LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098810.D
Acq On : 26 Sep 2017 4:45
Operator : SJ/JU
Sample : I5395-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-(0-5)

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	34	rVB	100189	147092	3.51%	0.412%
2	5.146	516	520	530	rVB	530140	719812	17.19%	2.018%
3	5.540	581	587	590	rBV	3419664	3897264	93.07%	10.928%
4	6.540	751	757	760	rBV	3471866	4036992	96.40%	11.320%
5	6.687	776	782	785	rBV	3978336	3954207	94.43%	11.088%
6	6.916	817	821	824	rBV	1084820	924252	22.07%	2.592%
7	7.069	843	847	851	rBV	3044881	2936962	70.14%	8.236%
8	7.475	911	916	919	rBV	2306336	2436060	58.17%	6.831%
9	8.198	1034	1039	1042	rBV	1343092	1257921	30.04%	3.527%
10	9.269	1216	1221	1225	rBV	4082647	4187536	100.00%	11.742%
11	9.657	1283	1287	1291	rBV	561349	476075	11.37%	1.335%
12	9.951	1332	1337	1341	rVB2	1557472	1334964	31.88%	3.743%
13	10.375	1406	1409	1412	rVB	79520	59290	1.42%	0.166%
14	10.739	1464	1471	1474	rBV	2285780	2254905	53.85%	6.323%
15	10.845	1486	1489	1495	rBV	96860	90375	2.16%	0.253%
16	11.439	1586	1590	1593	rBV	1503351	1231851	29.42%	3.454%
17	11.951	1674	1677	1681	rBV	67846	62540	1.49%	0.175%
18	12.833	1824	1827	1831	rVB	61151	49523	1.18%	0.139%
19	13.027	1855	1860	1863	rBV	3216944	3269834	78.08%	9.169%
20	13.904	2006	2009	2019	rBV	401574	369654	8.83%	1.037%
21	14.074	2035	2038	2042	rVB	961325	843445	20.14%	2.365%
22	14.533	2113	2116	2122	rBV2	38244	48290	1.15%	0.135%
23	14.927	2179	2183	2187	rVB	56637	62918	1.50%	0.176%
24	15.568	2286	2292	2298	rBV	662275	849758	20.29%	2.383%
25	16.033	2367	2371	2375	rVB2	34833	44732	1.07%	0.125%
26	16.080	2375	2379	2385	rBV6	44151	73242	1.75%	0.205%
27	16.545	2456	2458	2465	rVB4	24072	42276	1.01%	0.119%

Sum of corrected areas: 35661770

LSC Report - Integrated Chromatogram

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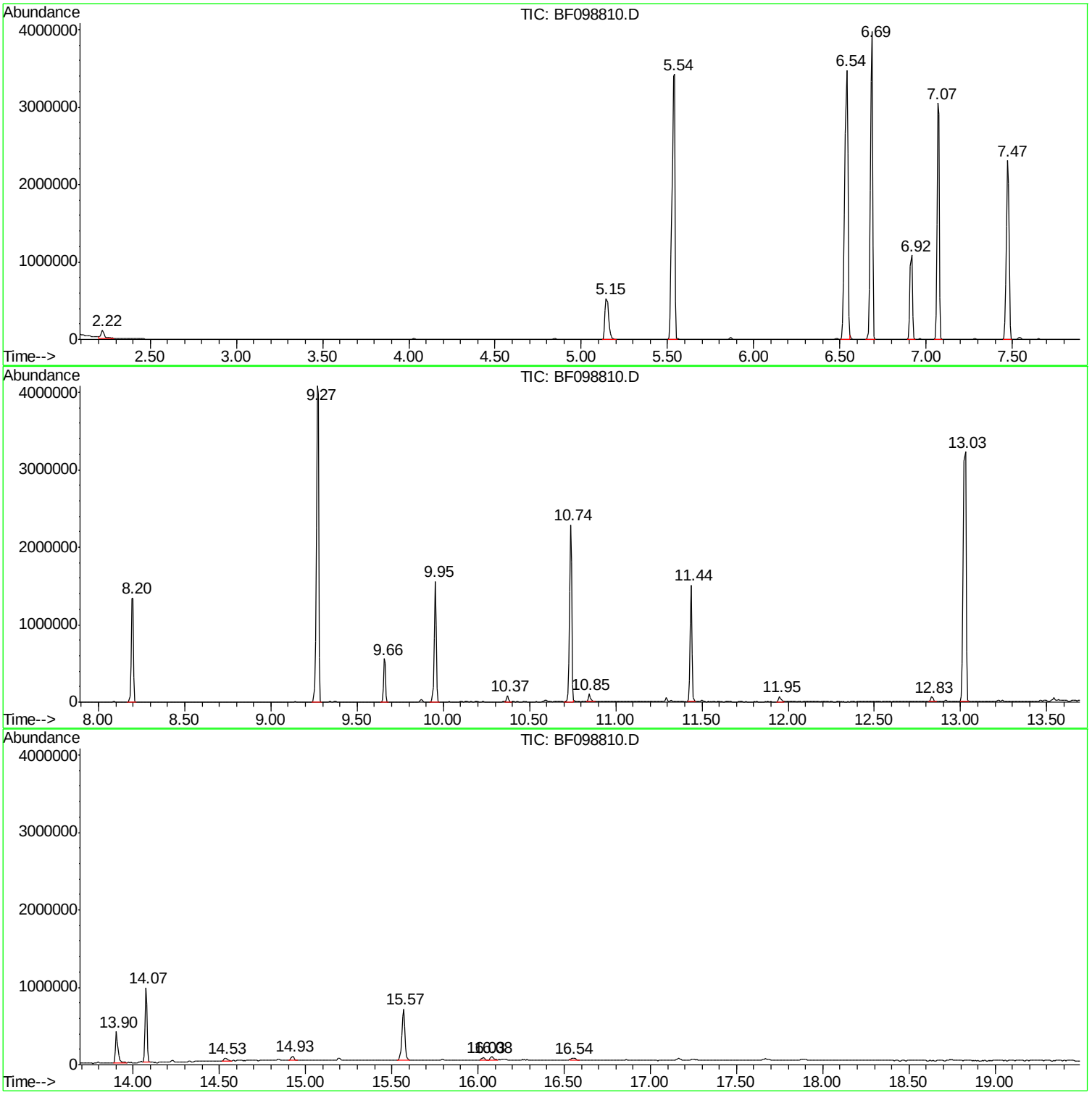
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5-(0-5)

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098810.D
Acq On : 26 Sep 2017 4:45
Operator : SJ/JU
Sample : I5395-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-(0-5)

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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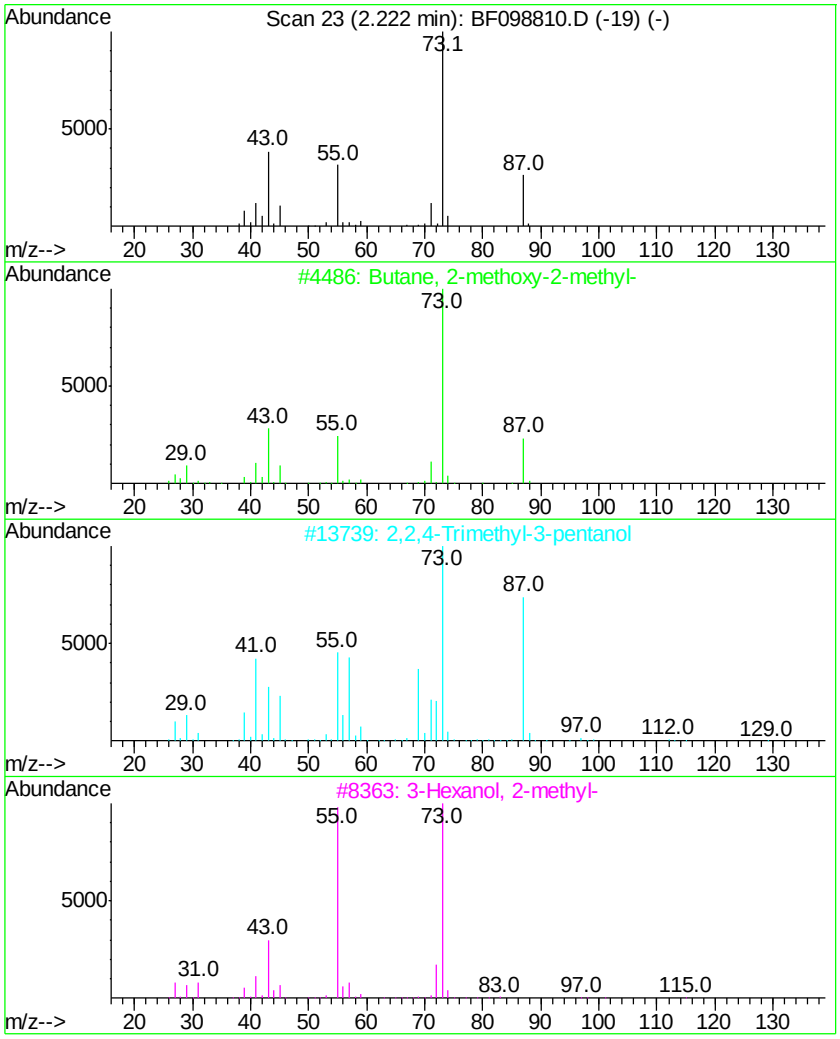
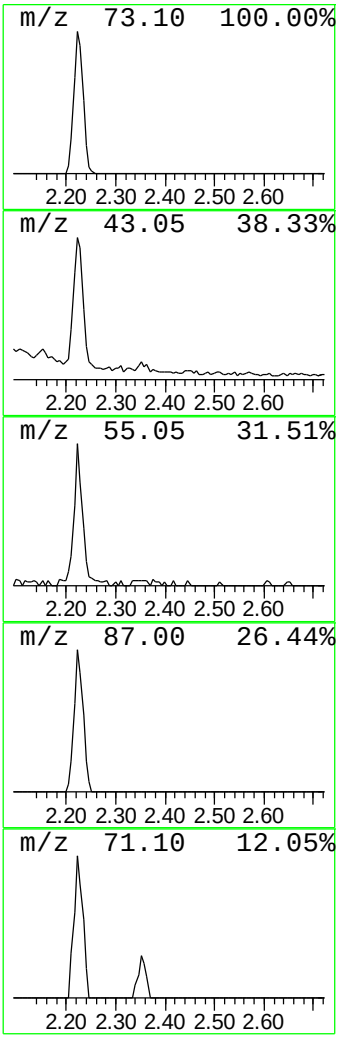
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.18 ng	147092	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





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Sample : I5395-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-(0-5)

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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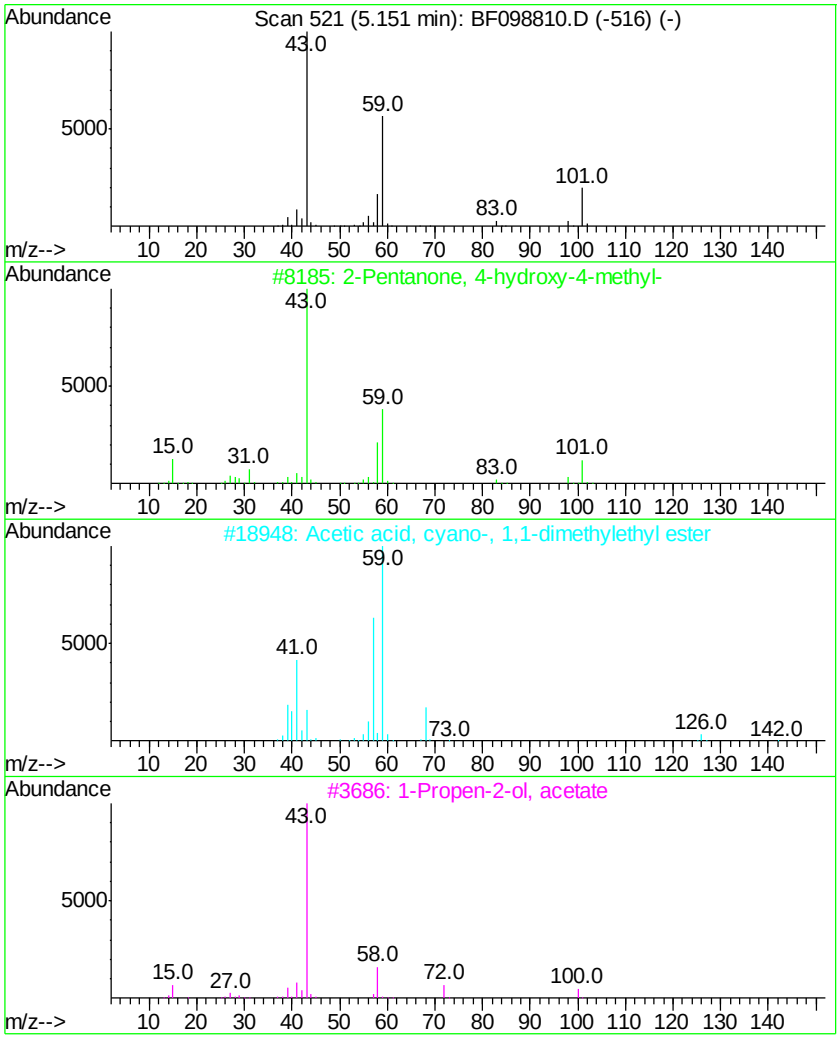
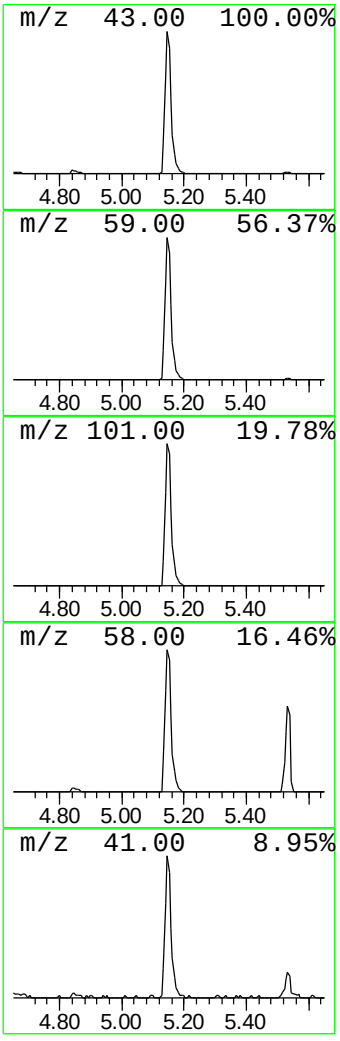
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.58 ng	719812	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	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	1,2-Butanediol	90	C4H10O2	000584-03-2	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098810.D
Acq On : 26 Sep 2017 4:45
Operator : SJ/JU
Sample : I5395-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-(0-5)

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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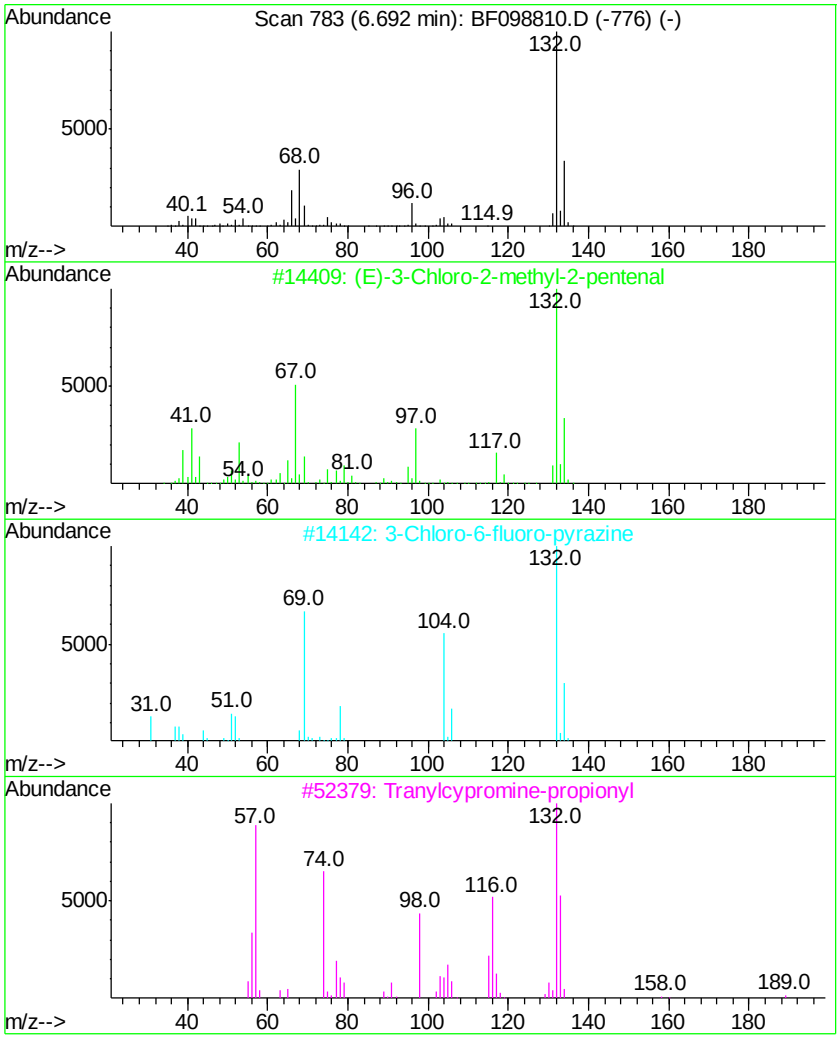
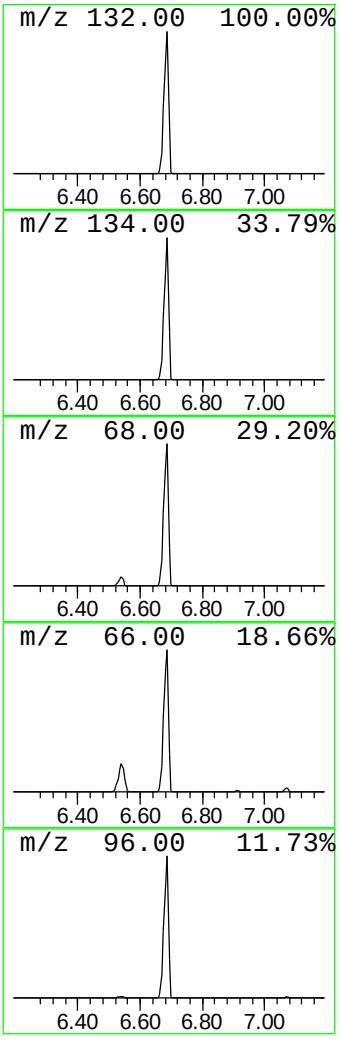
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.57 ng	3954210	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-(0-5)

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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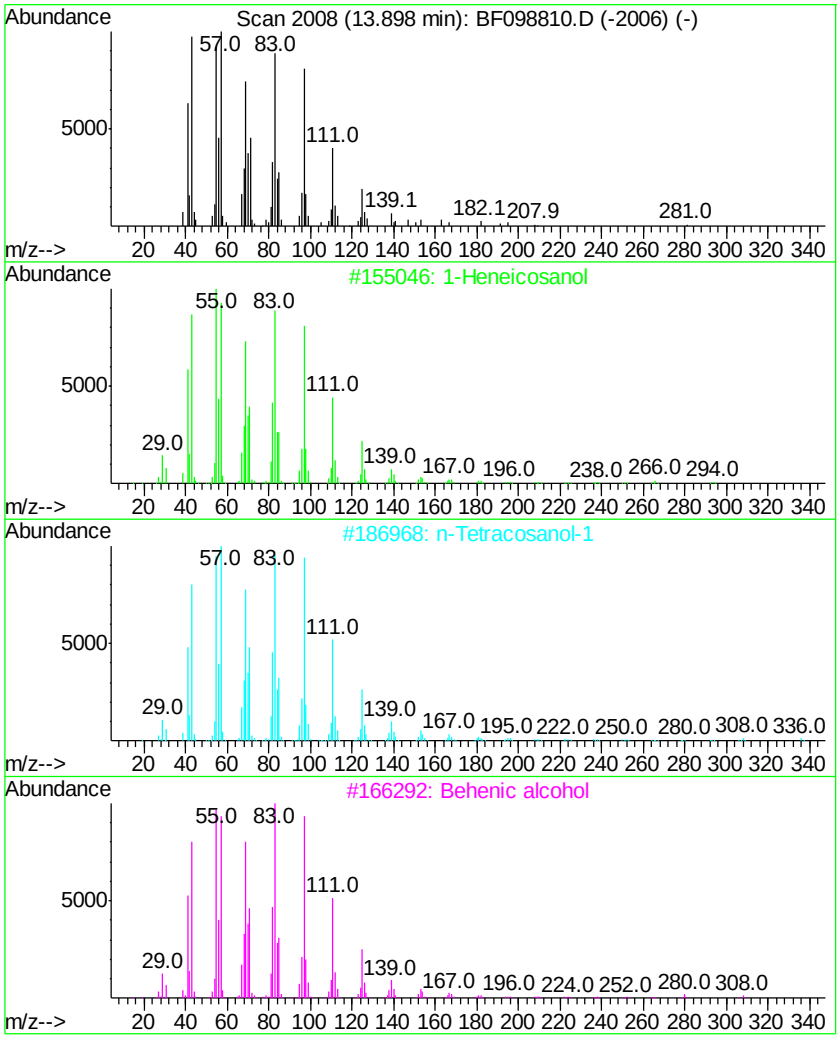
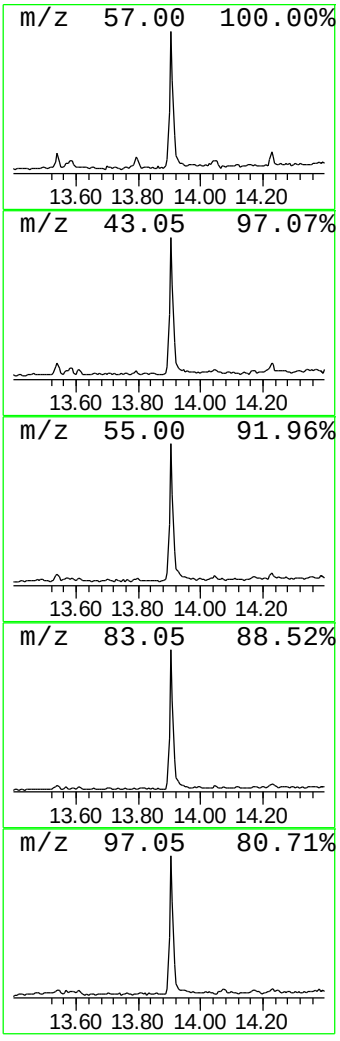
Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	8.77 ng	369654	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Operator : SJ/JU
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5-(0-5)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	3.2	ng	147092	1	6.92	924252	20.0
2-Pentanone, 4-hy...	5.15	15.6	ng	719812	1	6.92	924252	20.0
unknown6.69	6.69	85.6	ng	3954210	1	6.92	924252	20.0
1-Heneicosanol	13.90	8.8	ng	369654	5	14.07	843445	20.0