LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104369.D
Acq On : 9 Apr 2018 13:58
Operator : JU/SJ
Sample : J2237-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SC-1

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.516	409	413	417	rVB	39469	43134	1.22%	0.146%
2	5.022	490	499	508	rBV	115239	159055	4.49%	0.537%
3	5.416	560	566	569	rBV	3022592	3153941	89.12%	10.658%
4	6.434	732	739	742	rBV	2965176	3141729	88.77%	10.617%
5	6.575	757	763	766	rBV	3131334	3204131	90.54%	10.828%
6	6.804	798	802	805	rVB	989472	777346	21.97%	2.627%
7	6.963	824	829	832	rVB	2583563	2495983	70.53%	8.435%
8	7.369	892	898	901	rBV	2055014	1980856	55.97%	6.694%
9	8.086	1013	1020	1023	rBV	1298655	1061251	29.99%	3.586%
10	9.163	1198	1203	1206	rBV	3728960	3539002	100.00%	11.959%
11	9.557	1266	1270	1273	rBV	282614	231208	6.53%	0.781%
12	9.769	1304	1306	1310	rVB	49030	40539	1.15%	0.137%
13	9.839	1314	1318	1322	rVB	1267926	1138639	32.17%	3.848%
14	10.275	1389	1392	1394	rVB	83623	67404	1.90%	0.228%
15	10.633	1447	1453	1456	rBV	2132713	2129185	60.16%	7.195%
16	10.745	1469	1472	1478	rBV	90869	91863	2.60%	0.310%
17	11.192	1545	1548	1551	rBV	41232	38943	1.10%	0.132%
18	11.327	1567	1571	1574	rBV	1254418	1054099	29.79%	3.562%
19	11.857	1657	1661	1673	rBV2	265482	253909	7.17%	0.858%
20	12.816	1821	1824	1828	rVB	46737	37119	1.05%	0.125%
21	12.921	1837	1842	1845	rBV	2837042	2752075	77.76%	9.300%
22	13.810	1990	1993	2009	rBV	412048	393557	11.12%	1.330%
23	13.968	2014	2020	2024	rBV	825841	735096	20.77%	2.484%
24	14.451	2098	2102	2107	rBV4	31723	40361	1.14%	0.136%
25	14.827	2162	2166	2170	rVB	116561	113110	3.20%	0.382%
26	15.427	2263	2268	2273	rBV	639429	760381	21.49%	2.570%
27	15.945	2351	2356	2364	rBV5	55811	89675	2.53%	0.303%
28	17.445	2606	2611	2618	rVB7	33920	68142	1.93%	0.230%

Sum of corrected areas: 29591733

LSC Report - Integrated Chromatogram

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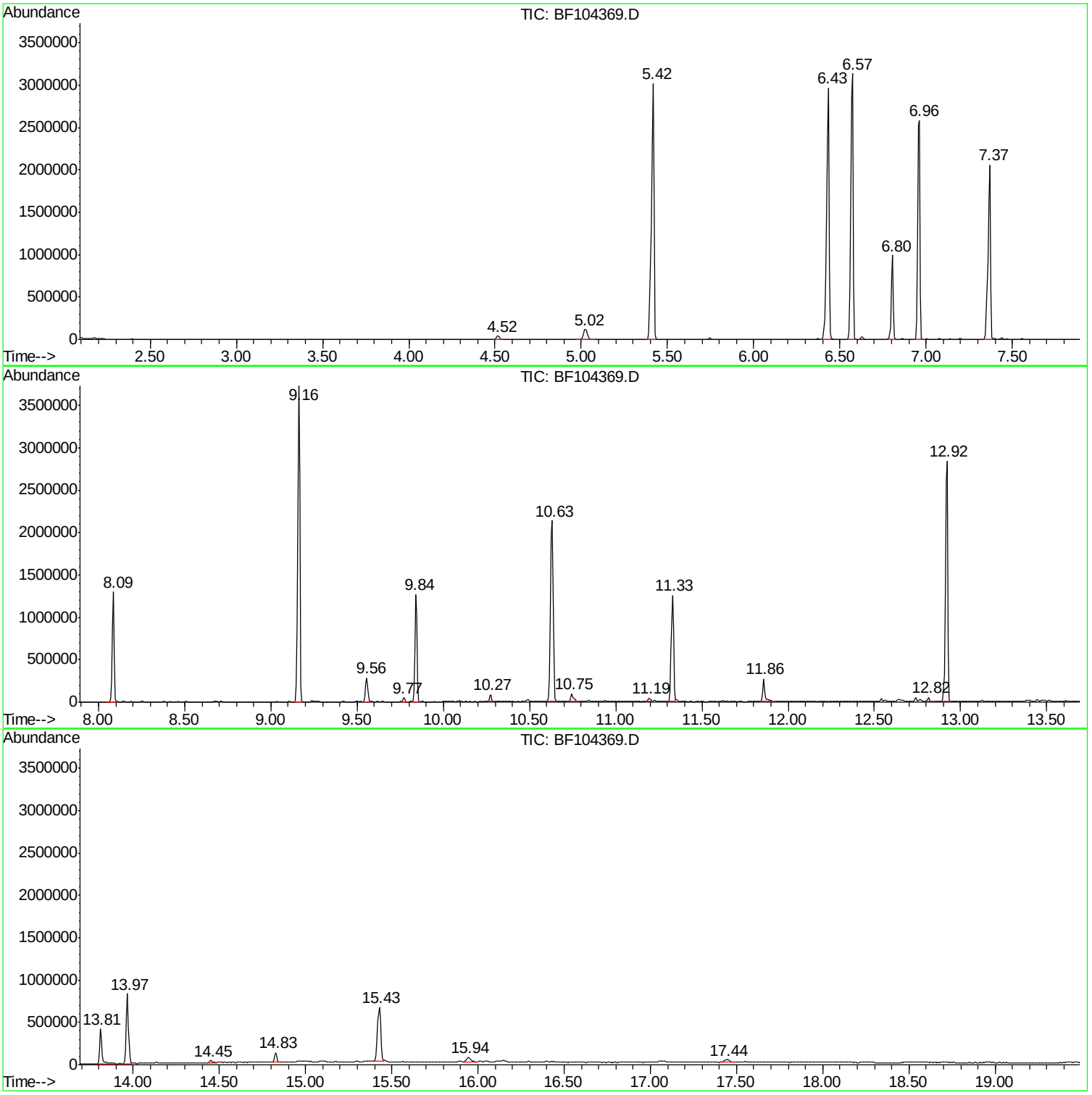
Instrument : BNA_F
ClientSampleId : SC-1

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



Library Search Compound Report

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Data File : BF104369.D
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Operator : JU/SJ
Sample : J2237-01
Misc :
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Instrument : BNA_F
ClientSampleId : SC-1

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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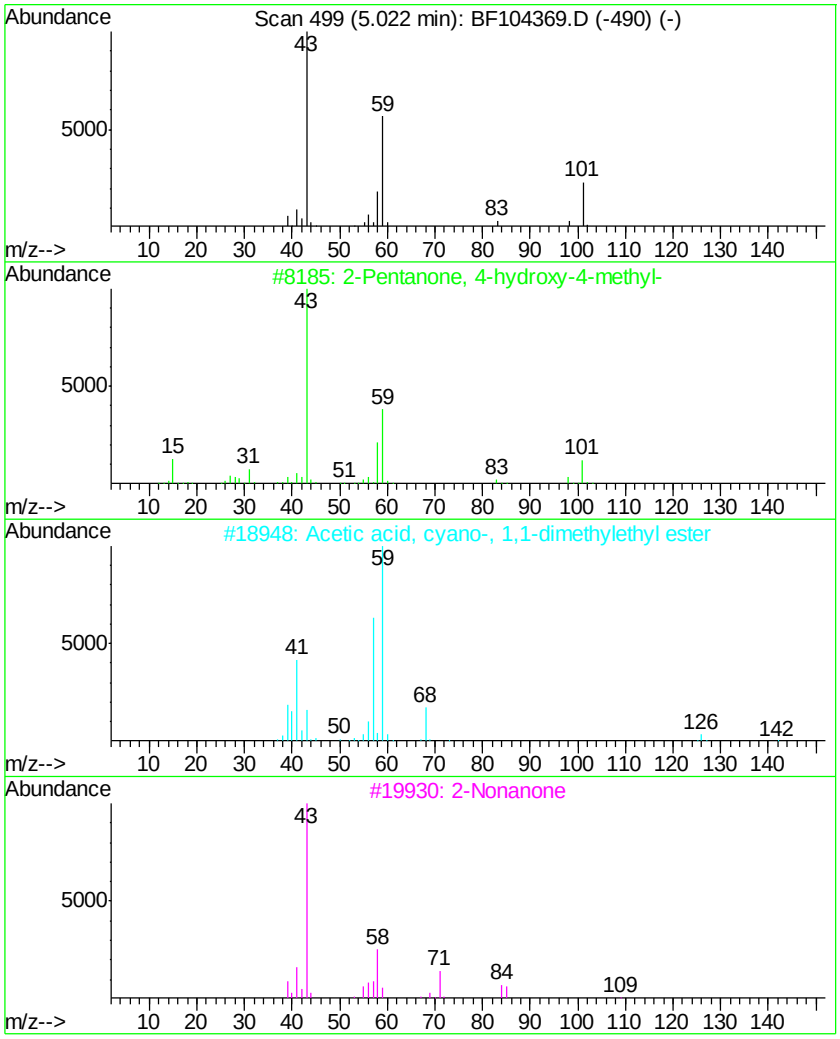
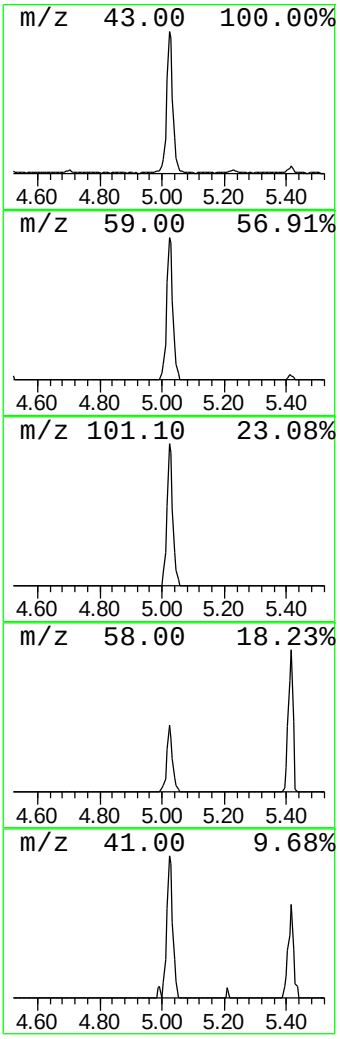
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.09 ng	159055	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2-Nonanone	142	C9H18O	000821-55-6	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
ClientSampleId : SC-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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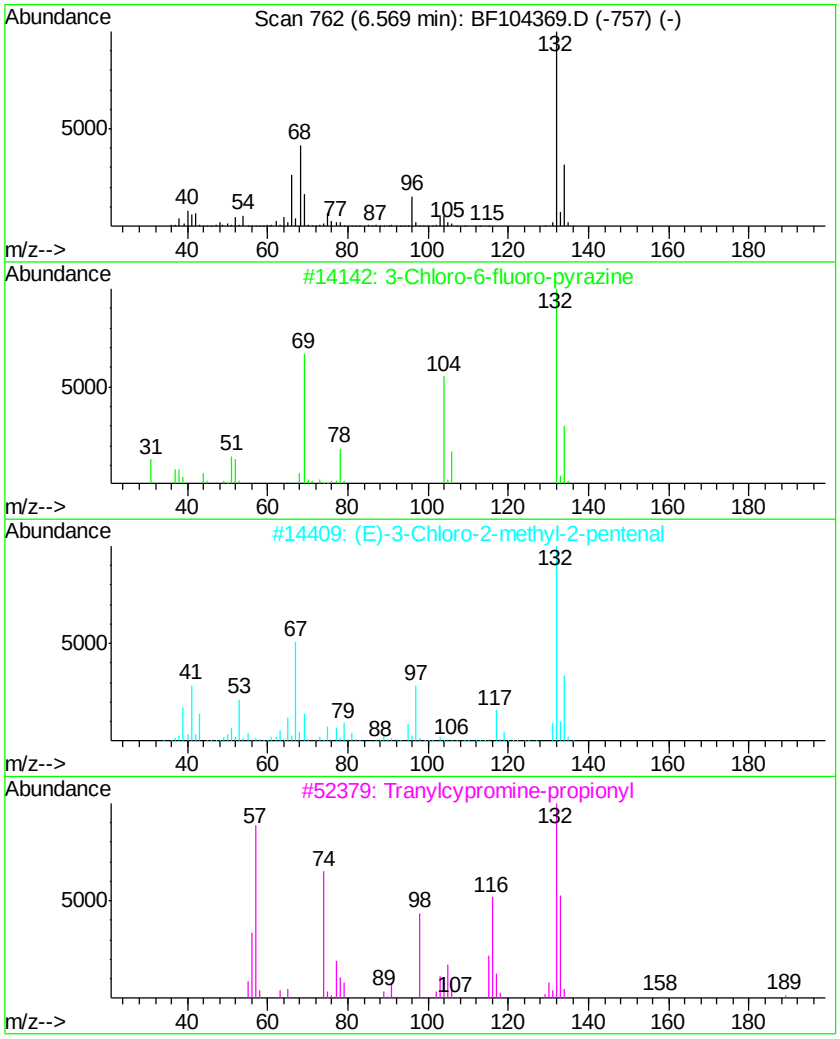
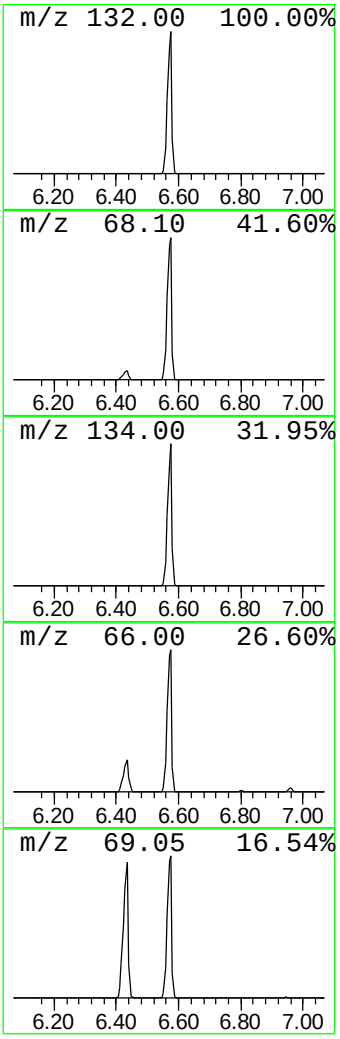
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	82.44 ng	3204130	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : J2237-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SC-1

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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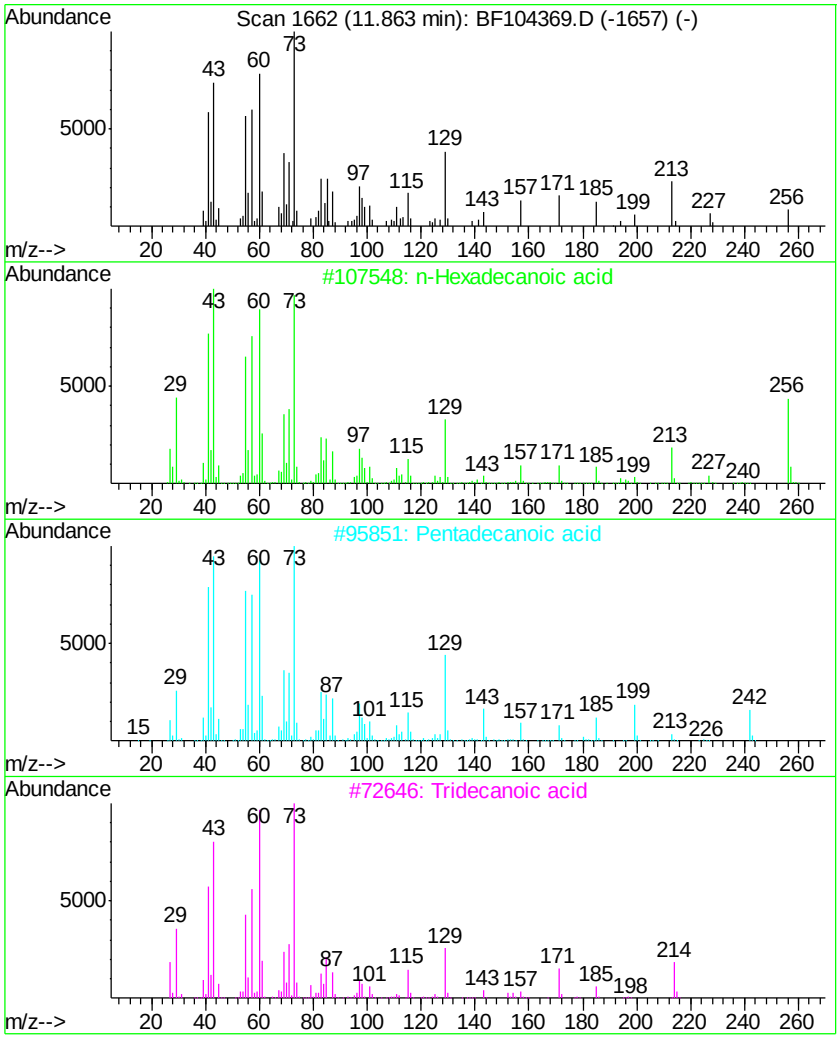
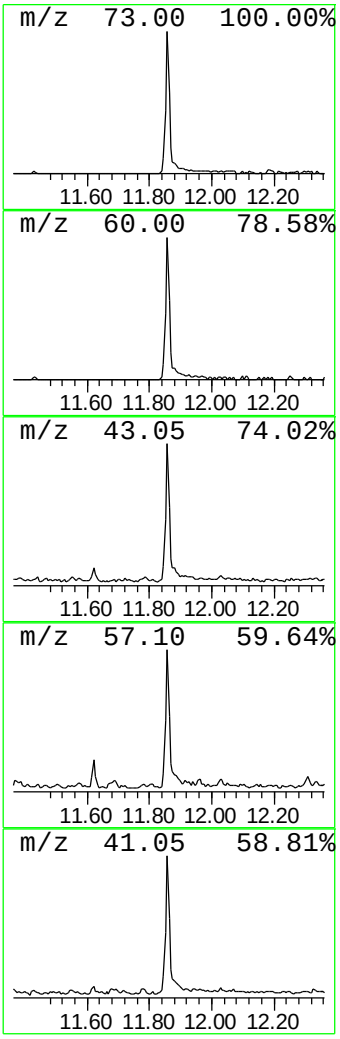
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.82 ng	253909	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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Sample : J2237-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
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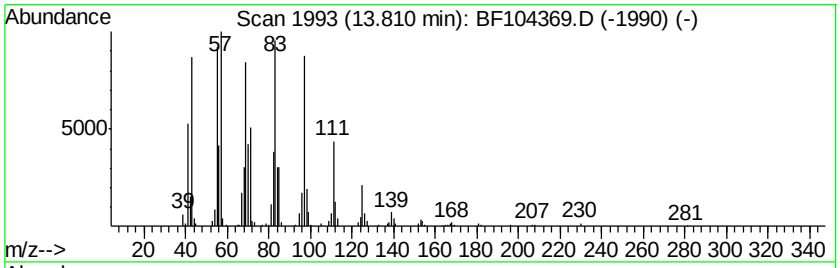
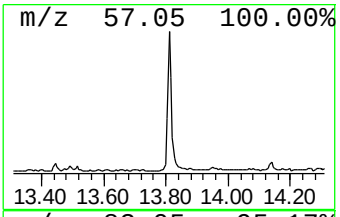
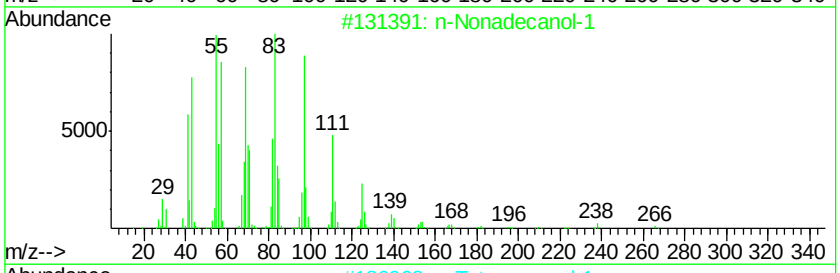
Peak Number 5 n-Nonadecanol-1 Concentration Rank 3

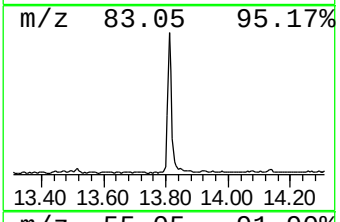
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	10.71 ng	393557	Chrysene-d12	13.97

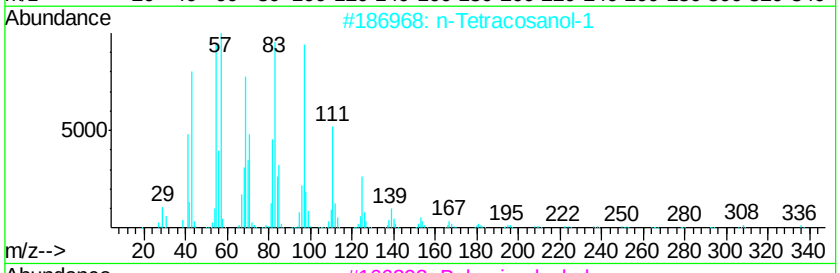
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94

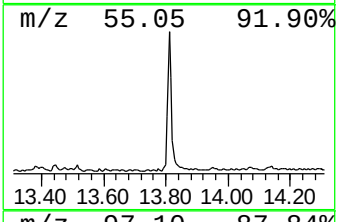


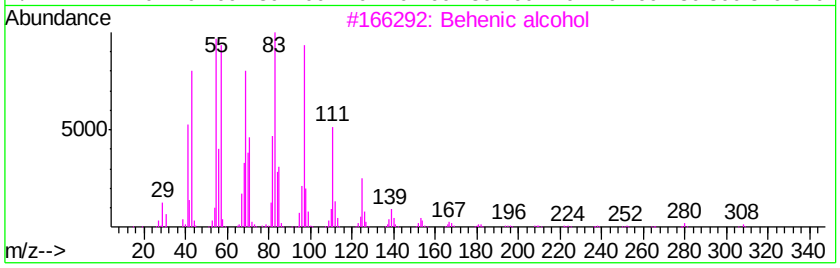


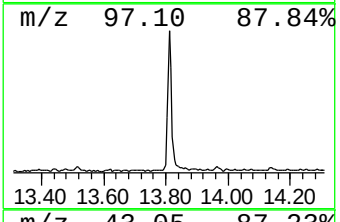


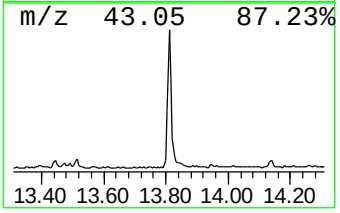












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

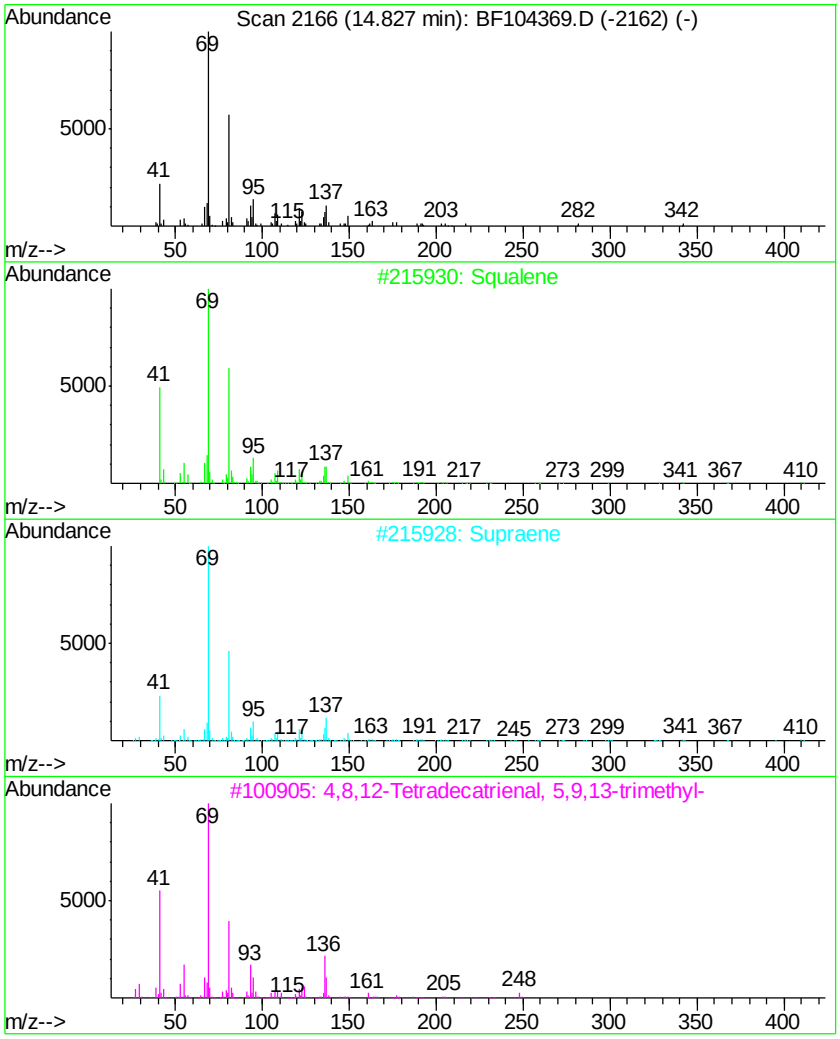
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

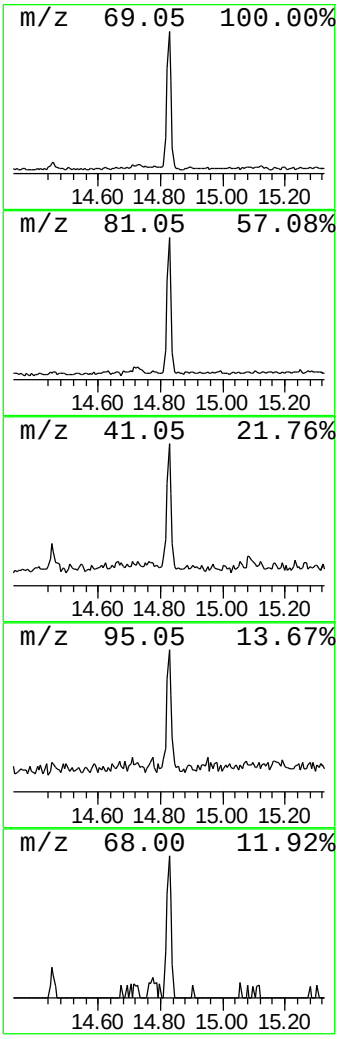
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.98 ng	113110	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





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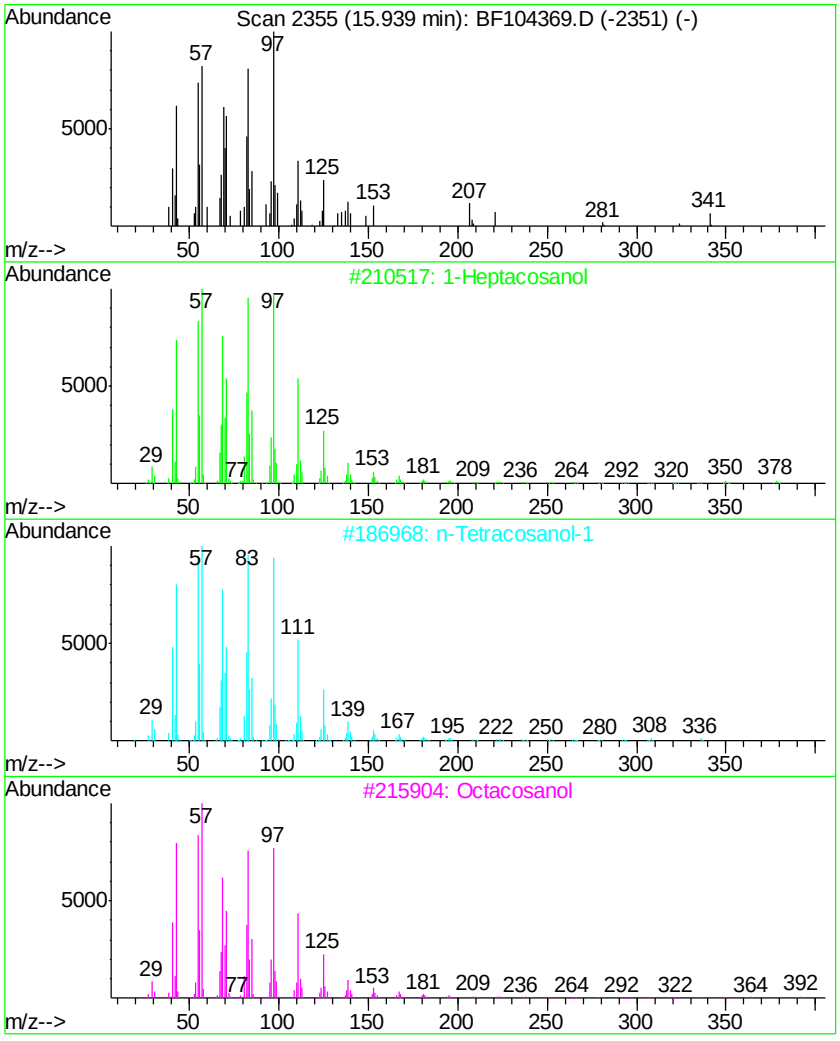
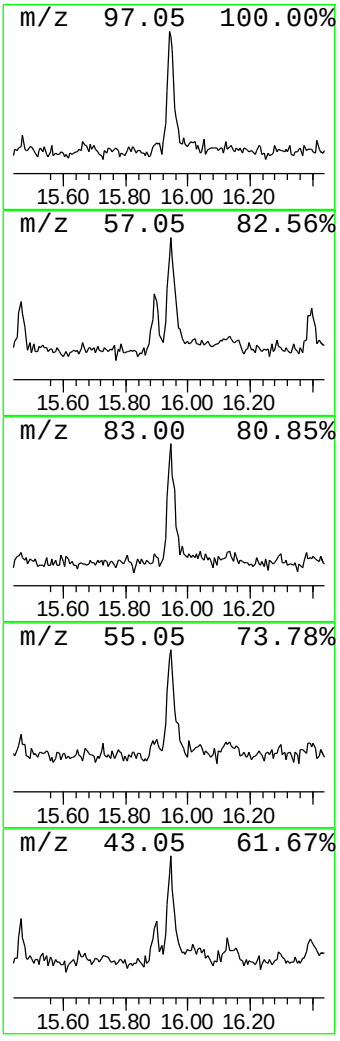
Peak Number 7 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.36 ng	89675	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Octacosanol	410	C28H58O	000557-61-9	94
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	4.1	ng	159055	1	6.80	777346	20.0
unknown6.57	6.57	82.4	ng	3204130	1	6.80	777346	20.0
n-Hexadecanoic acid	11.86	4.8	ng	253909	4	11.33	1054100	20.0
n-Nonadecanol-1	13.81	10.7	ng	393557	5	13.97	735096	20.0
Squalene	14.83	3.0	ng	113110	6	15.43	760381	20.0
1-Heptacosanol	15.94	2.4	ng	89675	6	15.43	760381	20.0