

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
 Data File : BF104363.D
 Acq On : 9 Apr 2018 11:20
 Operator : JU/SJ
 Sample : J2275-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-NARANJITO-S002-0001-02

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	124930	165772	4.83%	0.510%
2	5.416	560	566	569	rBV	3085319	3194752	93.01%	9.837%
3	5.745	618	622	628	rVB	63481	56008	1.63%	0.172%
4	6.434	732	739	742	rBV	2974971	3210240	93.46%	9.885%
5	6.569	757	762	766	rBV	3149704	3291062	95.82%	10.134%
6	6.804	798	802	805	rVB	1138018	925233	26.94%	2.849%
7	6.957	824	828	832	rVB	2616647	2468185	71.86%	7.600%
8	7.369	892	898	901	rBV	2150468	2056779	59.88%	6.333%
9	7.439	904	910	914	rVB	39587	38184	1.11%	0.118%
10	8.086	1016	1020	1023	rBV	1568680	1255876	36.56%	3.867%
11	9.163	1198	1203	1206	rBV	3691644	3434761	100.00%	10.576%
12	9.557	1266	1270	1273	rBV	522126	409768	11.93%	1.262%
13	9.769	1304	1306	1310	rVB	94755	79192	2.31%	0.244%
14	9.839	1314	1318	1322	rVV2	1500544	1396787	40.67%	4.301%
15	10.245	1384	1387	1389	rBV	41182	37052	1.08%	0.114%
16	10.275	1389	1392	1395	rVB	120674	95403	2.78%	0.294%
17	10.492	1424	1429	1432	rBV	44088	51188	1.49%	0.158%
18	10.633	1447	1453	1456	rBV	2325691	2245010	65.36%	6.913%
19	10.745	1469	1472	1481	rVB	116471	122294	3.56%	0.377%
20	11.192	1546	1548	1551	rBV2	80936	72081	2.10%	0.222%
21	11.327	1567	1571	1575	rBV	1591568	1349748	39.30%	4.156%
22	11.551	1604	1609	1611	rBV4	37694	42224	1.23%	0.130%
23	11.622	1618	1621	1624	rBV	57800	43176	1.26%	0.133%
24	11.686	1629	1632	1635	rVB	34230	40062	1.17%	0.123%
25	11.722	1635	1638	1643	rBV3	34205	40277	1.17%	0.124%
26	11.857	1657	1661	1665	rBV	567176	543401	15.82%	1.673%
27	12.027	1688	1690	1693	rBV	49941	44365	1.29%	0.137%
28	12.374	1746	1749	1753	rBV3	41008	41503	1.21%	0.128%
29	12.427	1754	1758	1761	rVV3	44864	64424	1.88%	0.198%
30	12.645	1792	1795	1799	rBV	95644	110940	3.23%	0.342%
31	12.921	1837	1842	1845	rBV	3025485	2962165	86.24%	9.121%
32	13.816	1990	1994	1997	rBV	480640	488031	14.21%	1.503%
33	13.968	2017	2020	2024	rVB	944021	874822	25.47%	2.694%
34	15.433	2265	2269	2274	rBV	686067	847008	24.66%	2.608%

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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	15.951	2355	2357	2365	rVB4	95433	154844	4.51%	0.477%
36	17.456	2609	2613	2622	rVB4	106581	223539	6.51%	0.688%

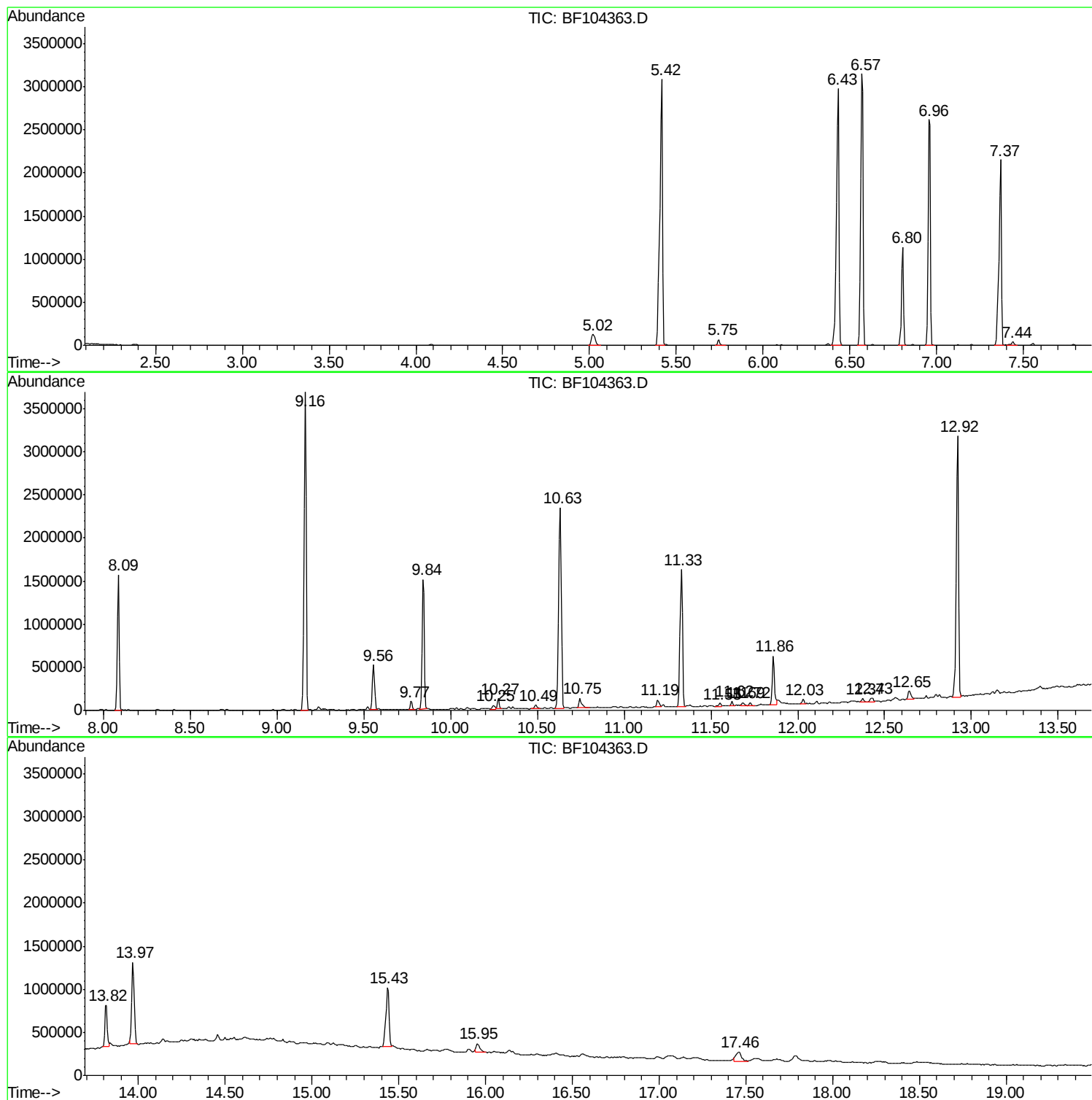
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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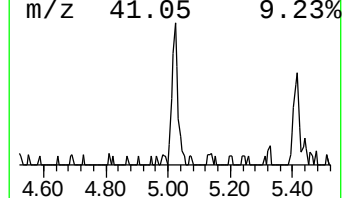
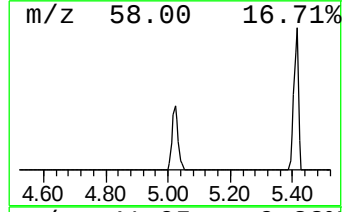
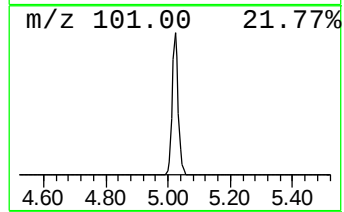
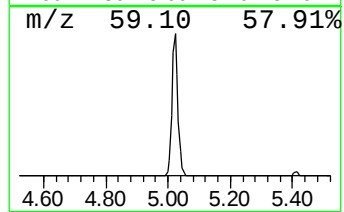
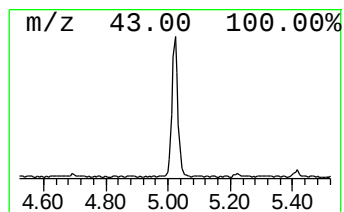
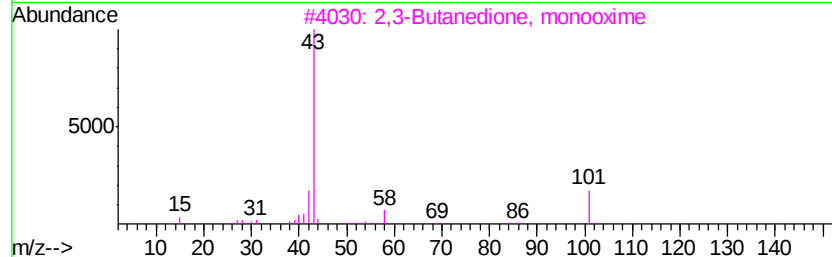
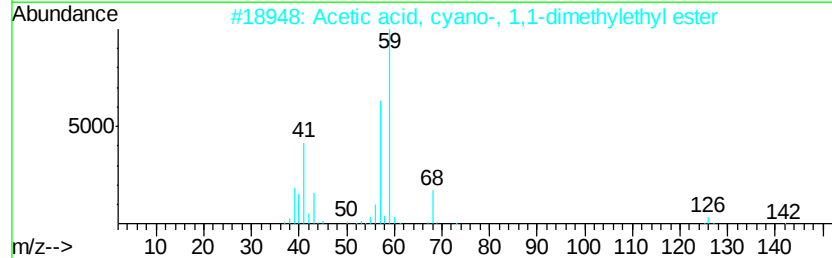
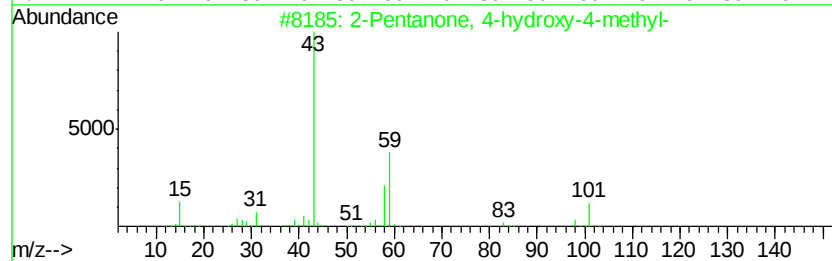
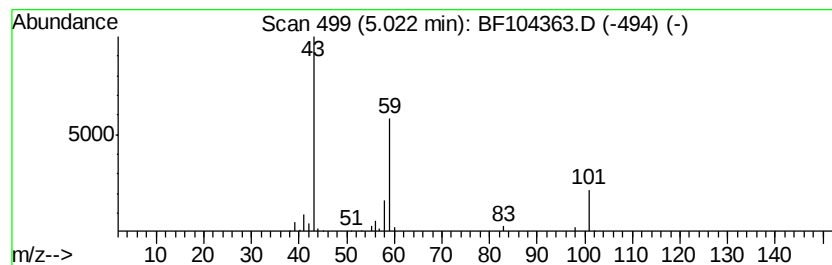
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.58 ng	165772	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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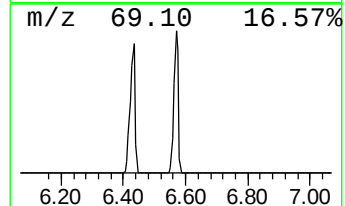
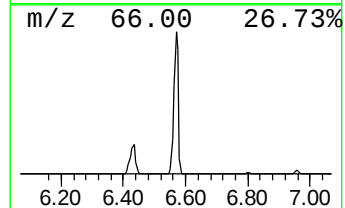
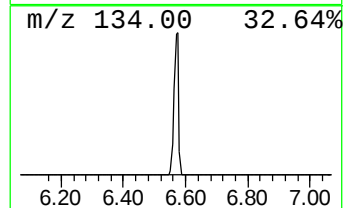
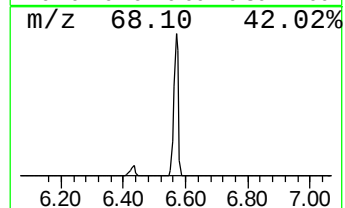
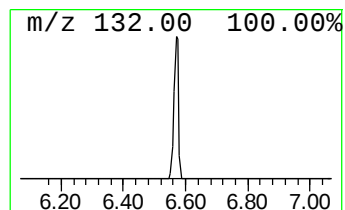
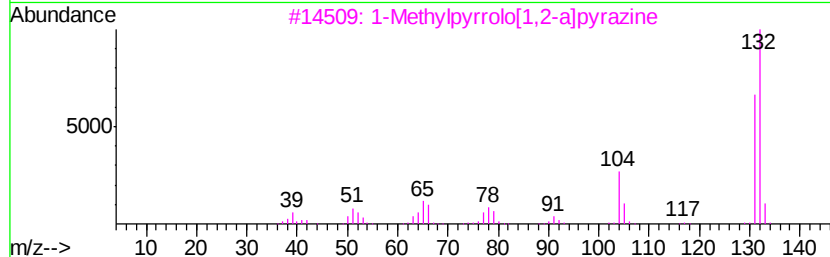
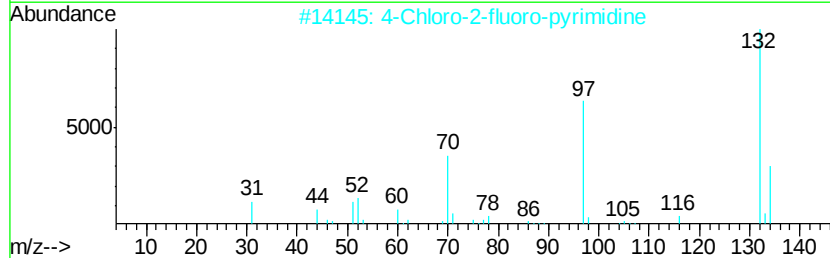
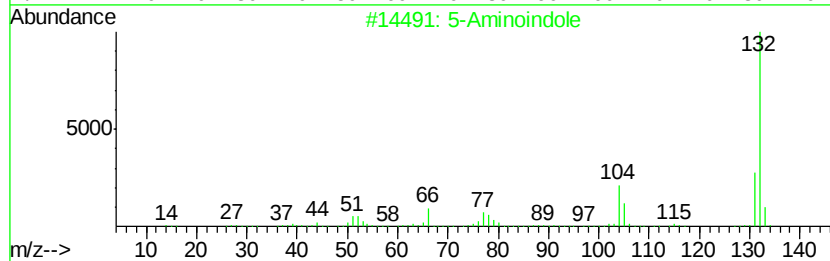
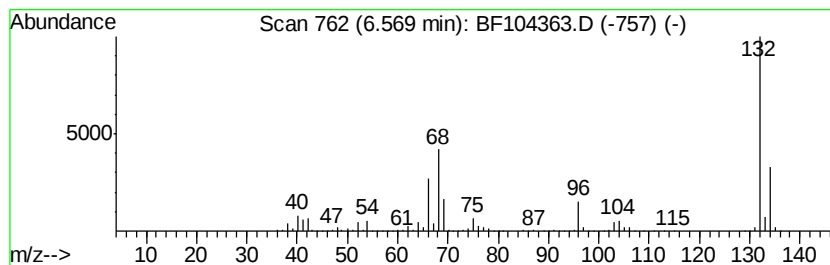
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.14 ng	3291060	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminoindole	132	C8H8N2	005192-03-0	12
2			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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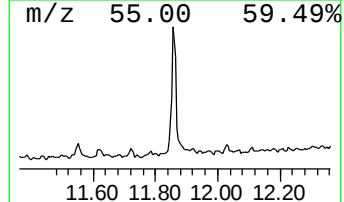
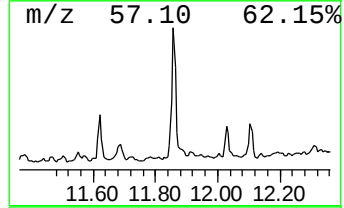
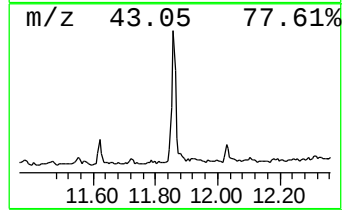
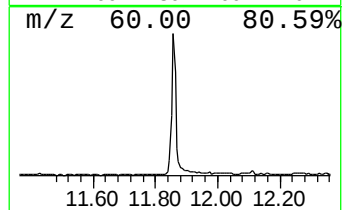
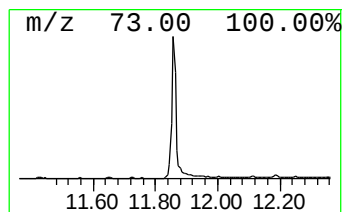
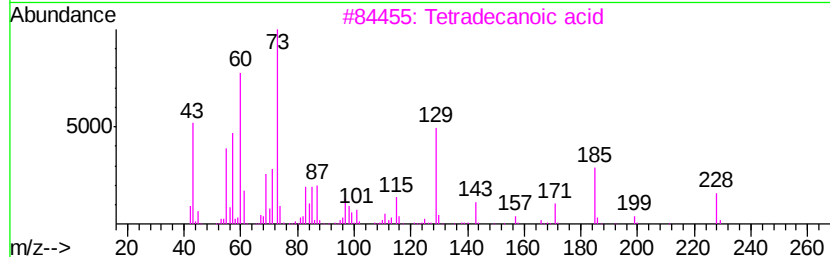
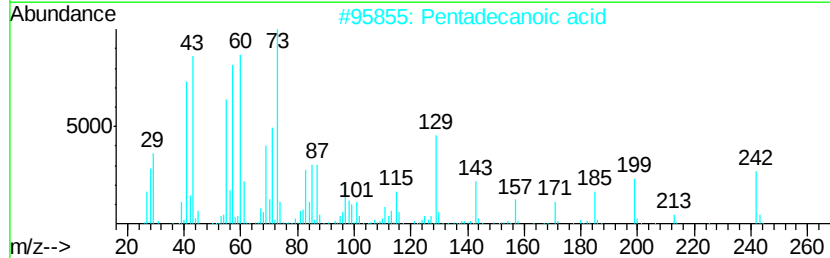
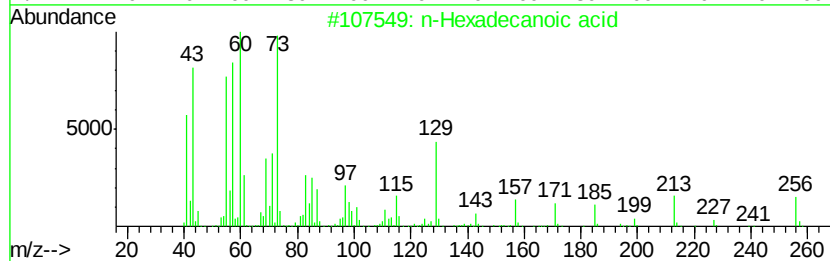
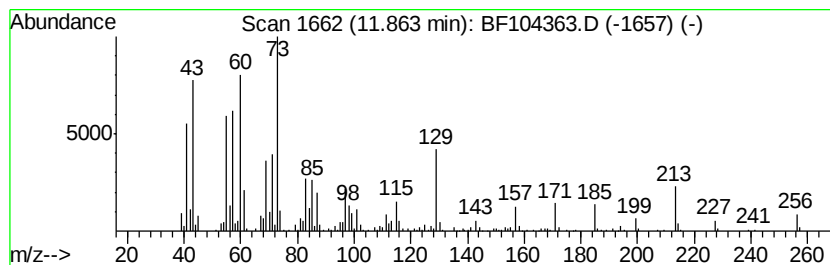
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	8.05 ng	543401	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		Nonanoic acid	158	C9H18O2	000112-05-0	43



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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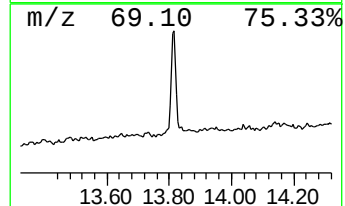
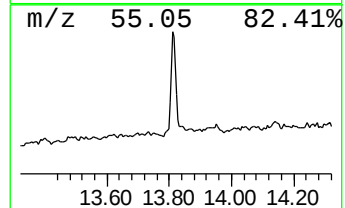
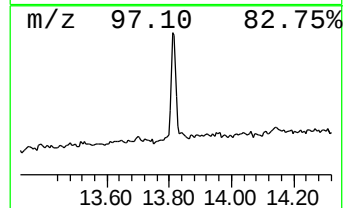
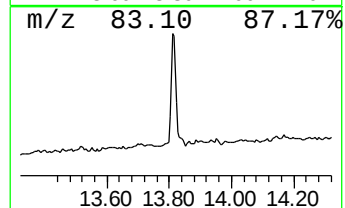
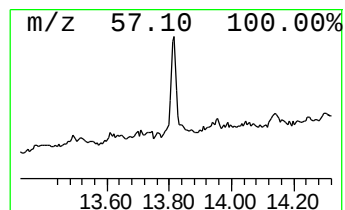
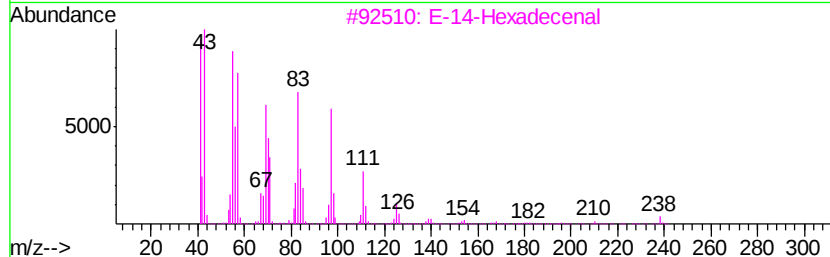
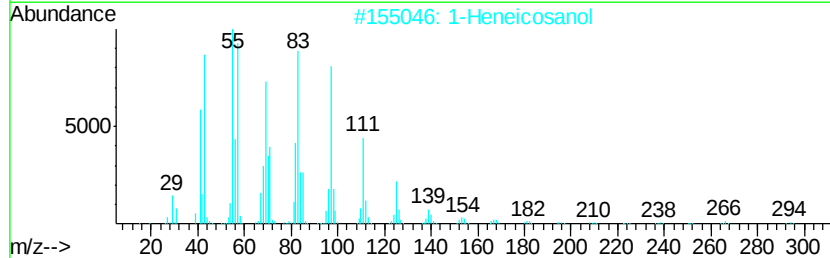
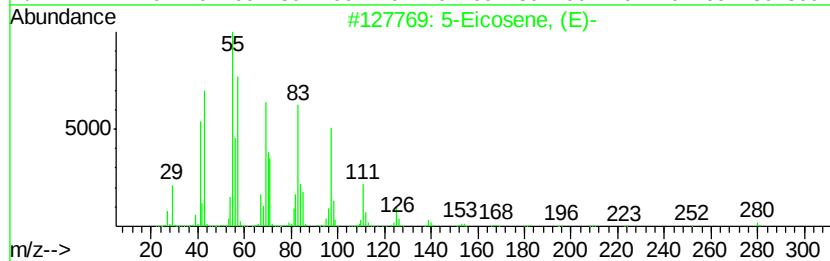
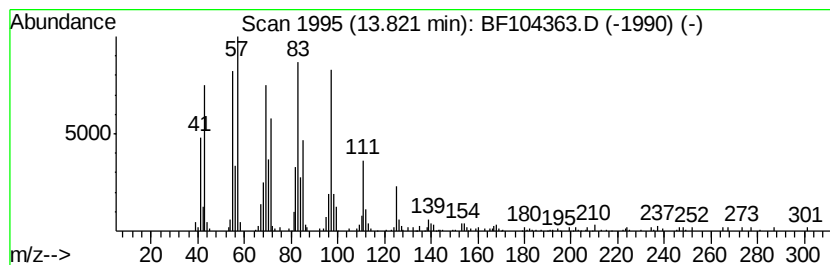
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	11.16 ng	488031	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	E-14-Hexadecenal		238	C16H30O	330207-53-9	95
4	Cyclopentadecane		210	C15H30	000295-48-7	94
5	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	94



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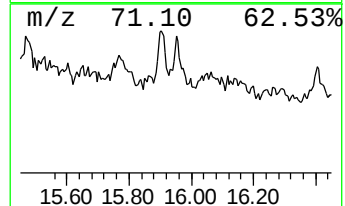
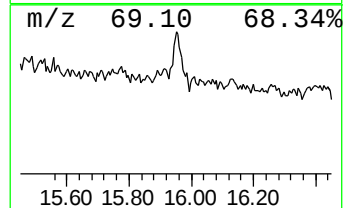
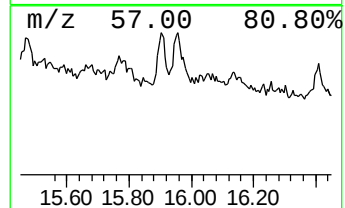
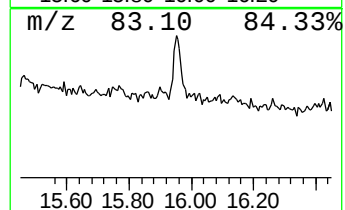
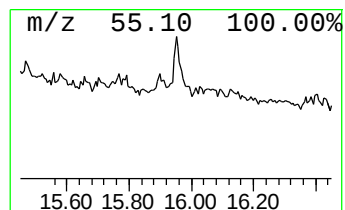
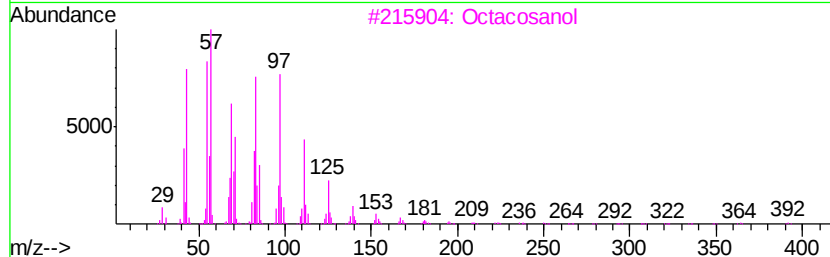
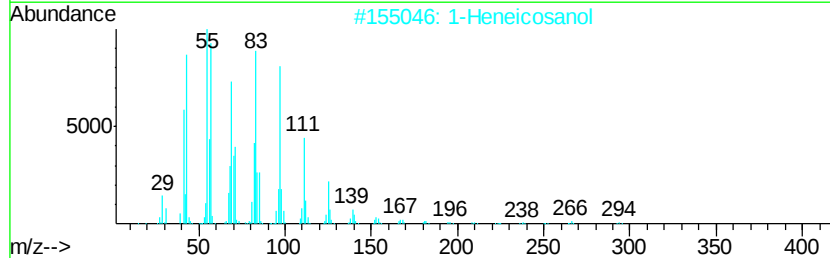
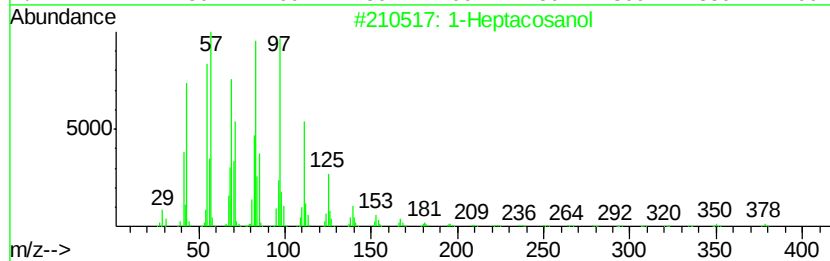
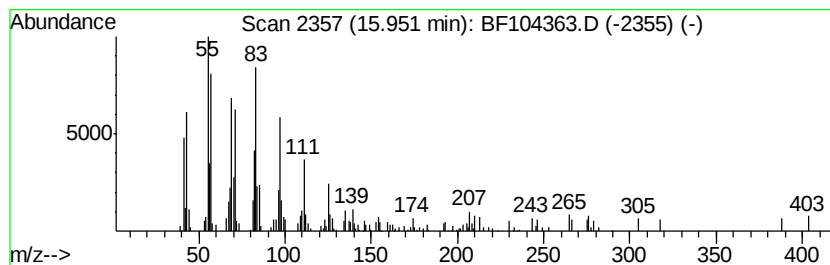
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Peak Number 6 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.95	3.66 ng	154844	Perylene-d12	15.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
Data File : BF104363.D
Acq On : 9 Apr 2018 11:20
Operator : JU/SJ
Sample : J2275-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-NARANJITO-S002-0001-02

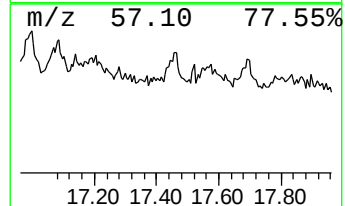
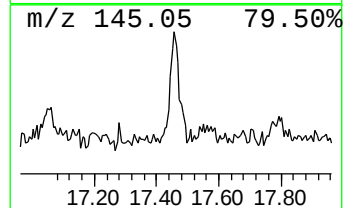
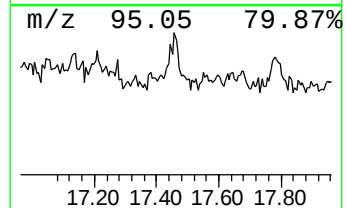
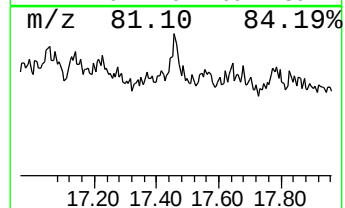
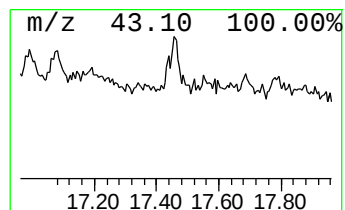
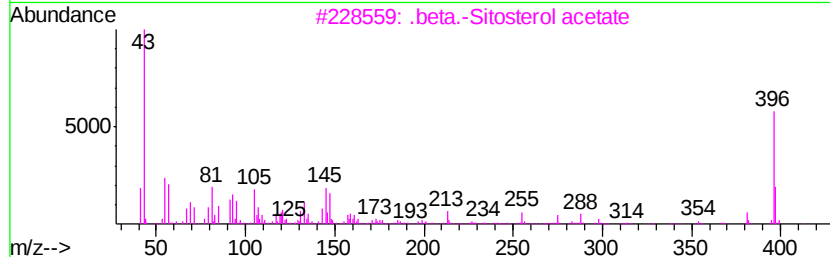
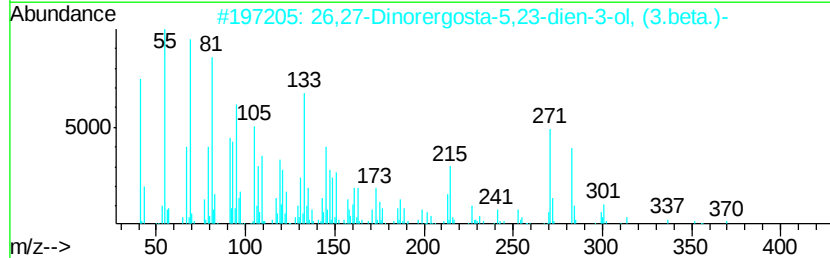
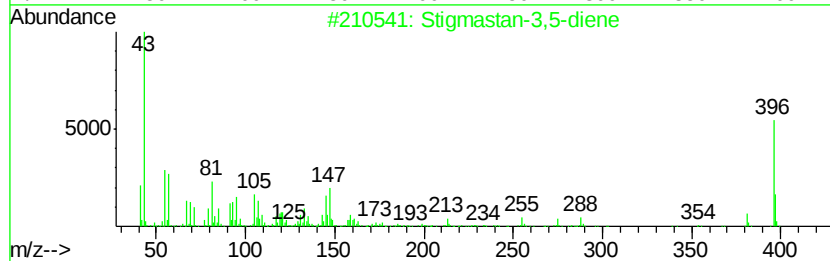
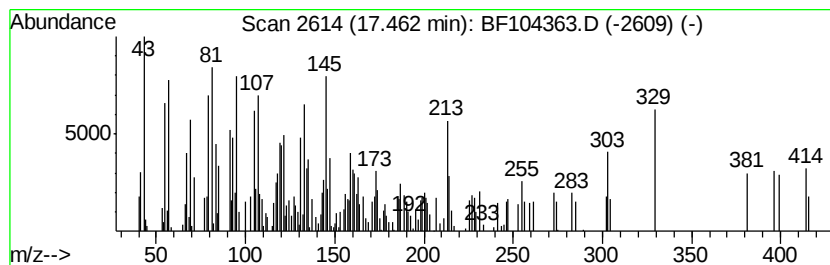
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.46 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	5.28 ng	223539	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	35
2		26,27-Dinorergosta-5,23-dien-3-o...	370	C26H42O	035882-88-3	23
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	17
4		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	16
5		5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	16



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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-NARANJITO-S002-0001-02

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	3.6	ng	165772	1	6.80	925233	20.0
unknown6.57	6.57	71.1	ng	3291060	1	6.80	925233	20.0
n-Hexadecanoic acid	11.86	8.1	ng	543401	4	11.33	1349750	20.0
5-Eicosene, (E)-	13.82	11.2	ng	488031	5	13.97	874822	20.0
1-Heptacosanol	15.95	3.7	ng	154844	6	15.43	847008	20.0
unknown17.46	17.46	5.3	ng	223539	6	15.43	847008	20.0