

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
 Data File : BF104360.D
 Acq On : 9 Apr 2018 10:01
 Operator : JU/SJ
 Sample : J2275-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-NARANJITO-S002-0001-01

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.022	494	499	506	rVB	136982	176896	5.36%	0.545%
2	5.416	560	566	569	rBV	3015507	3128326	94.70%	9.637%
3	5.745	618	622	627	rBV	70756	58900	1.78%	0.181%
4	6.434	732	739	742	rBV	2797082	3159588	95.65%	9.733%
5	6.569	757	762	766	rBV	3069461	3205460	97.04%	9.874%
6	6.804	798	802	805	rBV	1097767	895135	27.10%	2.757%
7	6.957	824	828	832	rBV	2659438	2413957	73.08%	7.436%
8	7.369	892	898	901	rBV	2032301	1991010	60.27%	6.133%
9	7.439	904	910	913	rVB	46395	44666	1.35%	0.138%
10	8.087	1015	1020	1023	rBV	1445339	1220563	36.95%	3.760%
11	9.163	1198	1203	1206	rBV	3704573	3303282	100.00%	10.176%
12	9.551	1266	1269	1273	rBV	445017	375289	11.36%	1.156%
13	9.769	1303	1306	1309	rVB	105678	78145	2.37%	0.241%
14	9.839	1314	1318	1322	rBV2	1581187	1350439	40.88%	4.160%
15	10.245	1384	1387	1389	rBV	47796	44462	1.35%	0.137%
16	10.269	1389	1391	1394	rVB	113059	90044	2.73%	0.277%
17	10.492	1424	1429	1431	rBV	36436	41187	1.25%	0.127%
18	10.628	1447	1452	1455	rBV	2241305	2187702	66.23%	6.739%
19	10.745	1469	1472	1477	rBV	107903	118896	3.60%	0.366%
20	11.192	1545	1548	1551	rBV2	83843	74711	2.26%	0.230%
21	11.327	1567	1571	1574	rBV	1554115	1312942	39.75%	4.044%
22	11.551	1605	1609	1611	rBV3	42253	44553	1.35%	0.137%
23	11.622	1618	1621	1624	rVB	45460	35773	1.08%	0.110%
24	11.722	1635	1638	1643	rVB3	36099	45403	1.37%	0.140%
25	11.857	1656	1661	1669	rBV2	749242	776664	23.51%	2.392%
26	12.027	1688	1690	1693	rVB	46552	39302	1.19%	0.121%
27	12.374	1746	1749	1753	rBV3	57869	59519	1.80%	0.183%
28	12.422	1754	1757	1760	rVV3	31276	40210	1.22%	0.124%
29	12.563	1779	1781	1785	rVB3	44649	42015	1.27%	0.129%
30	12.639	1790	1794	1804	rBV	237502	315655	9.56%	0.972%
31	12.916	1837	1841	1845	rBV	2892119	2975144	90.07%	9.165%
32	13.121	1874	1876	1878	rBV	48005	35456	1.07%	0.109%
33	13.392	1920	1922	1925	rVB2	60975	54719	1.66%	0.169%
34	13.810	1990	1993	1996	rBV	465119	439709	13.31%	1.355%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.839	1996	1998	2001	rVB	132191	110316	3.34%	0.340%
36	13.968	2016	2020	2023	rVB	1087510	983326	29.77%	3.029%
37	15.421	2263	2267	2271	rBV	682857	840507	25.44%	2.589%
38	15.939	2352	2355	2363	rVB4	88788	161414	4.89%	0.497%
39	17.439	2605	2610	2618	rVB4	93652	191456	5.80%	0.590%

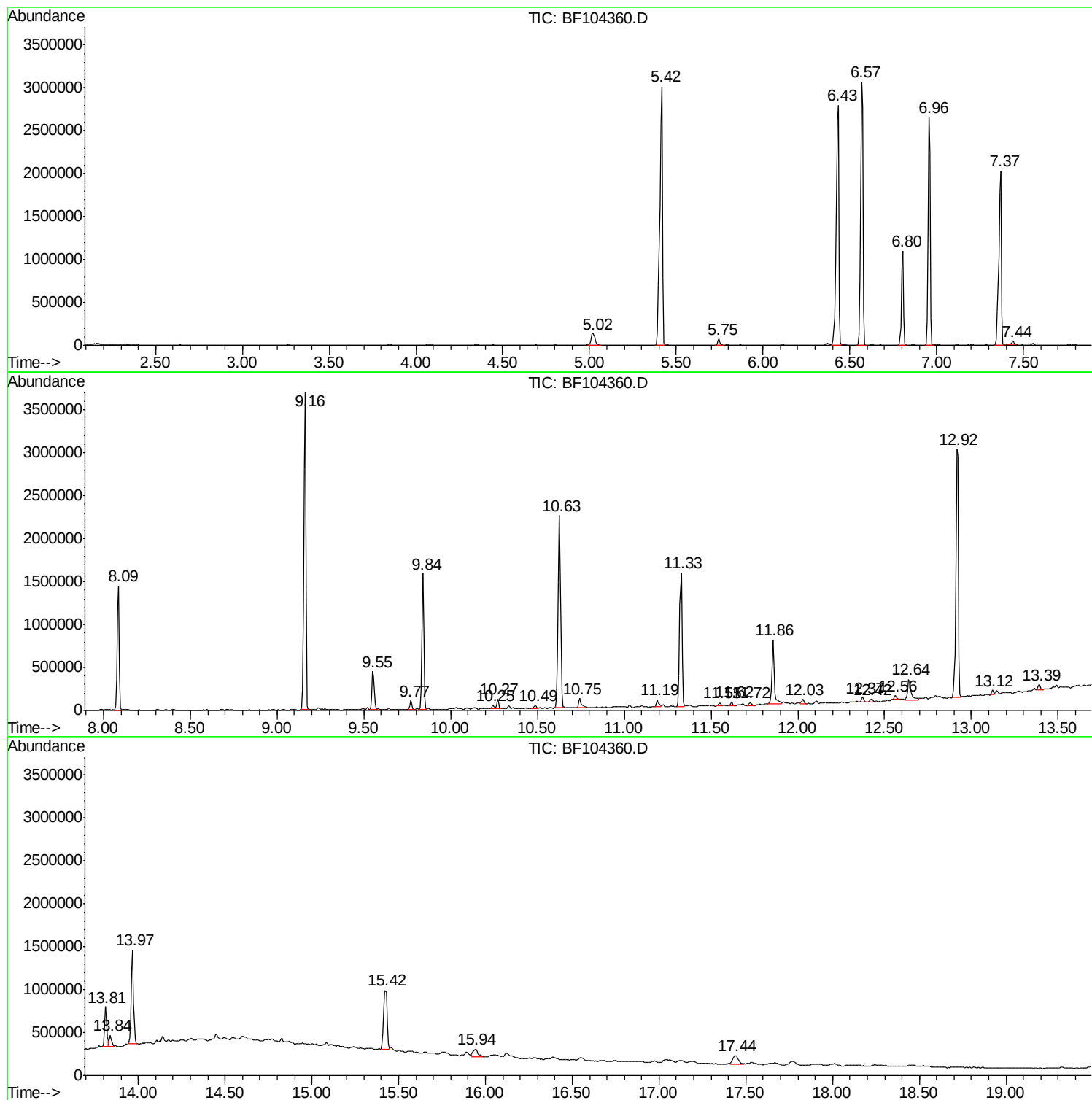
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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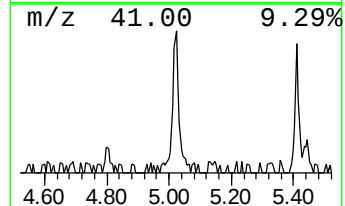
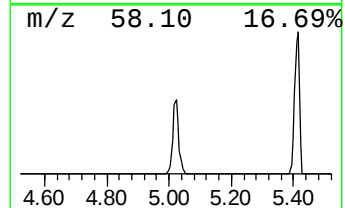
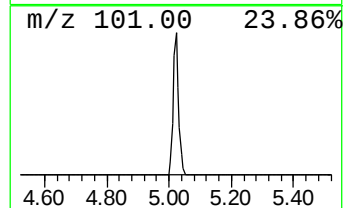
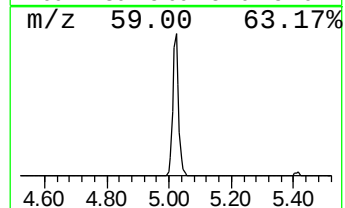
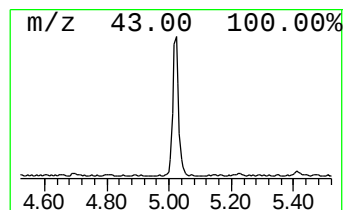
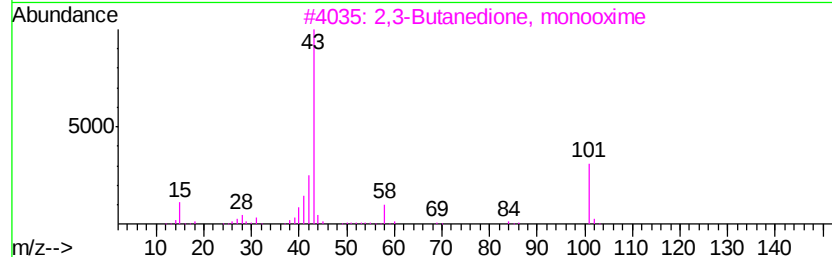
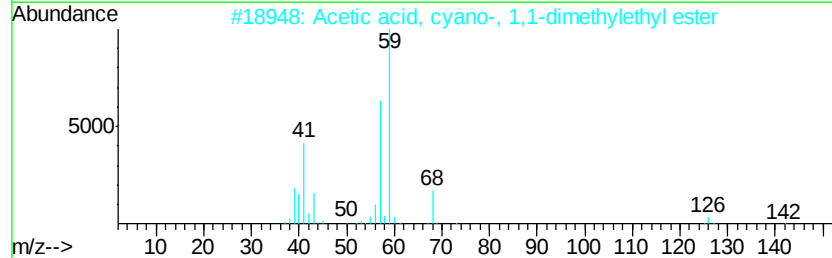
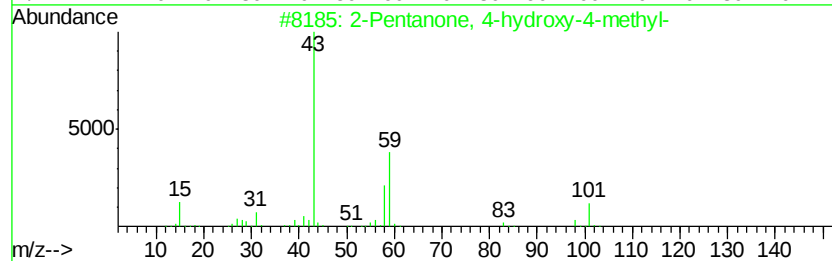
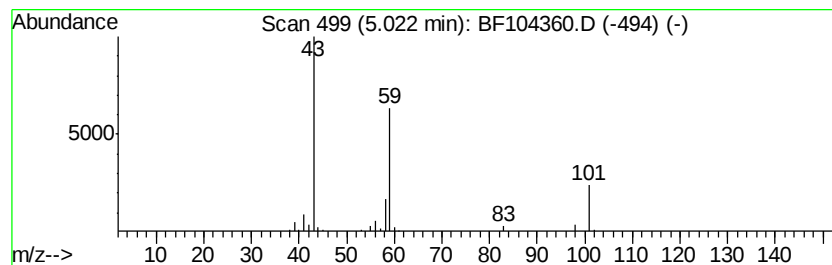
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.95 ng	176896	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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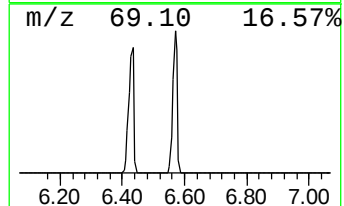
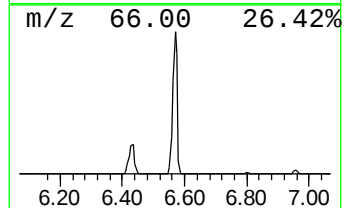
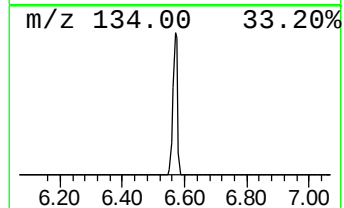
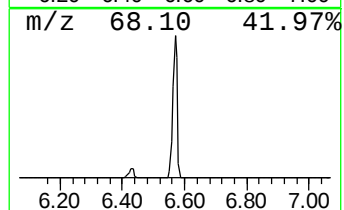
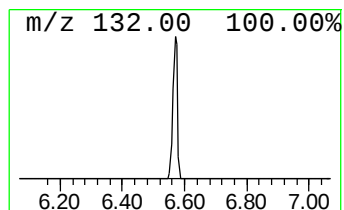
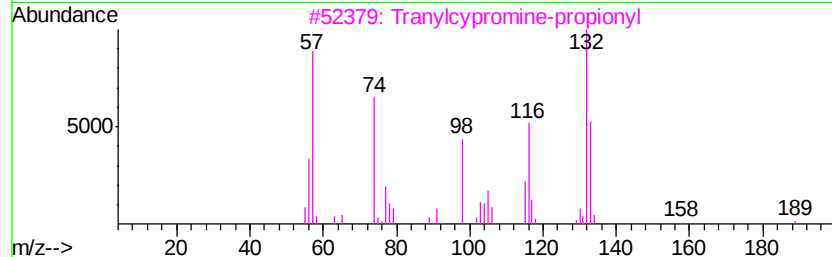
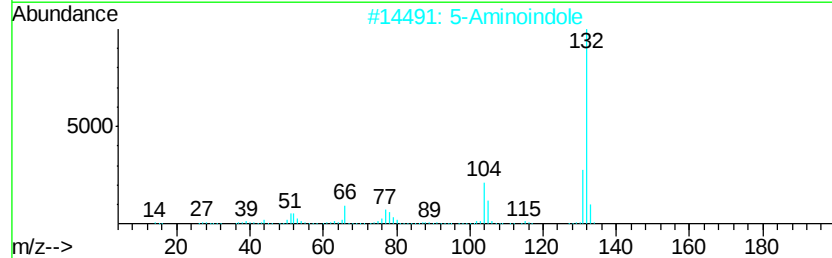
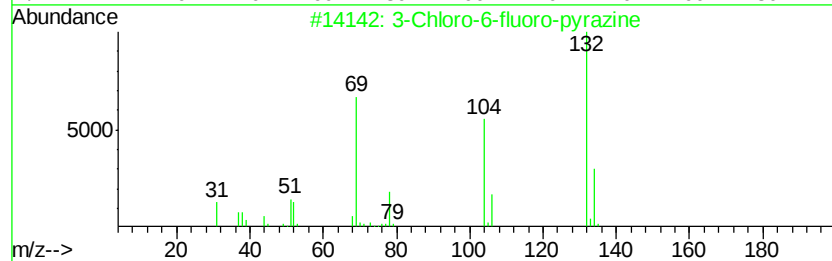
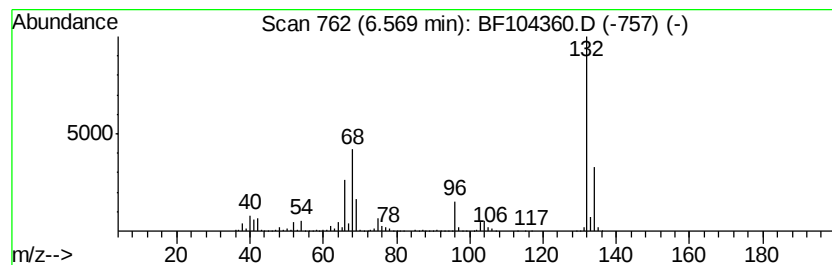
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.62 ng	3205460	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5	Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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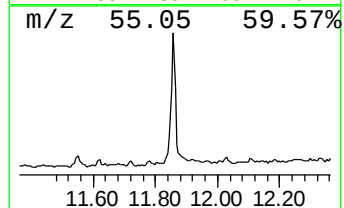
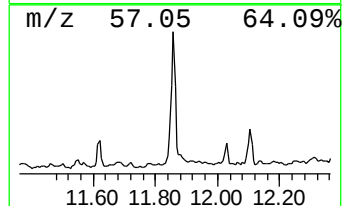
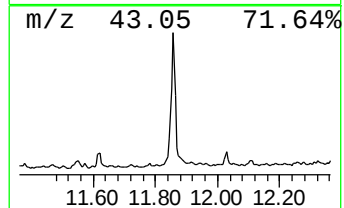
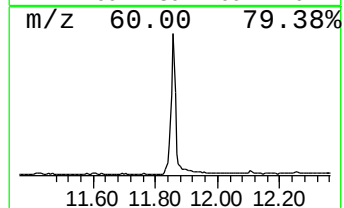
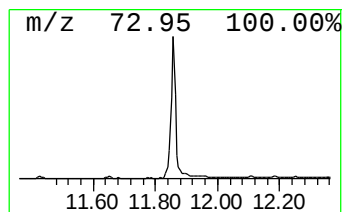
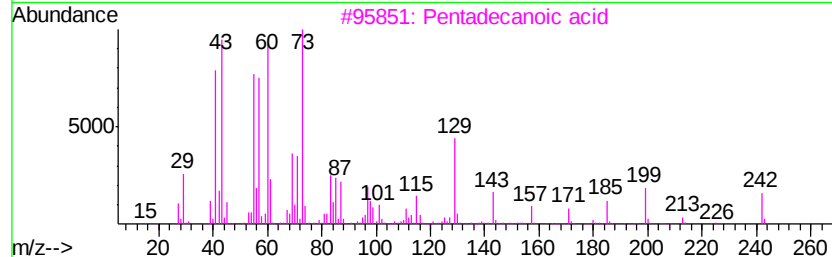
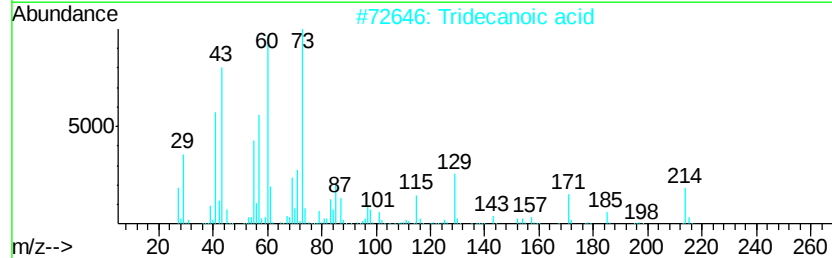
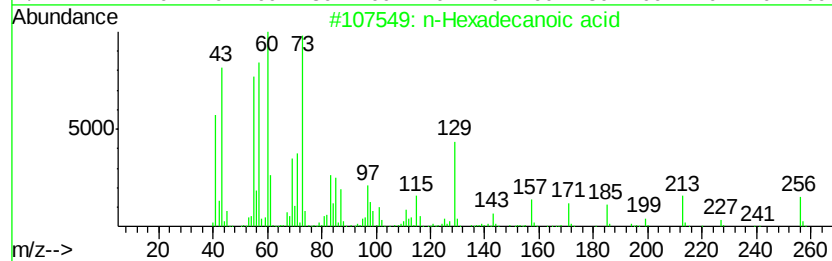
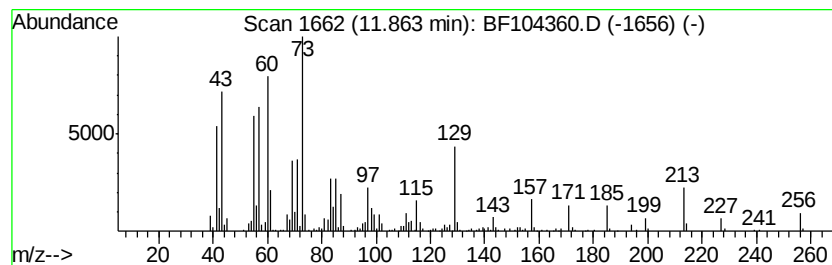
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	11.83 ng	776664	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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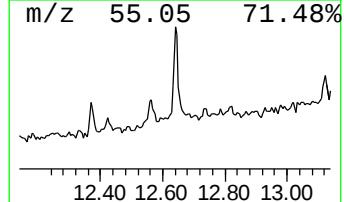
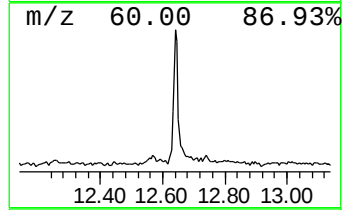
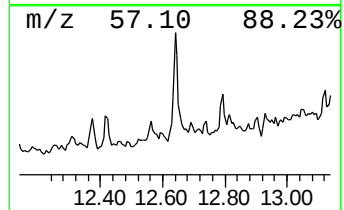
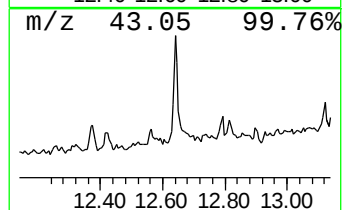
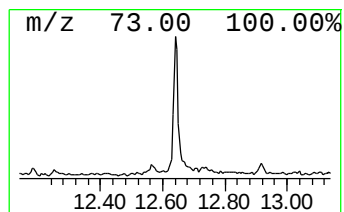
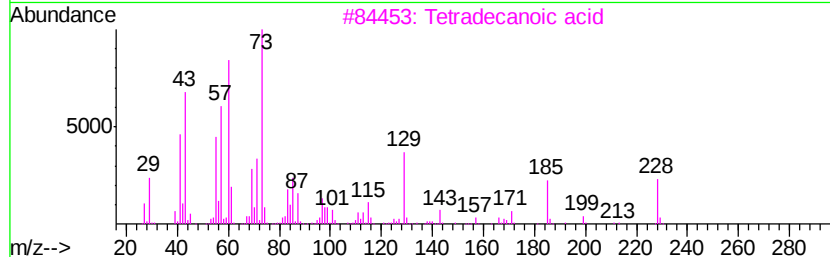
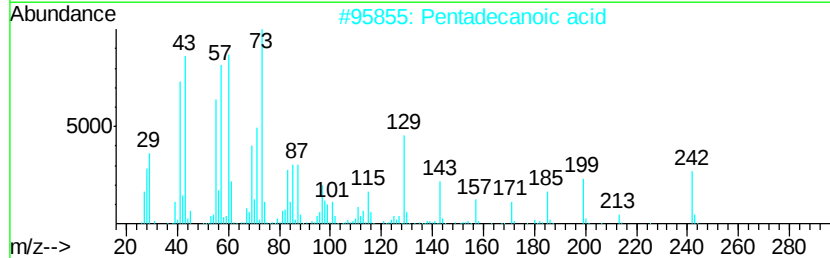
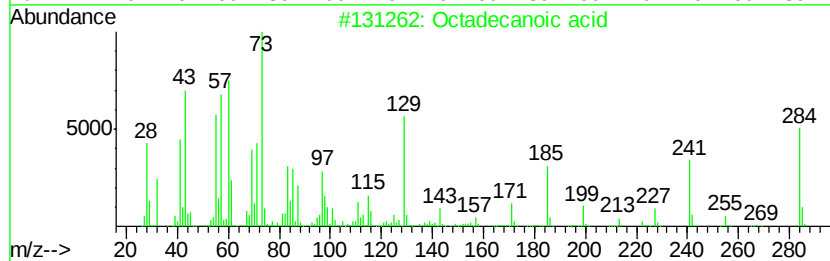
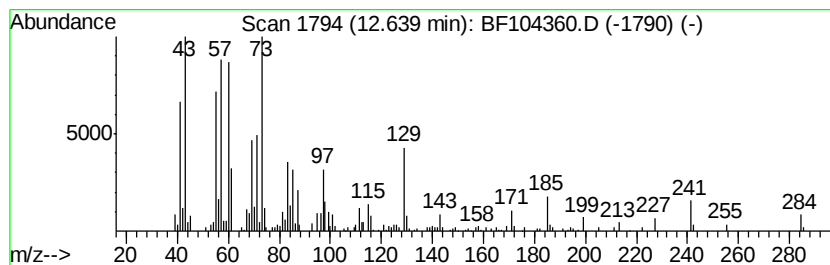
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.64	4.81 ng	315655	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



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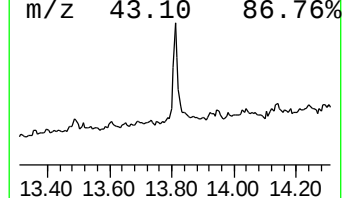
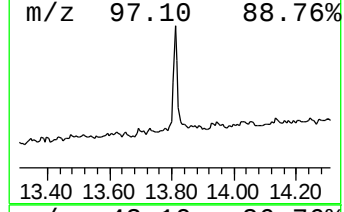
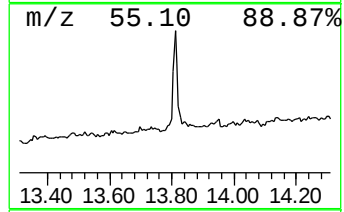
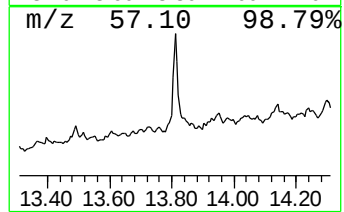
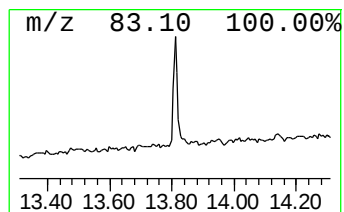
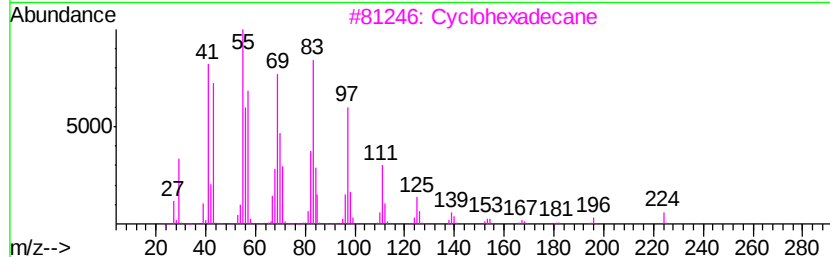
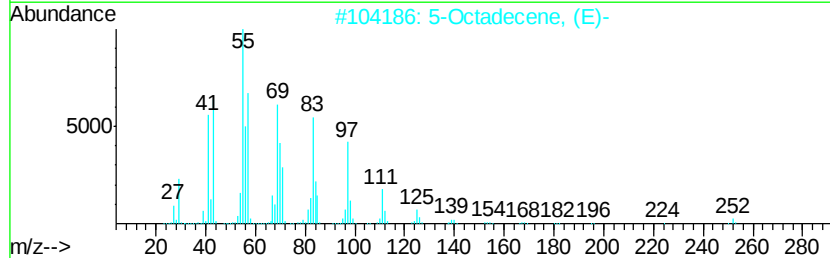
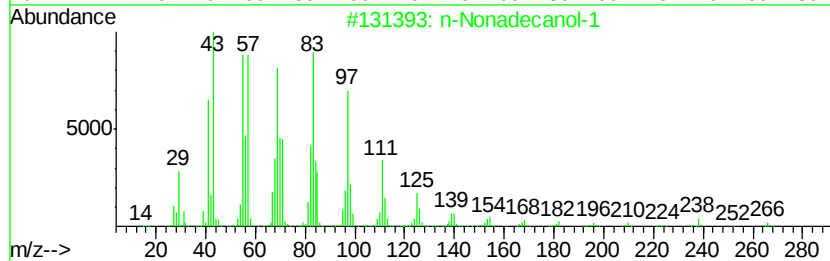
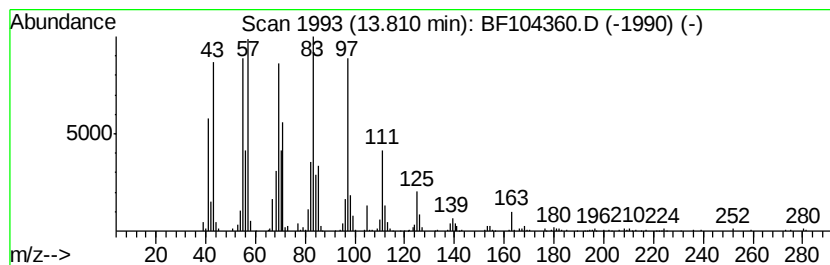
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	8.94 ng	439709	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	Cyclohexadecane	224	C16H32	000295-65-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104360.D
Acq On : 9 Apr 2018 10:01
Operator : JU/SJ
Sample : J2275-01
Misc :
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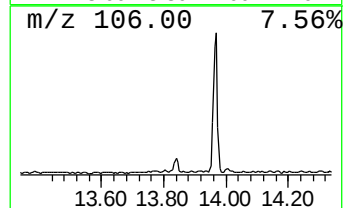
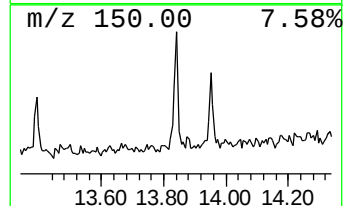
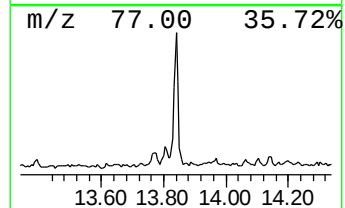
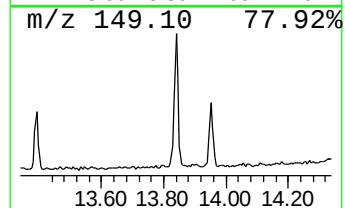
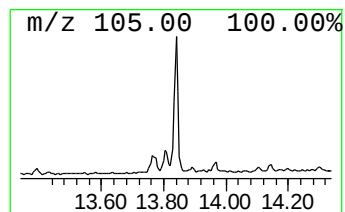
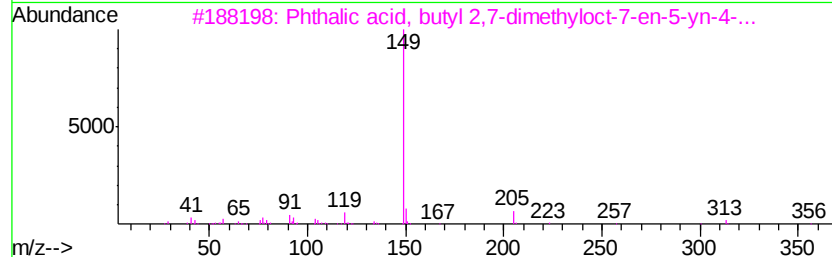
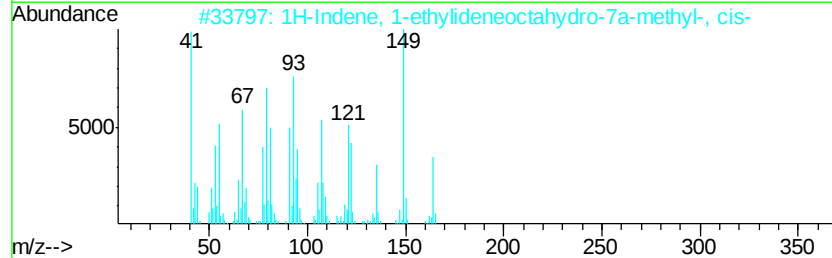
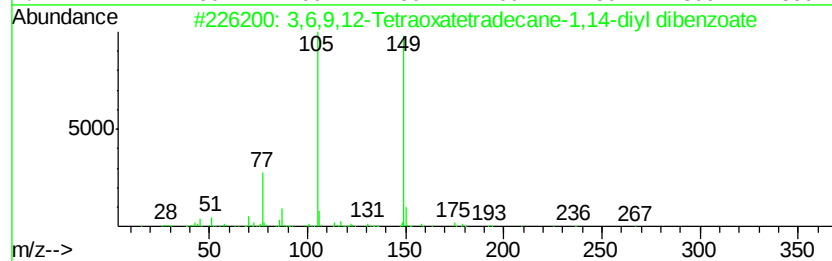
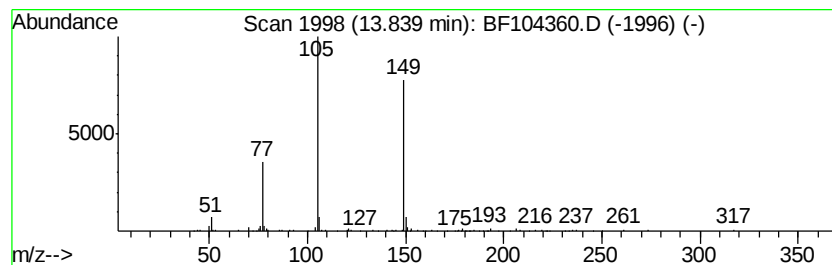
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N-NARANJITO-S002-0001-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3,6,9,12-Tetraoxatetradecan... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.84	2.24 ng	110316	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
2	1H-Indene, 1-ethylideneoctahydro...	164	C12H20	056362-87-9	53
3	Phthalic acid, butyl 2,7-dimethy...	356	C22H28O4	1000315-49-0	50
4	1,2-Benzenedicarboxylic acid, bi...	250	C14H18O4	000605-45-8	47
5	1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104360.D
Acq On : 9 Apr 2018 10:01
Operator : JU/SJ
Sample : J2275-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-NARANJITO-S002-0001-01

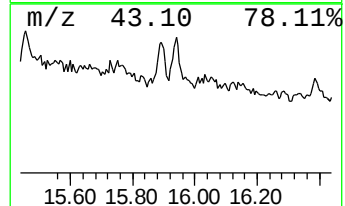
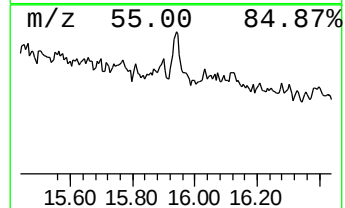
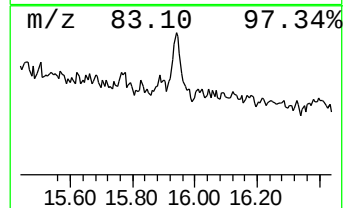
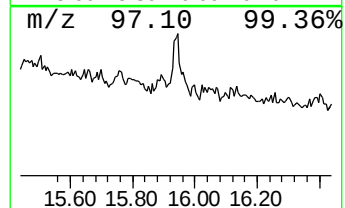
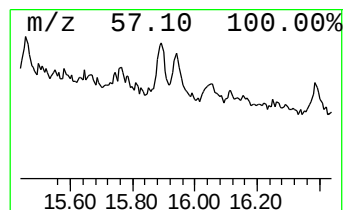
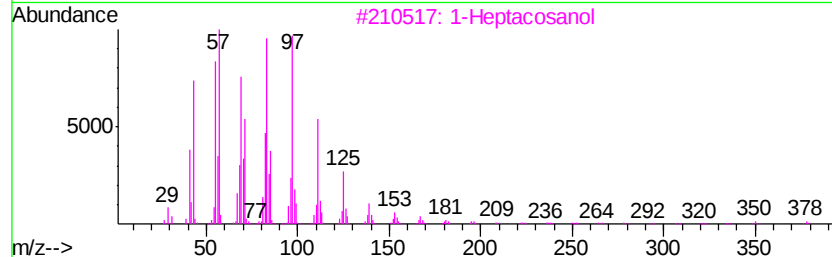
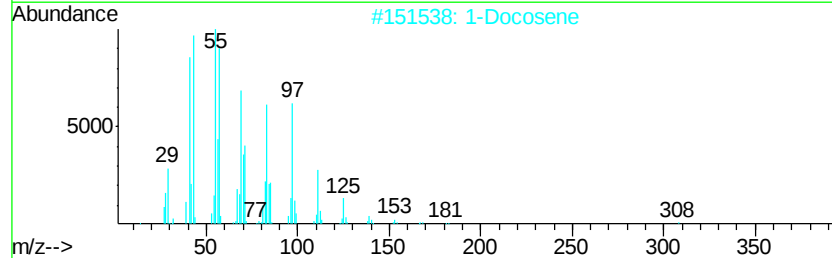
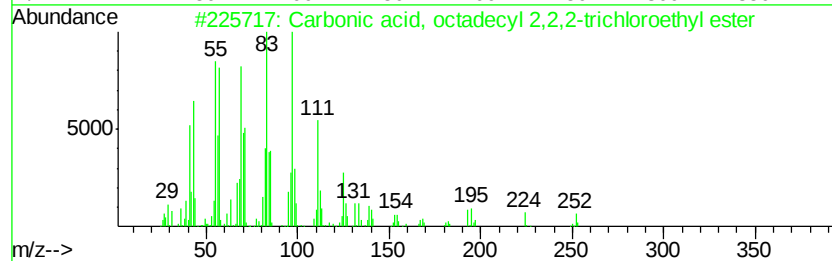
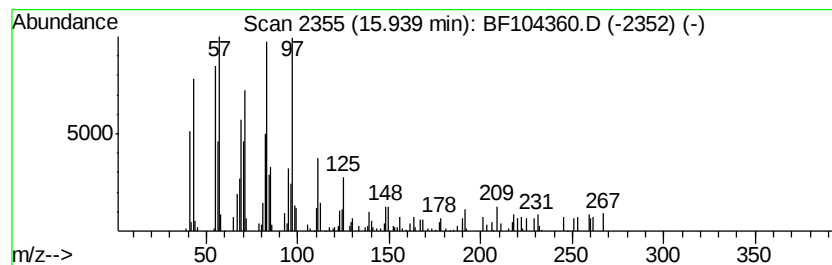
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Carbonic acid, octadecyl 2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.84 ng	161414	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87
2		1-Docosene	308	C22H44	001599-67-3	83
3		1-Heptacosanol	396	C27H56O	002004-39-9	81
4		Trihexadecyl borate	735	C48H99B03	002665-11-4	80
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
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Operator : JU/SJ
Sample : J2275-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-NARANJITO-S002-0001-01

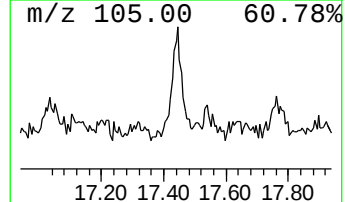
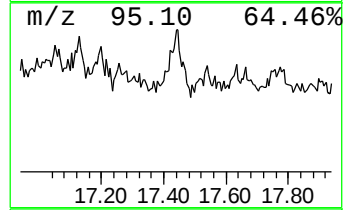
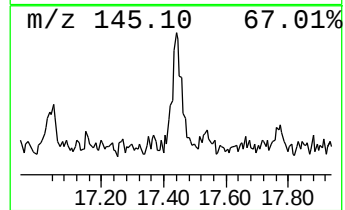
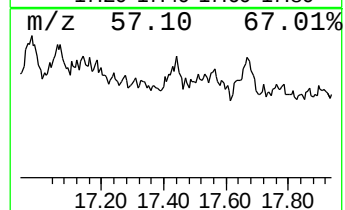
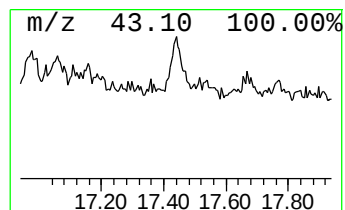
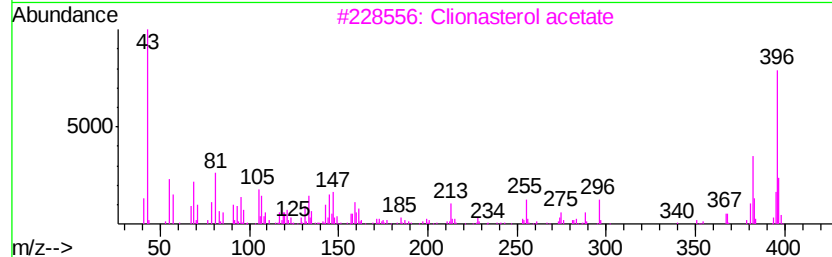
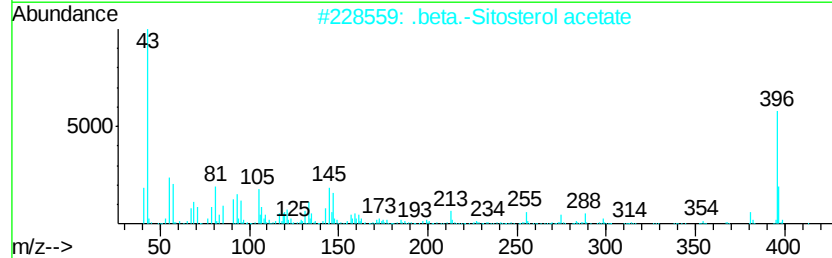
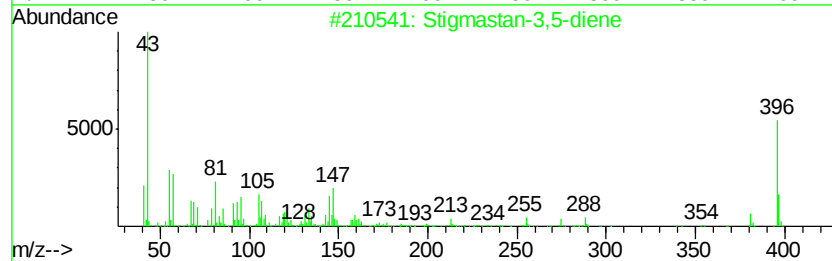
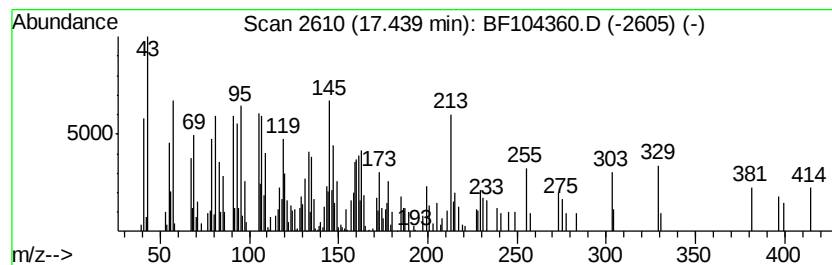
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.44 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	4.56 ng	191456	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	25
2		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	22
3		Clionasterol acetate	456	C31H52O2	004651-54-1	14
4		Pren-5-ene-3,12,14,17,20-pentol...	366	C21H34O5	028417-32-5	11
5		Trilostane	329	C20H27NO3	013647-35-3	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104360.D
Acq On : 9 Apr 2018 10:01
Operator : JU/SJ
Sample : J2275-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	4.0	ng	176896	1	6.80	895135	20.0
unknown6.57	6.57	71.6	ng	3205460	1	6.80	895135	20.0
n-Hexadecanoic acid	11.86	11.8	ng	776664	4	11.33	1312940	20.0
Octadecanoic acid	12.64	4.8	ng	315655	4	11.33	1312940	20.0
n-Nonadecanol-1	13.81	8.9	ng	439709	5	13.97	983326	20.0
3,6,9,12-Tetraoxa...	13.84	2.2	ng	110316	5	13.97	983326	20.0
Carbonic acid, oc...	15.94	3.8	ng	161414	6	15.42	840507	20.0
unknown17.44	17.44	4.6	ng	191456	6	15.42	840507	20.0