LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098861.D
Acq On : 27 Sep 2017 14:17
Operator : SJ/JU
Sample : I5434-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : UT5400534

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-BF092317.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	2.222	19	23	33	rVB	119403	178270	4.75%	0.528%
2	5.146	516	520	532	rVB	602707	794020	21.14%	2.352%
3	5.540	581	587	590	rBV	3277114	3500832	93.22%	10.372%
4	6.540	751	757	760	rBV	3212568	3755398	100.00%	11.126%
5	6.687	776	782	785	rBV	3659337	3676180	97.89%	10.891%
6	6.916	817	821	824	rVB	1073927	931675	24.81%	2.760%
7	7.069	843	847	850	rBV	2565314	2214030	58.96%	6.559%
8	7.475	911	916	919	rBV	2265597	2289193	60.96%	6.782%
9	8.192	1034	1038	1042	rBV	1401474	1279922	34.08%	3.792%
10	9.269	1216	1221	1224	rBV	3884172	3515404	93.61%	10.415%
11	9.657	1283	1287	1290	rBV	596451	487982	12.99%	1.446%
12	9.951	1333	1337	1341	rVB	1671817	1403690	37.38%	4.159%
13	10.369	1406	1408	1411	rVB	72360	62052	1.65%	0.184%
14	10.739	1466	1471	1474	rBV	2266510	2130944	56.74%	6.313%
15	10.845	1486	1489	1494	rBV	95317	88202	2.35%	0.261%
16	11.439	1586	1590	1593	rBV	1637247	1368024	36.43%	4.053%
17	11.951	1672	1677	1682	rBV2	44440	43959	1.17%	0.130%
18	13.021	1855	1859	1863	rVB	3314253	3465348	92.28%	10.267%
19	13.904	2005	2009	2018	rBV	278184	271961	7.24%	0.806%
20	14.074	2034	2038	2042	rVB	1080474	921990	24.55%	2.732%
21	14.539	2113	2117	2123	rBV2	40917	55985	1.49%	0.166%
22	14.827	2162	2166	2172	rBV	233687	261225	6.96%	0.774%
23	15.192	2224	2228	2230	rBV	35989	38654	1.03%	0.115%
24	15.568	2286	2292	2298	rBV	618515	817025	21.76%	2.421%
25	16.027	2365	2370	2375	rBV	37621	56132	1.49%	0.166%
26	16.080	2375	2379	2388	rVV7	23128	44856	1.19%	0.133%
27	17.668	2640	2649	2658	rBV9	41241	100364	2.67%	0.297%

Sum of corrected areas: 33753317

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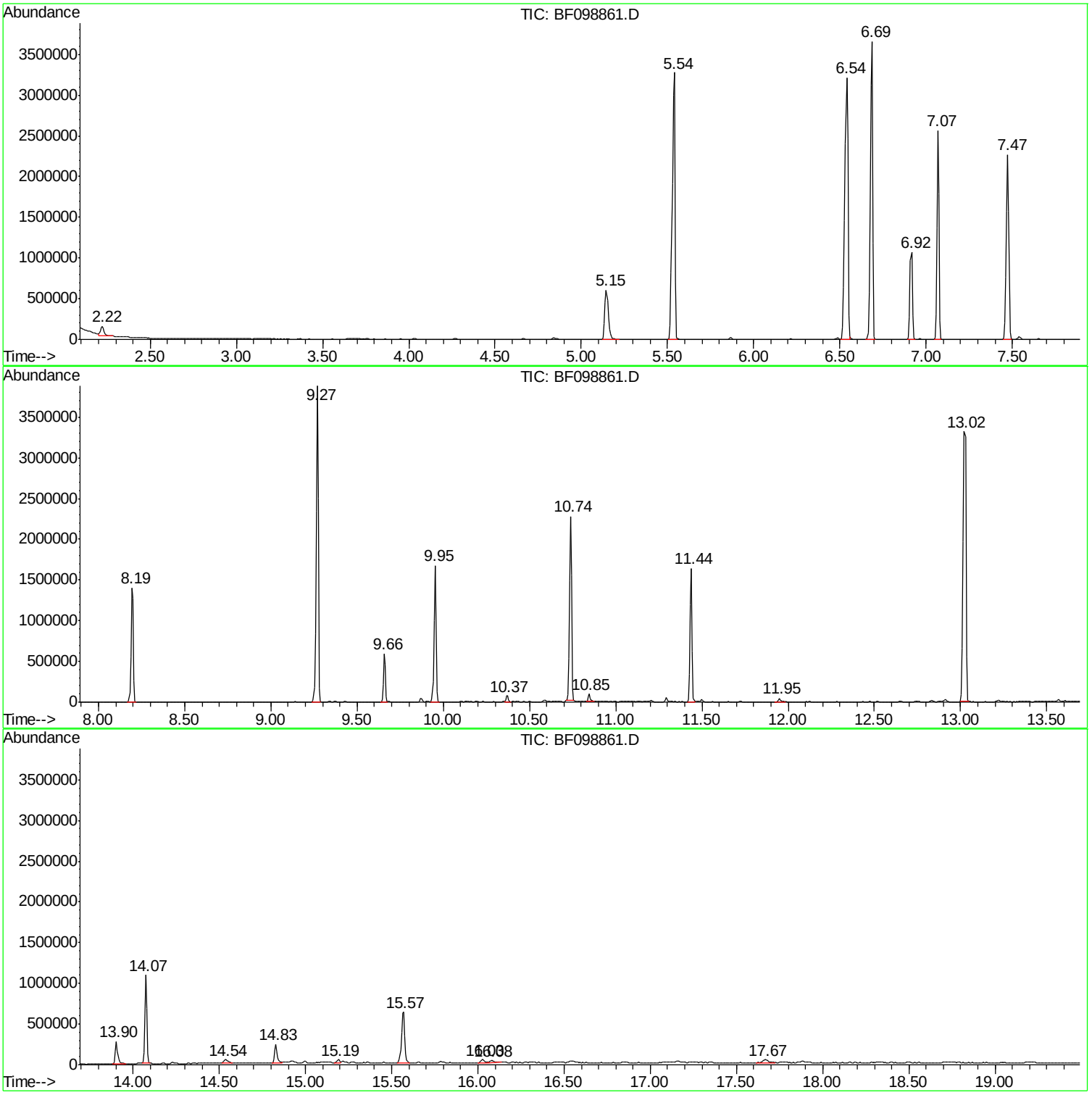
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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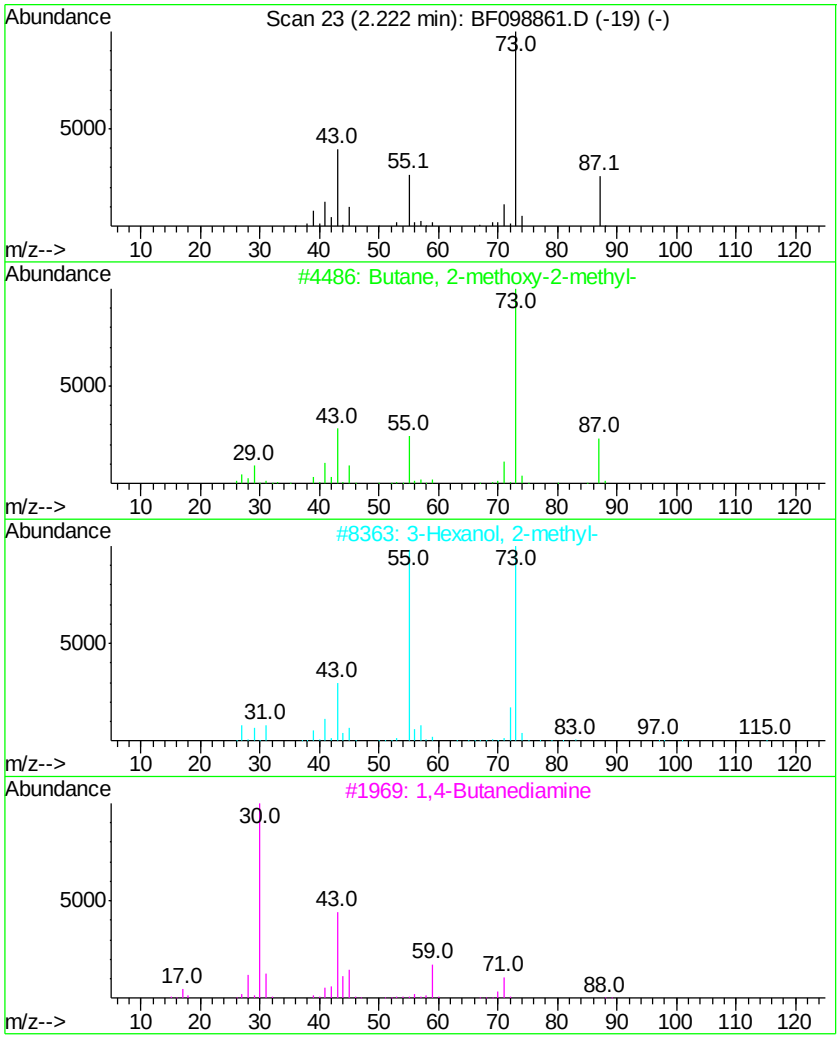
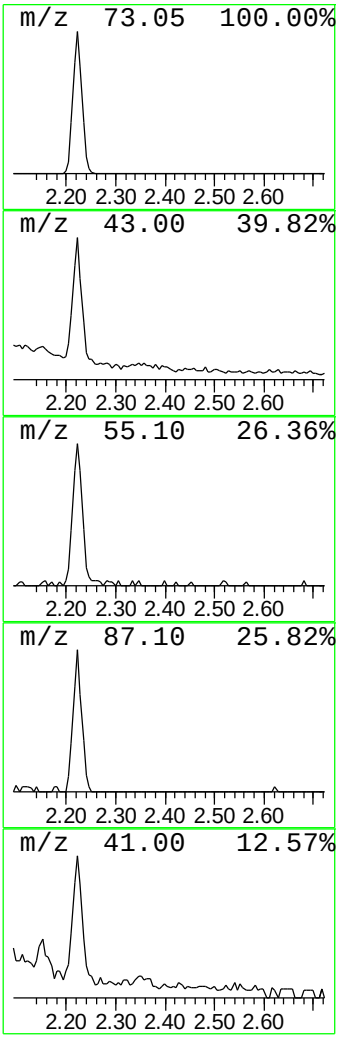
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.83 ng	178270	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





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Instrument : BNA_F
ClientSampleId : UT5400534

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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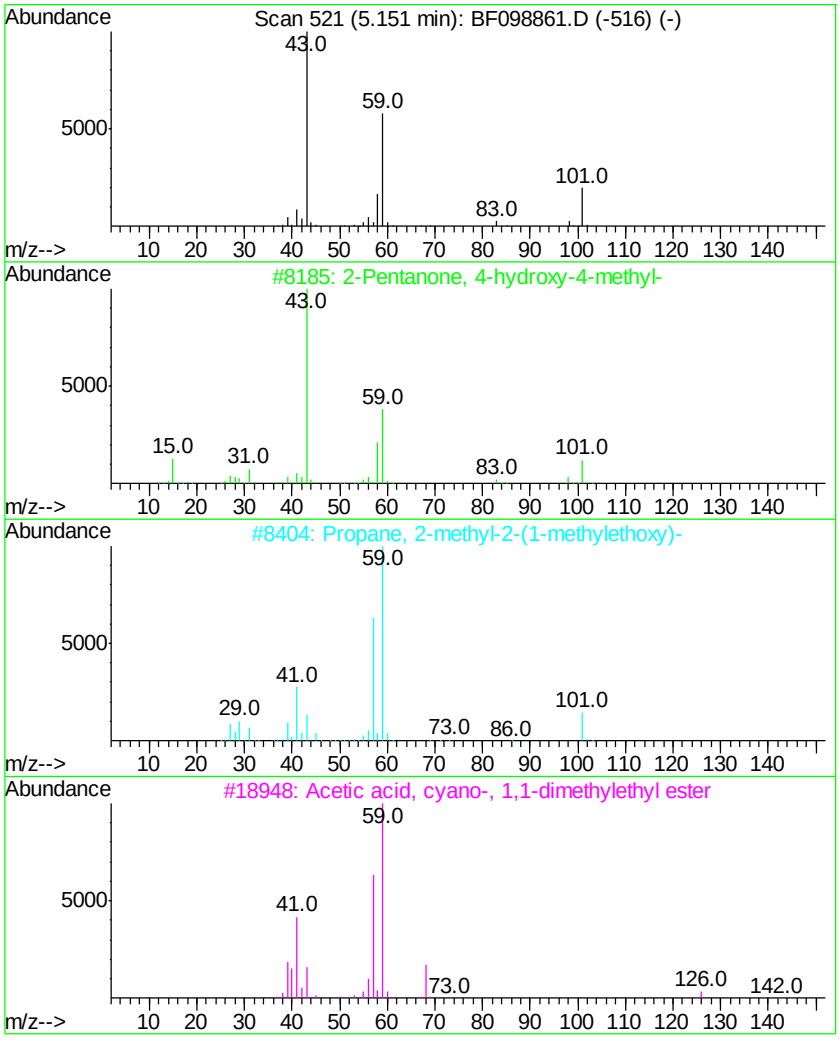
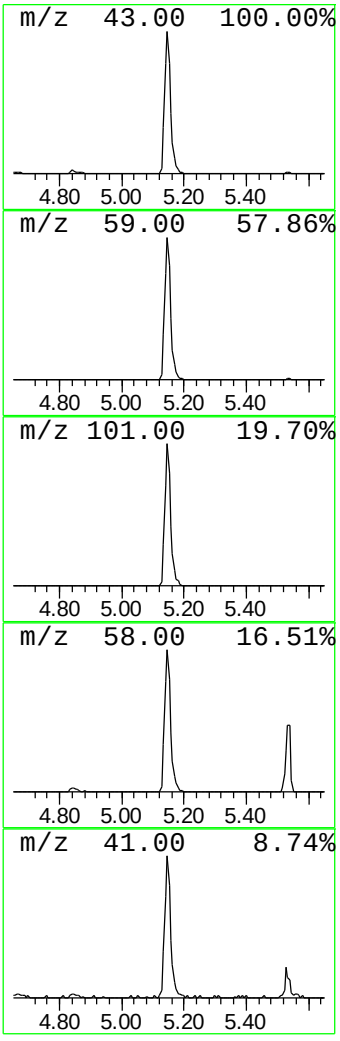
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	17.05 ng	794020	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





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Sample : I5434-13
Misc :
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Instrument : BNA_F
ClientSampleId : UT5400534

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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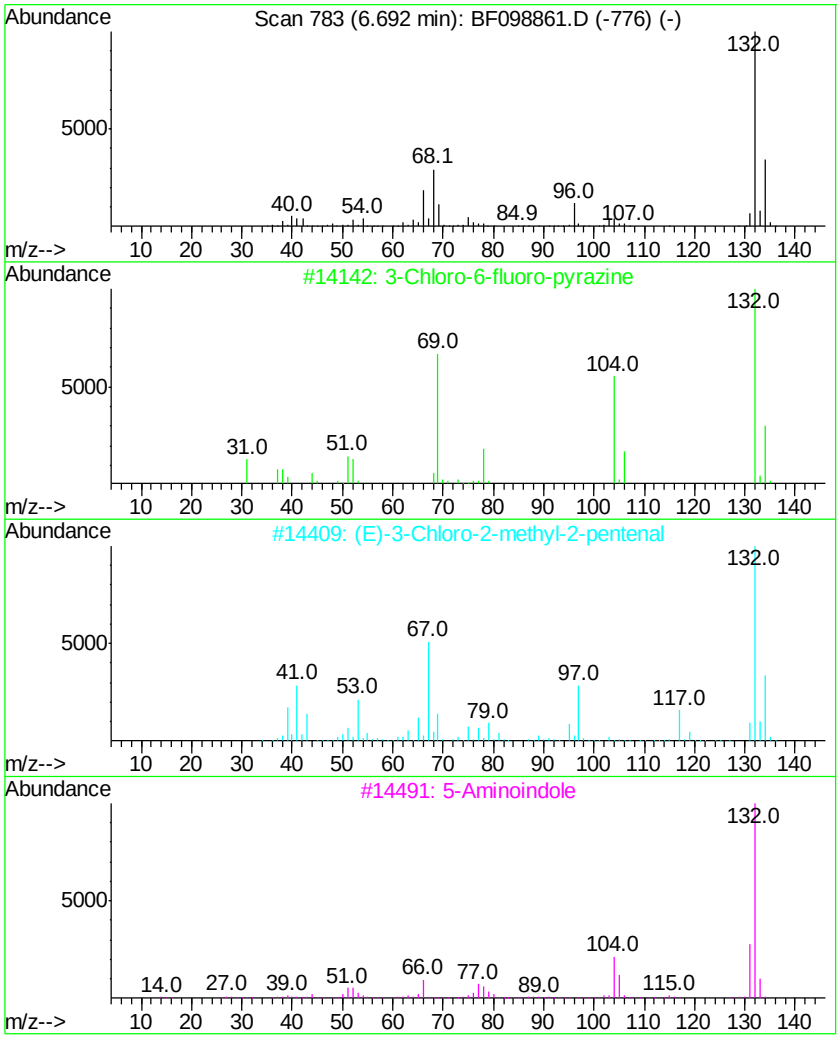
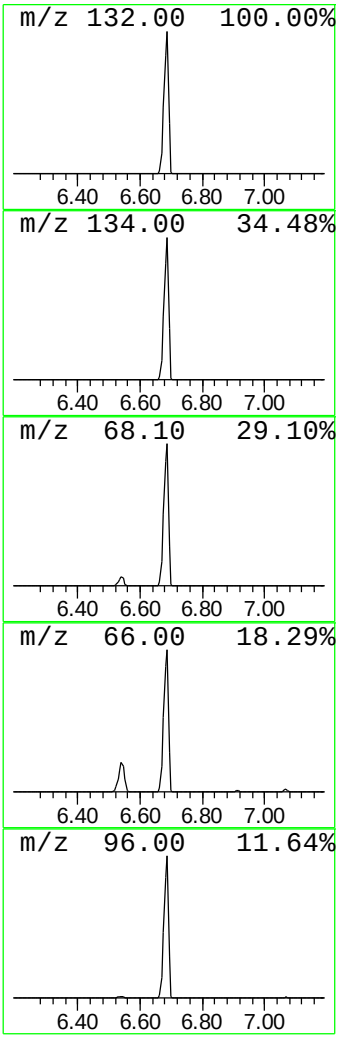
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	78.92 ng	3676180	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Xenon	132	Xe	007440-63-3	9





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Instrument : BNA_F
ClientSampleId : UT5400534

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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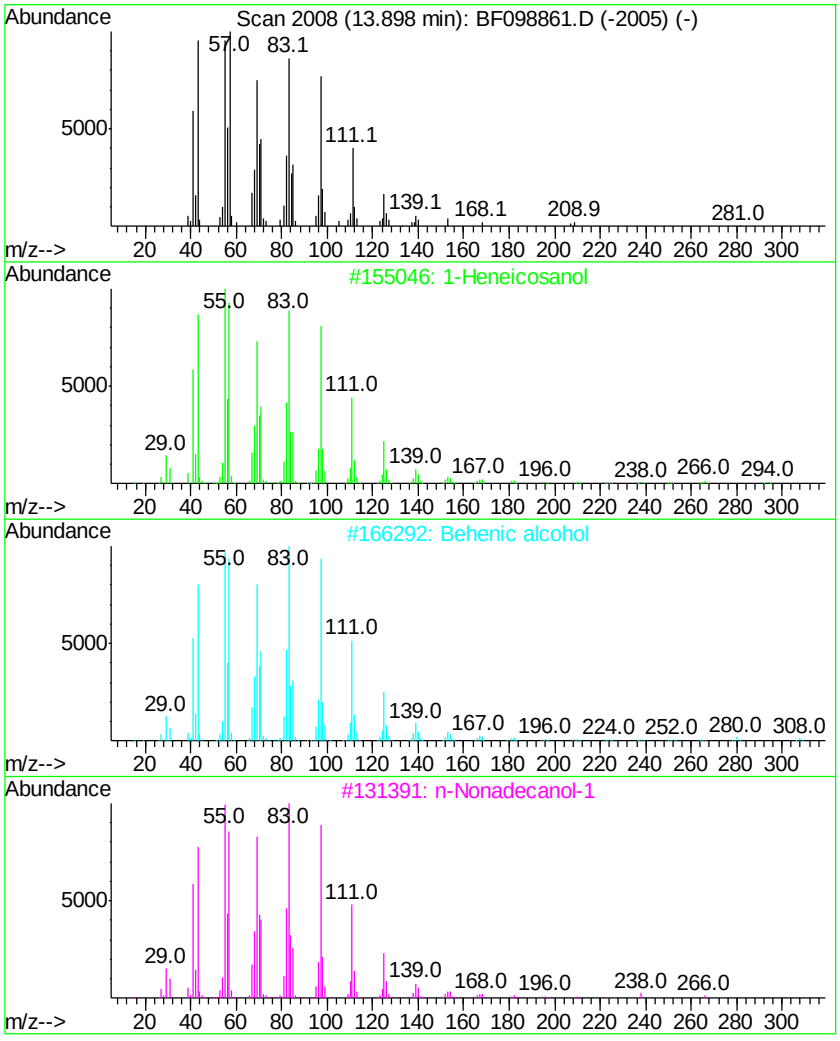
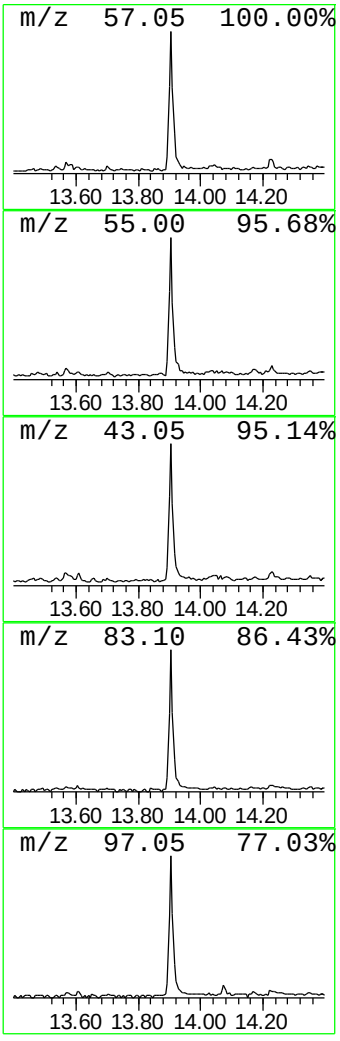
Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.90 ng	271961	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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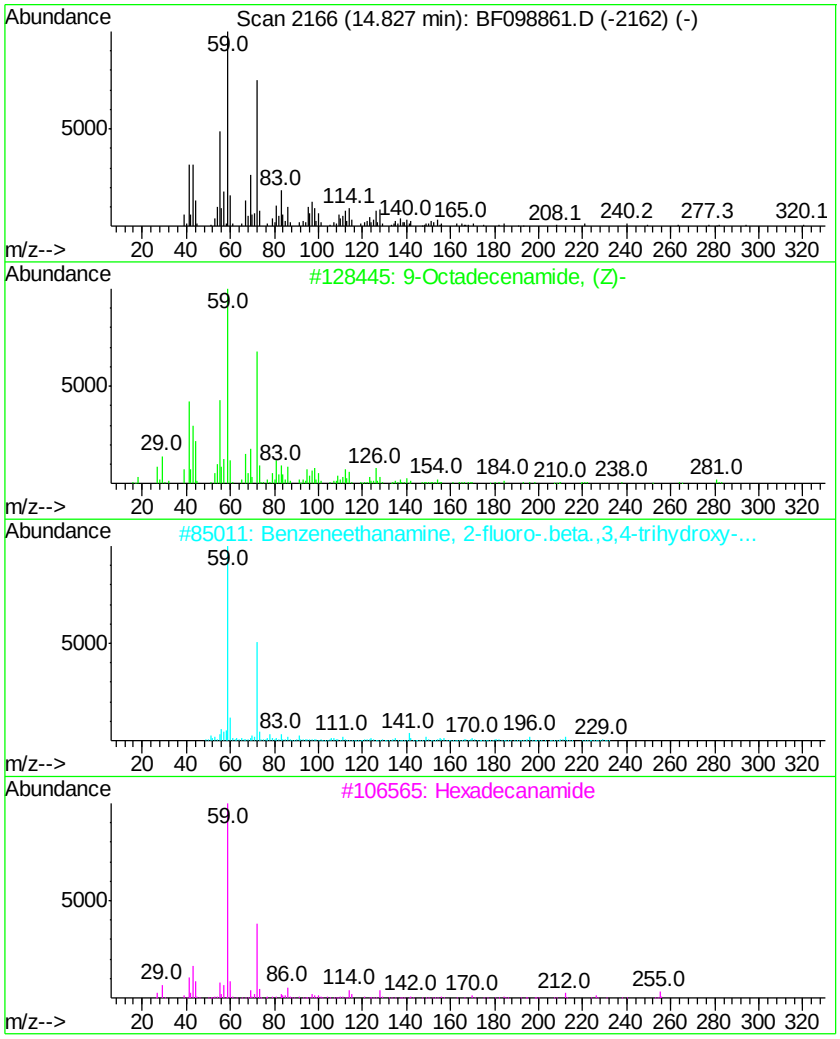
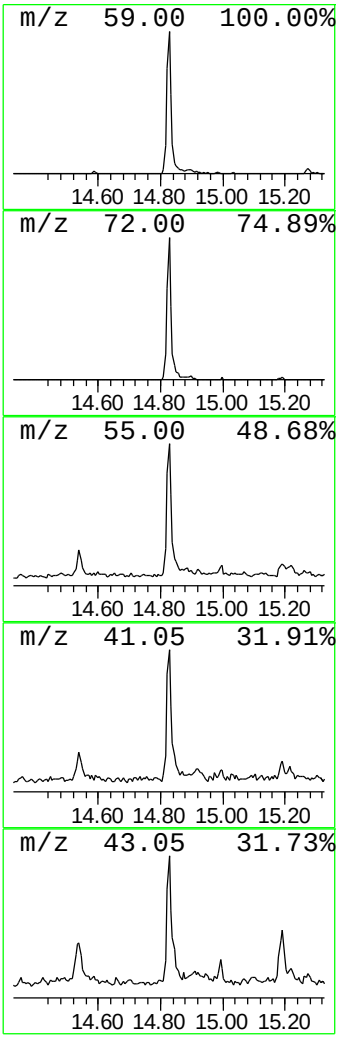
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	6.39 ng	261225	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	50
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	Decanamide-	171	C10H21NO	002319-29-1	47





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Instrument : BNA_F
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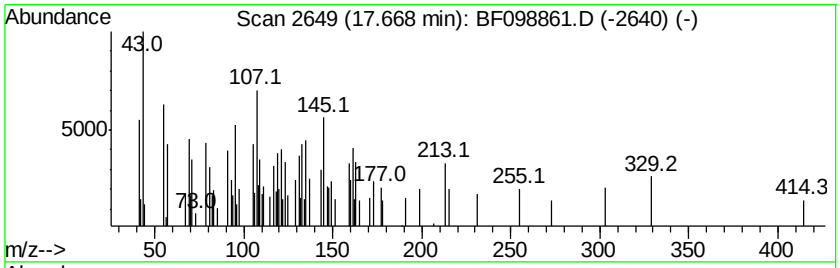
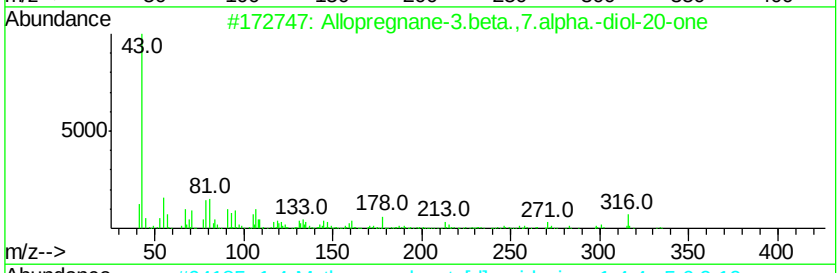
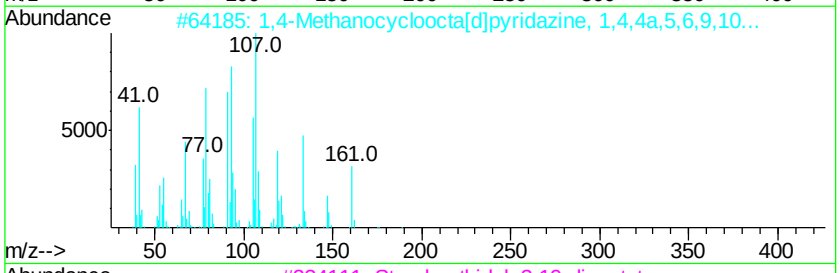
Peak Number 7 unknown17.67 Concentration Rank 7

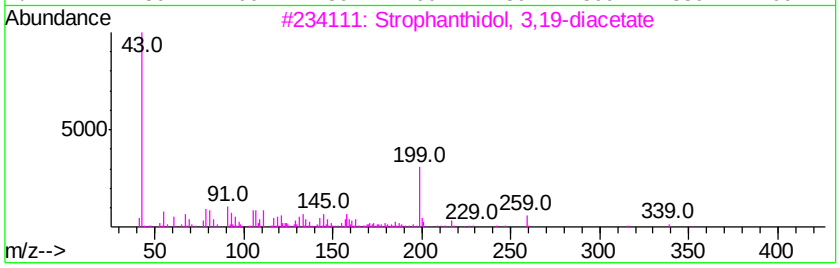
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	2.46 ng	100364	Perylene-d12	15.57

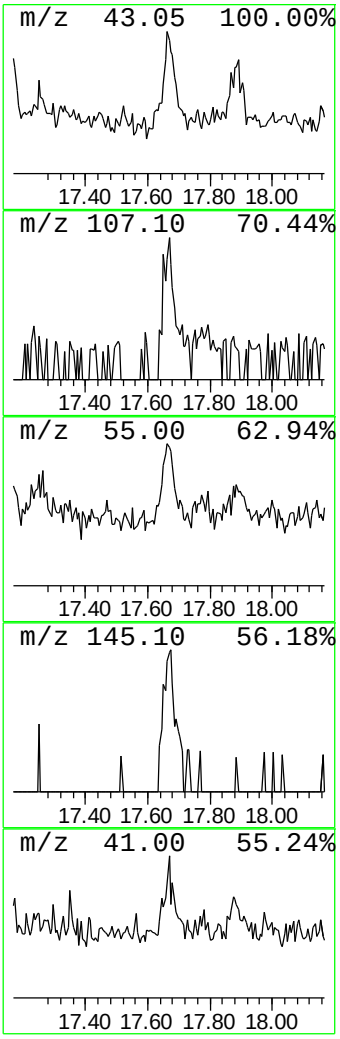
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allopregnane-3.beta.,7.alpha.-di...	334	C21H34O3	000566-20-1	37
2	1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	27
3	Strophanthidol, 3,19-diacetate	490	C27H38O8	083349-11-5	25
4	3,7-Cyclodecadien-1-one, 3,7-dim...	218	C15H22O	006902-91-6	14
5	Alloaromadendrene	204	C15H24	025246-27-9	14











Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	3.8	ng	178270	1	6.92	931675	20.0
2-Pentanone, 4-hy...	5.15	17.1	ng	794020	1	6.92	931675	20.0
unknown6.69	6.69	78.9	ng	3676180	1	6.92	931675	20.0
1-Heneicosanol	13.90	5.9	ng	271961	5	14.07	921990	20.0
9-Octadecenamide,...	14.83	6.4	ng	261225	6	15.57	817025	20.0
unknown17.67	17.67	2.5	ng	100364	6	15.57	817025	20.0