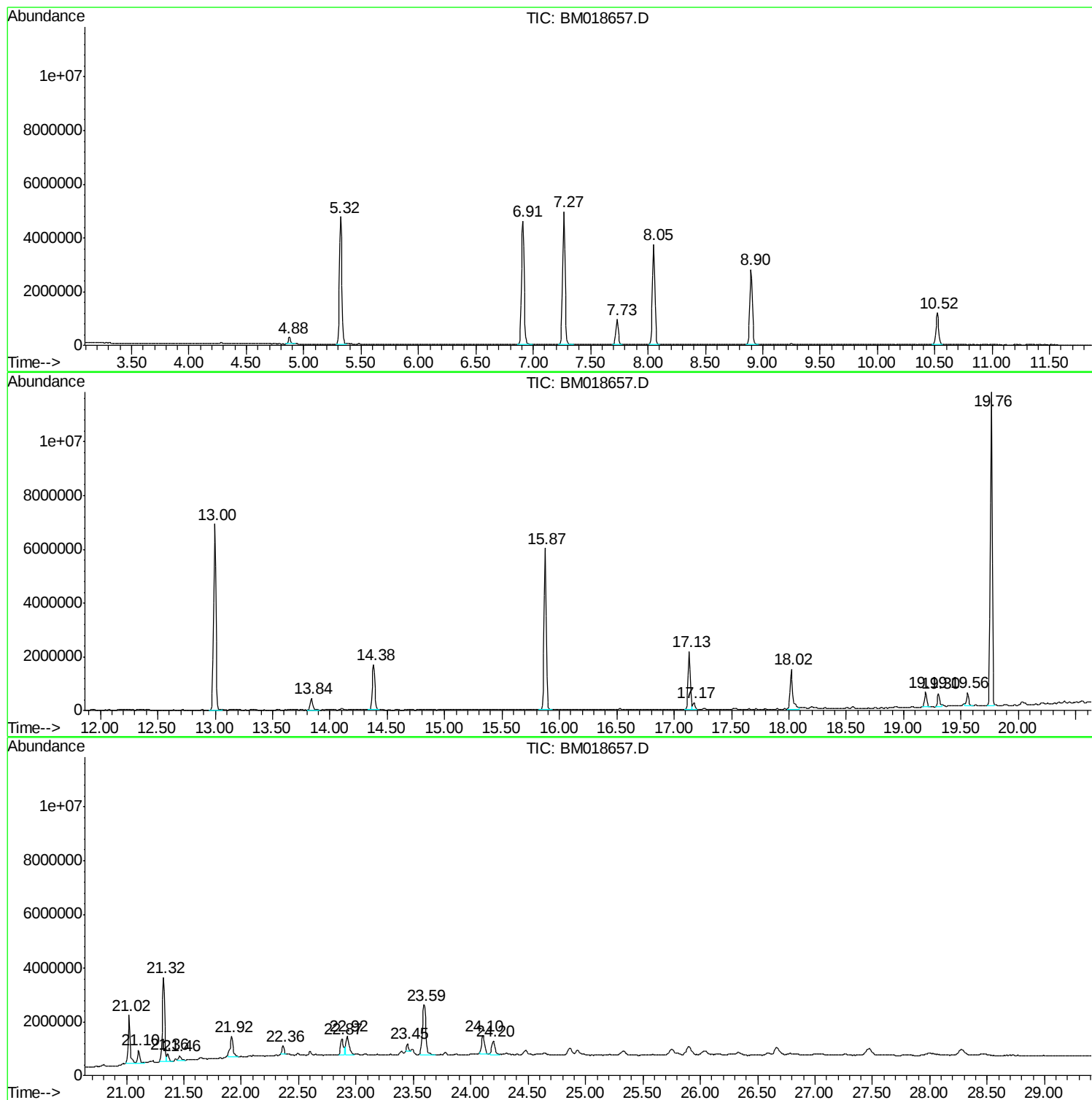
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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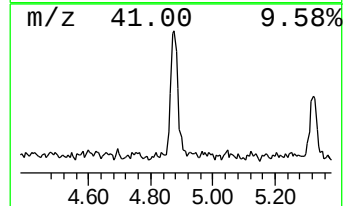
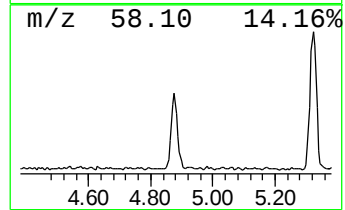
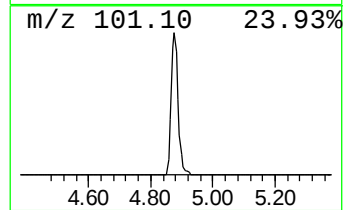
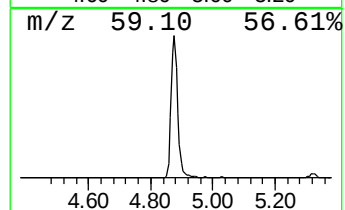
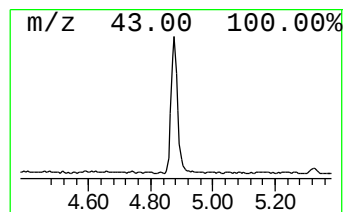
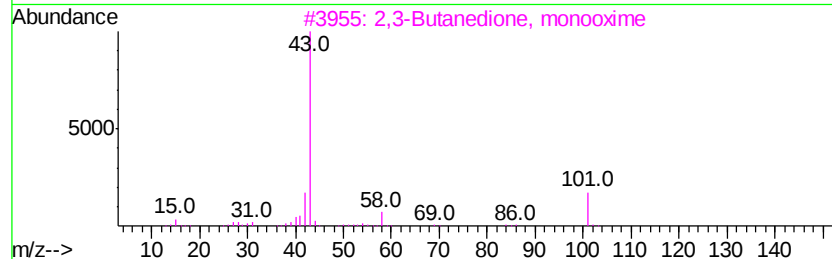
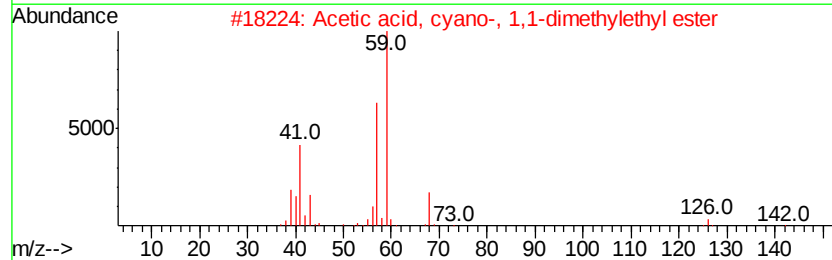
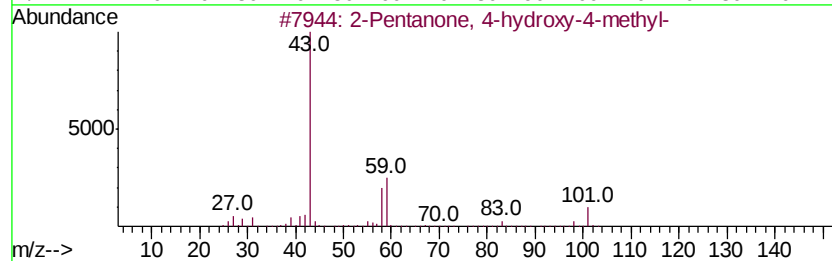
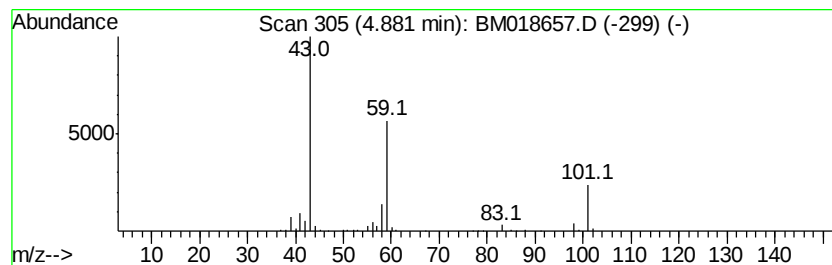
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	4.89 ng	364046	1,4-Dichlorobenzene-d4	7.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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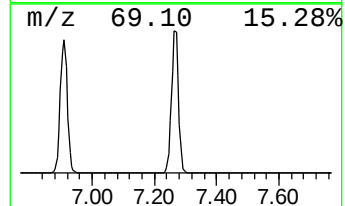
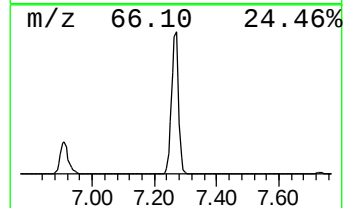
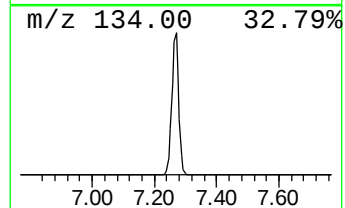
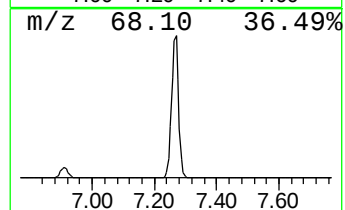
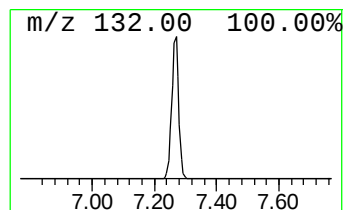
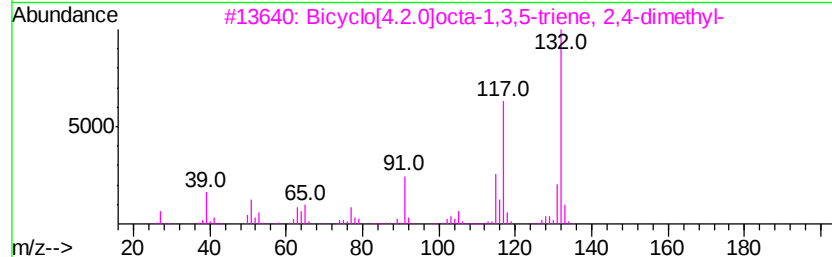
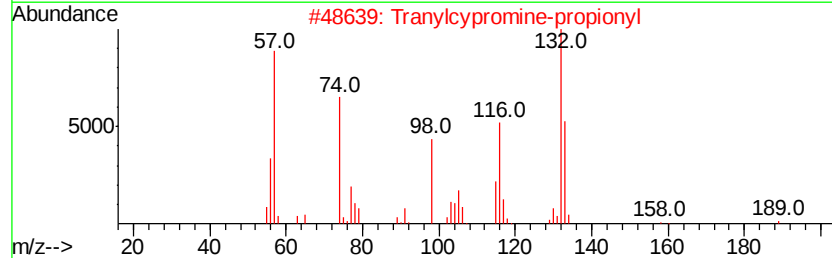
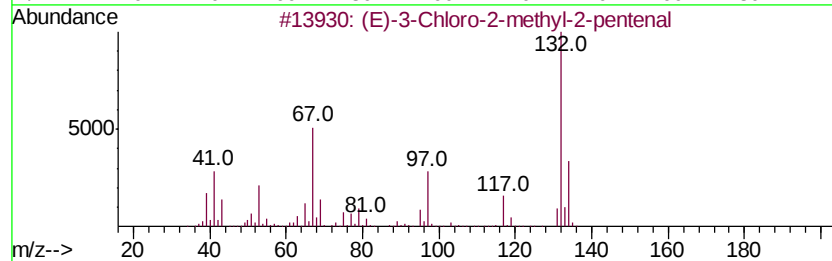
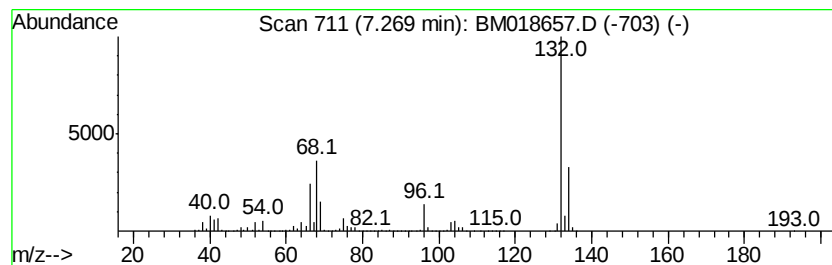
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	104.48 ng	7775050	1,4-Dichlorobenzene-d4	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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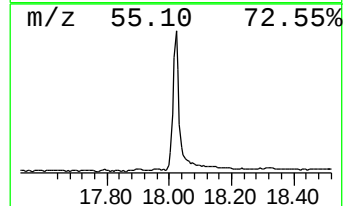
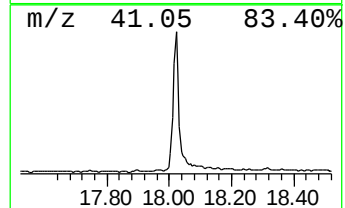
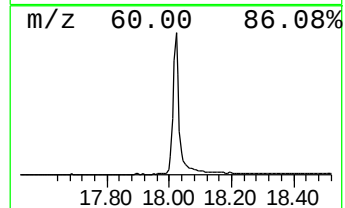
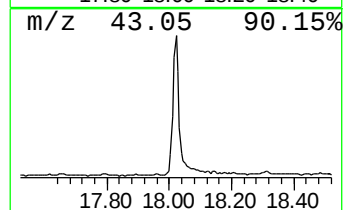
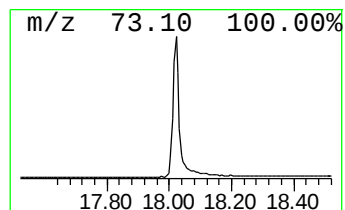
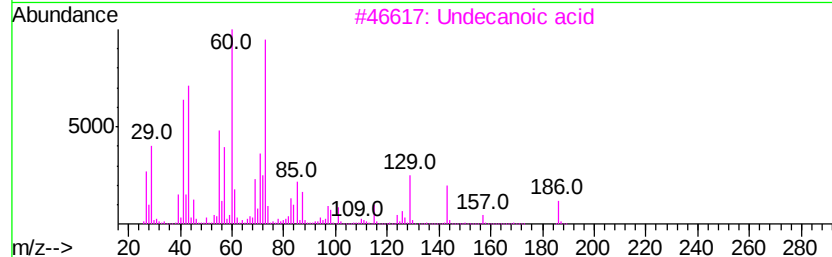
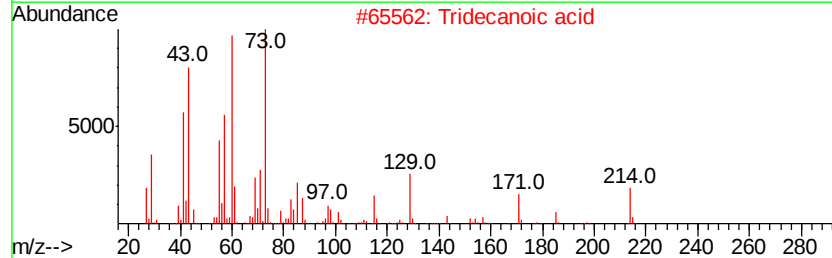
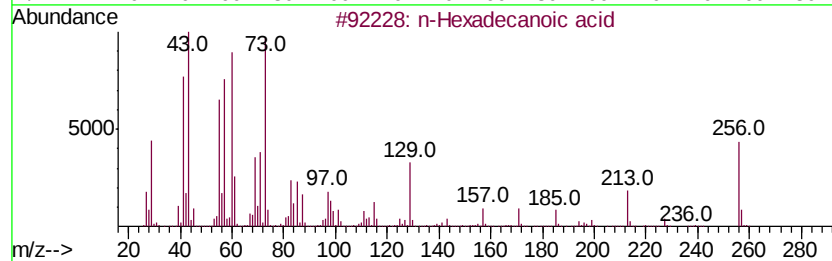
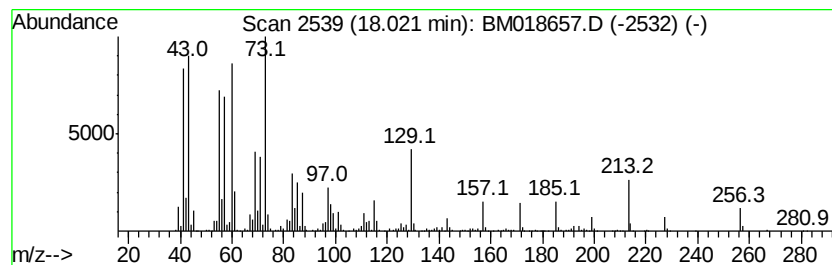
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	15.33 ng	2345230	Phenanthrene-d10	17.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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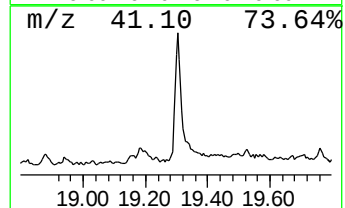
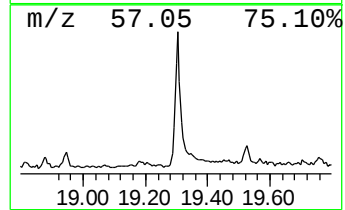
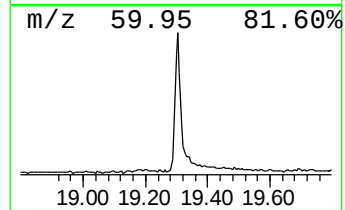
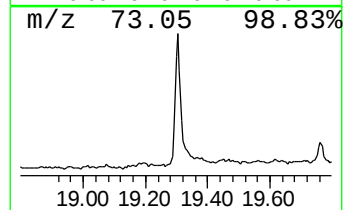
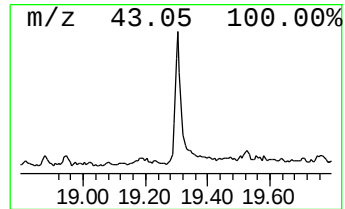
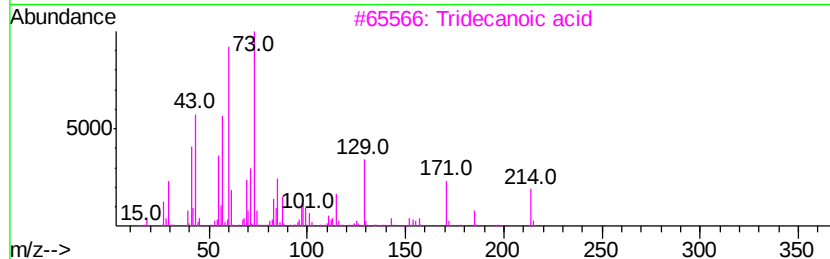
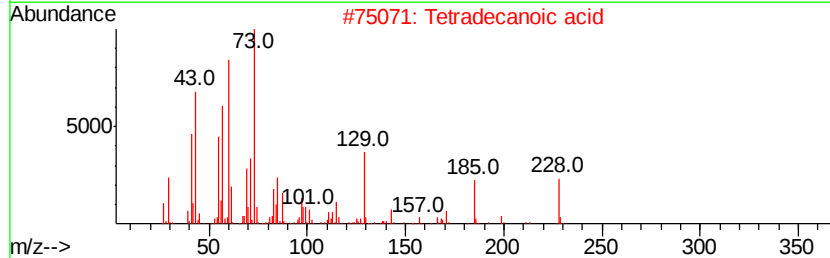
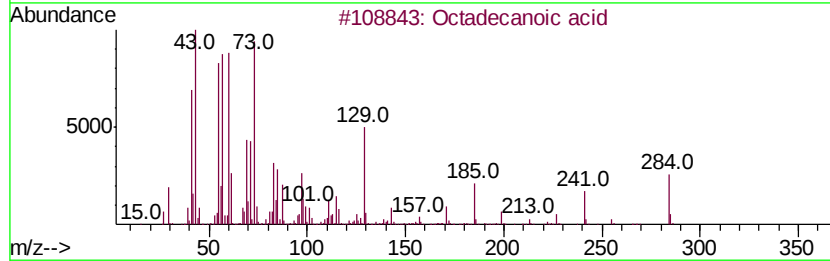
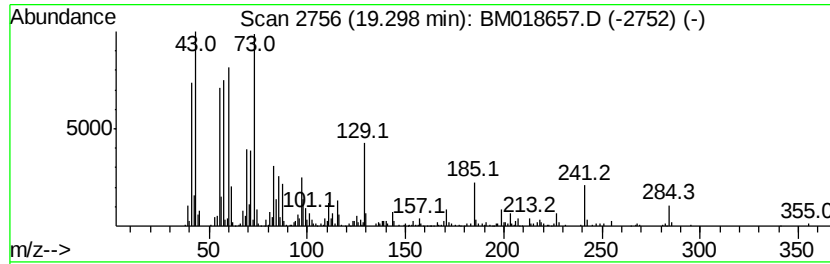
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	3.39 ng	700232	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	72



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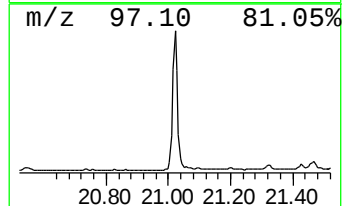
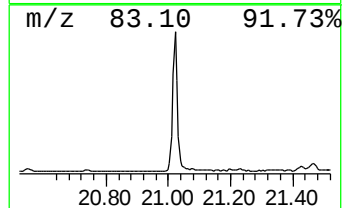
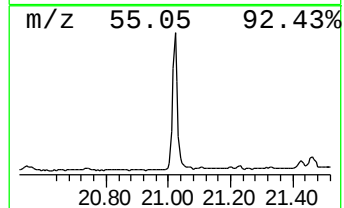
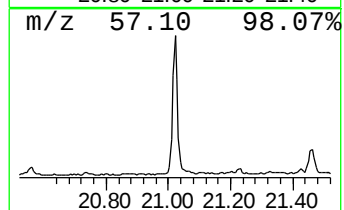
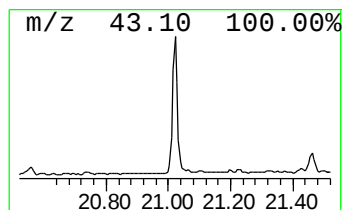
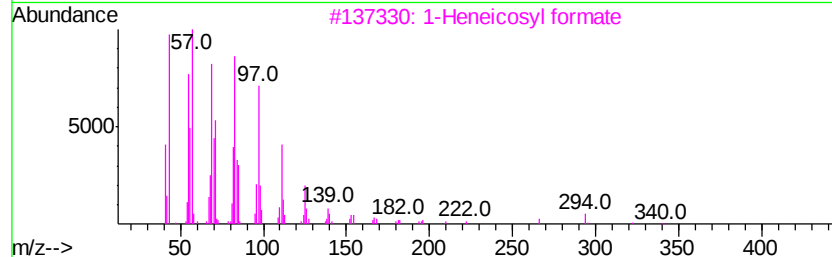
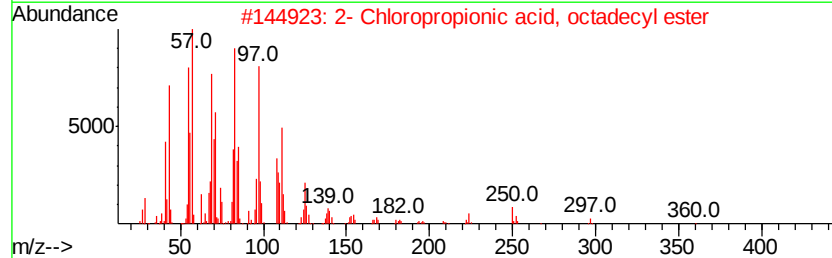
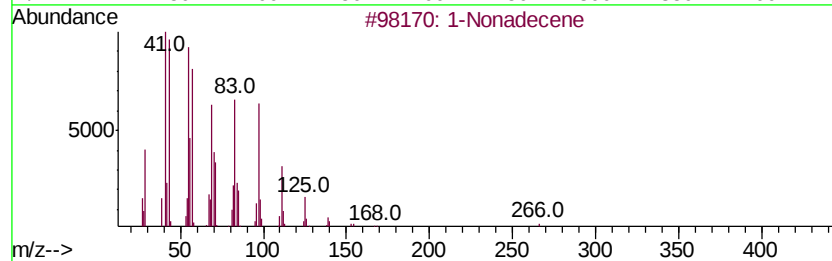
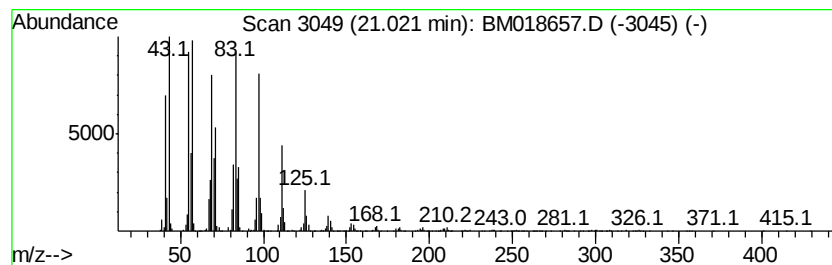
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.02	10.28 ng	2120610	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	98
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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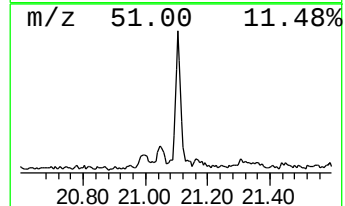
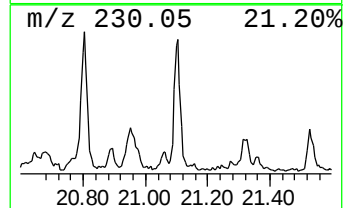
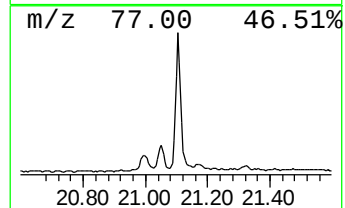
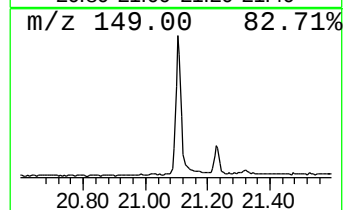
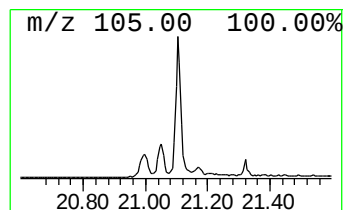
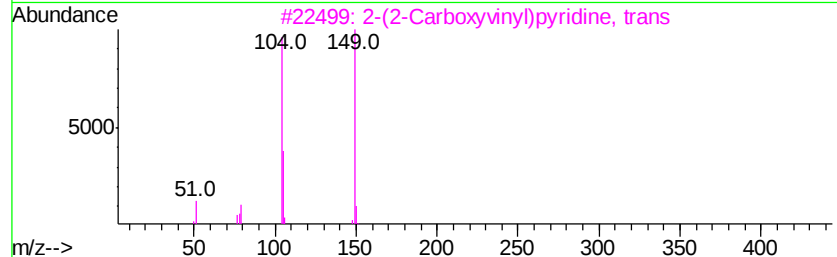
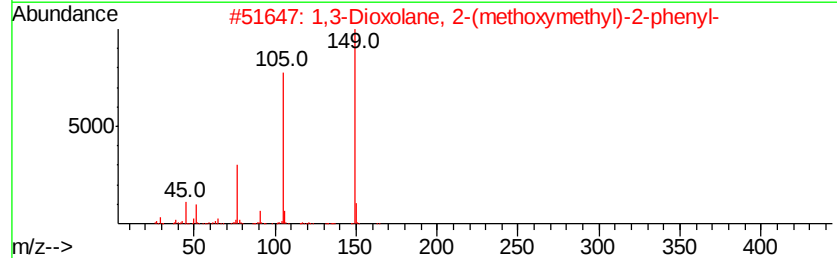
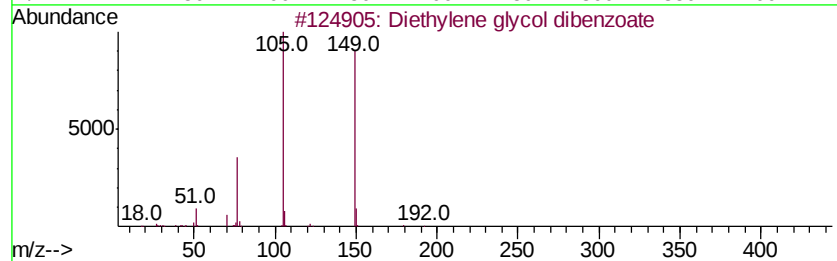
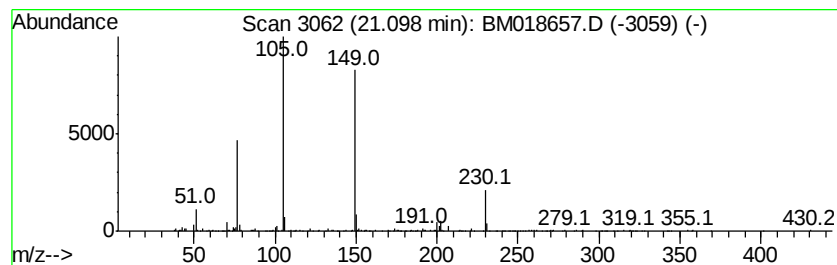
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.97 ng	613135	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
3		2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4		2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5		Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM012519\
Data File : BM018657.D
Acq On : 25 Jan 2019 17:57
Operator : JU/SJ
Sample : K1157-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-04-011519

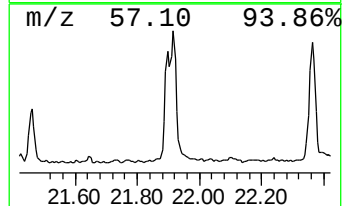
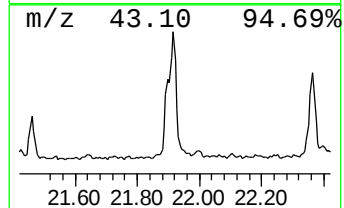
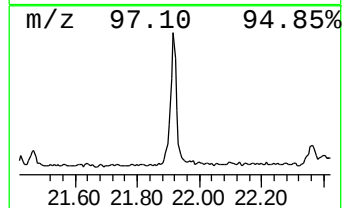
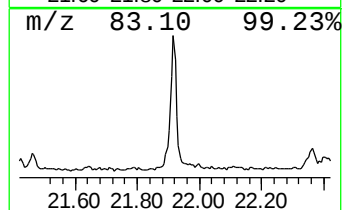
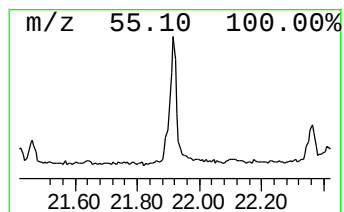
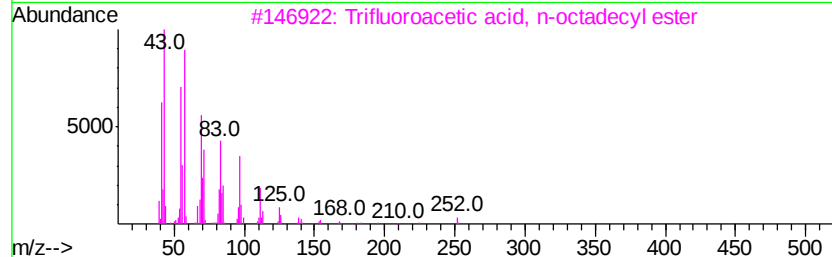
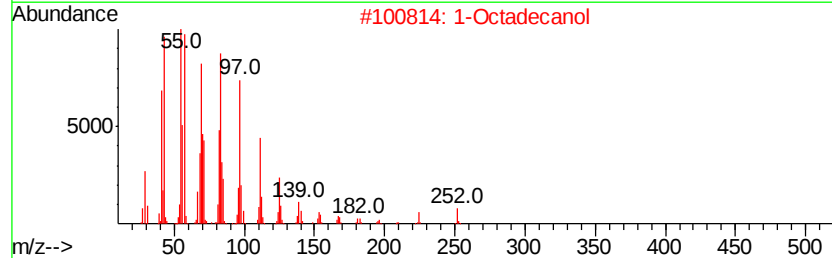
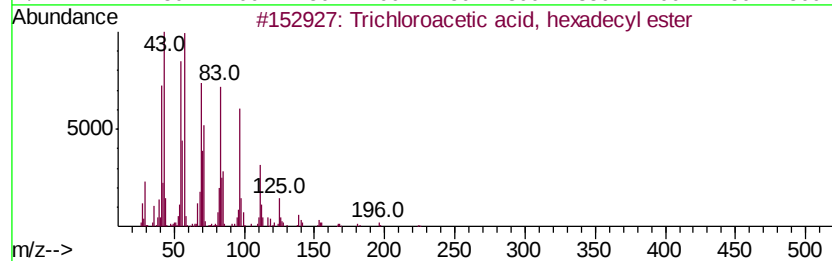
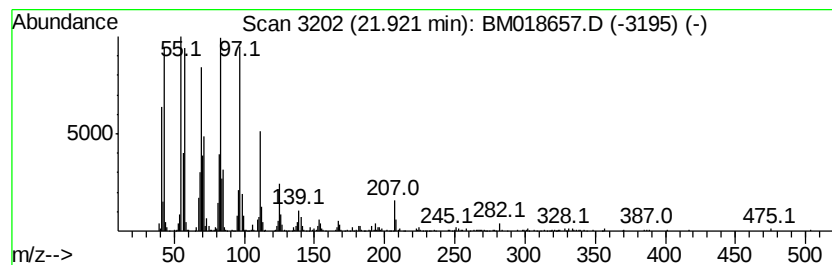
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.92	6.42 ng	1325500	Chrysene-d12	21.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2			1-Octadecanol	270	C18H38O	000112-92-5	87
3			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	87
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5			2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM012519\
Data File : BM018657.D
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Operator : JU/SJ
Sample : K1157-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-04-011519

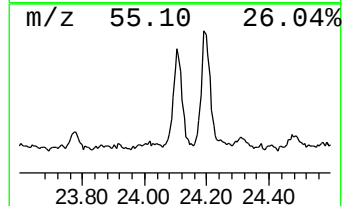
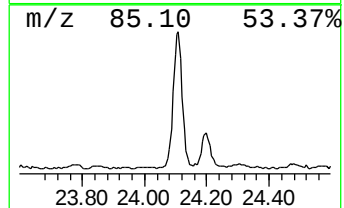
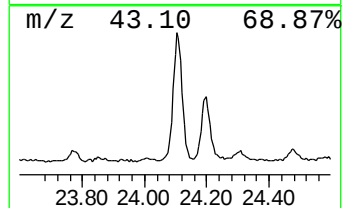
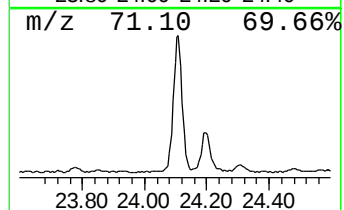
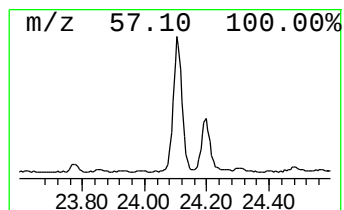
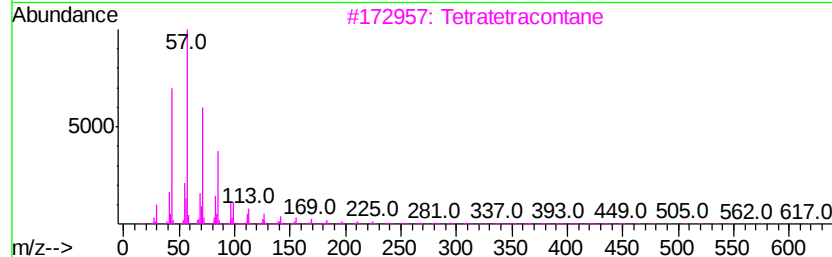
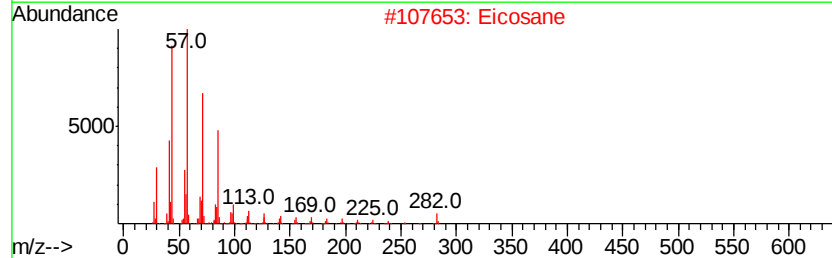
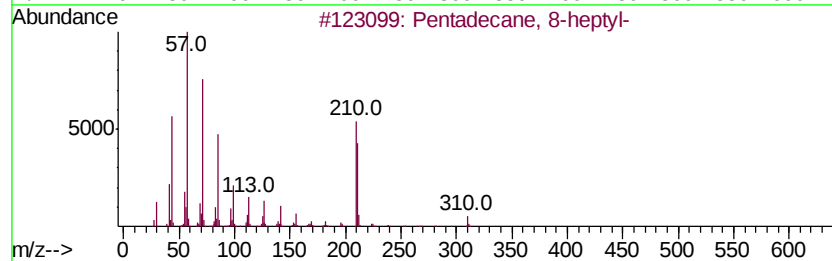
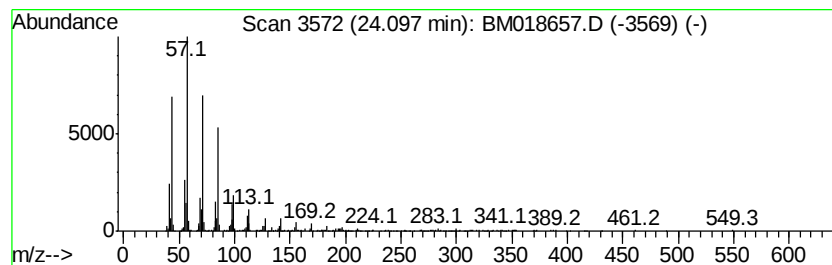
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.10	6.90 ng	1315450	Perylene-d12	23.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	96
2		Eicosane	282	C20H42	000112-95-8	95
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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Acq On : 25 Jan 2019 17:57
Operator : JU/SJ
Sample : K1157-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-04-011519

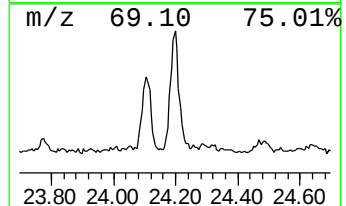
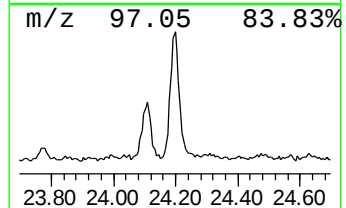
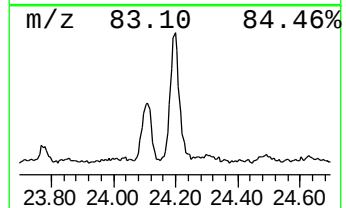
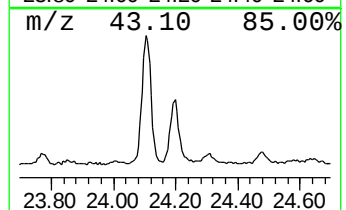
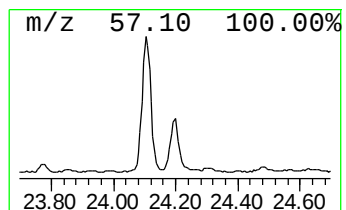
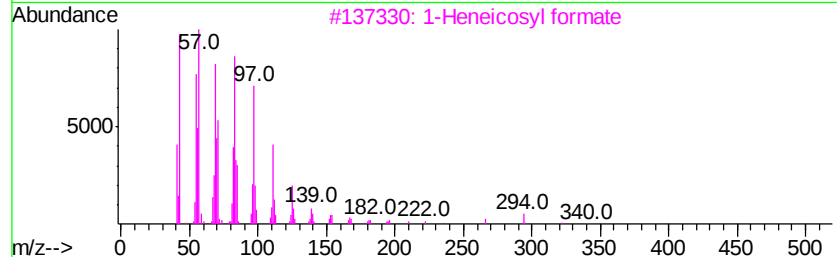
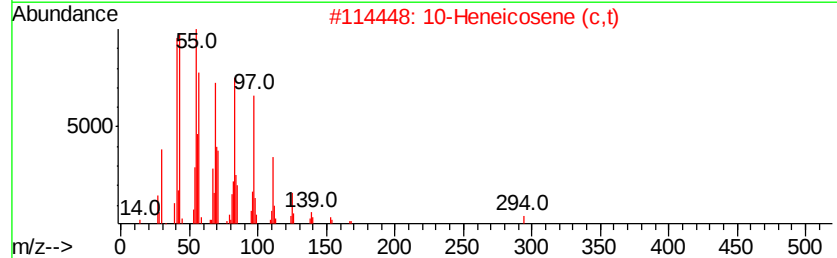
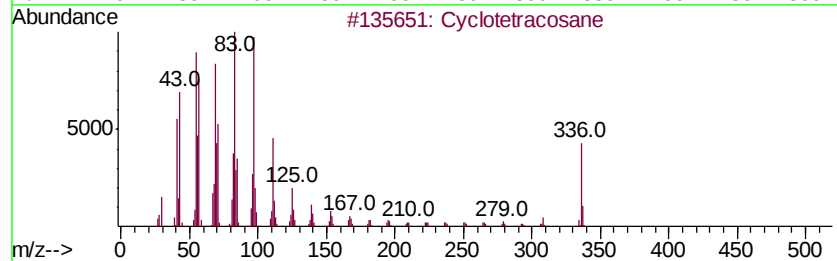
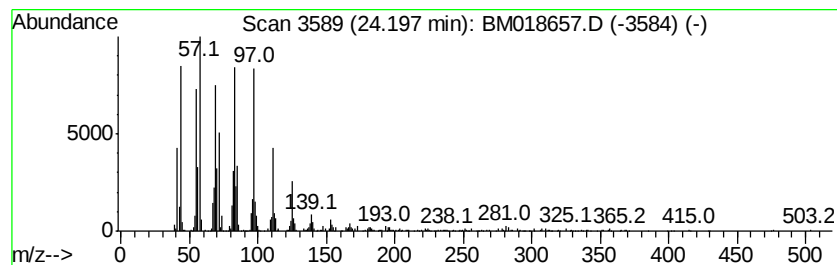
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.20	5.15 ng	981783	Perylene-d12	23.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	96
2			10-Heneicosene (c,t)	294	C21H42	095008-11-0	83
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	83
4			1-Docosene	308	C22H44	001599-67-3	76
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM012519\
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 Sample : K1157-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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...	4.88	4.9	ng	364046	1	7.73	1488400	20.0
unknown7.27	7.27	104.5	ng	7775050	1	7.73	1488400	20.0
n-Hexadecanoic acid	18.02	15.3	ng	2345230	4	17.13	3059420	20.0
Octadecanoic acid	19.30	3.4	ng	700232	5	21.32	4126370	20.0
1-Nonadecene	21.02	10.3	ng	2120610	5	21.32	4126370	20.0
Diethylene glycol...	21.10	3.0	ng	613135	5	21.32	4126370	20.0
Trichloroacetic a...	21.92	6.4	ng	1325500	5	21.32	4126370	20.0
Pentadecane, 8-he...	24.10	6.9	ng	1315450	6	23.59	3815020	20.0
Cyclotetracosane	24.20	5.2	ng	981783	6	23.59	3815020	20.0