LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043016\
Data File : BF086539.D
Acq On : 30 Apr 2016 23:32
Operator : UM/SJ
Sample : H2740-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-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-BF042716.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	2.430	27	30	41	rVB2	22662	69072	1.47%	0.206%
2	4.922	246	248	256	rBV	80589	107676	2.29%	0.321%
3	5.356	283	286	288	rBV	1486491	1933182	41.12%	5.767%
4	5.767	319	322	331	rVB	23195	50083	1.07%	0.149%
5	6.396	374	377	386	rBV	1449893	1538417	32.73%	4.589%
6	6.533	386	389	391	rBV	3349727	3590633	76.38%	10.711%
7	6.762	407	409	419	rBV	837260	922078	19.62%	2.751%
8	6.922	420	423	425	rBV	3427647	3181513	67.68%	9.491%
9	7.333	455	459	461	rBV	2765394	2959055	62.95%	8.827%
10	7.447	466	469	473	rVB	103371	178331	3.79%	0.532%
11	7.585	479	481	485	rVB	40303	58418	1.24%	0.174%
12	7.870	502	506	513	rVB4	23667	59264	1.26%	0.177%
13	8.053	519	522	524	rBV	1046906	1121716	23.86%	3.346%
14	8.179	530	533	538	rVB2	23628	59227	1.26%	0.177%
15	8.430	549	555	556	rBV	72293	141293	3.01%	0.421%
16	8.476	558	559	564	rVB	42235	49348	1.05%	0.147%
17	9.128	613	616	619	rBV	4108410	4332351	92.16%	12.924%
18	9.528	649	651	653	rBV	104277	134685	2.87%	0.402%
19	9.802	672	675	677	rBV	1470243	1365503	29.05%	4.073%
20	10.248	710	714	715	rBV2	49530	87719	1.87%	0.262%
21	10.465	730	733	736	rBV	26823	53743	1.14%	0.160%
22	10.591	741	744	746	rBV	2833896	3034323	64.55%	9.052%
23	10.716	753	755	761	rVB	93190	138624	2.95%	0.414%
24	11.162	792	794	795	rBV	68017	65233	1.39%	0.195%
25	11.276	802	804	807	rBV2	1020060	1284844	27.33%	3.833%
26	11.459	817	820	826	rBV	133622	148464	3.16%	0.443%
27	12.865	940	943	946	rBV	3434780	4700822	100.00%	14.023%
28	13.791	1019	1024	1032	rBV4	19595	59393	1.26%	0.177%
29	13.905	1032	1034	1046	rVV	844354	1175441	25.01%	3.506%
30	15.300	1153	1156	1173	rVB	562004	871613	18.54%	2.600%
31	15.585	1176	1181	1190	rVV3	11350	50167	1.07%	0.150%

Sum of corrected areas: 33522231

LSC Report - Integrated Chromatogram

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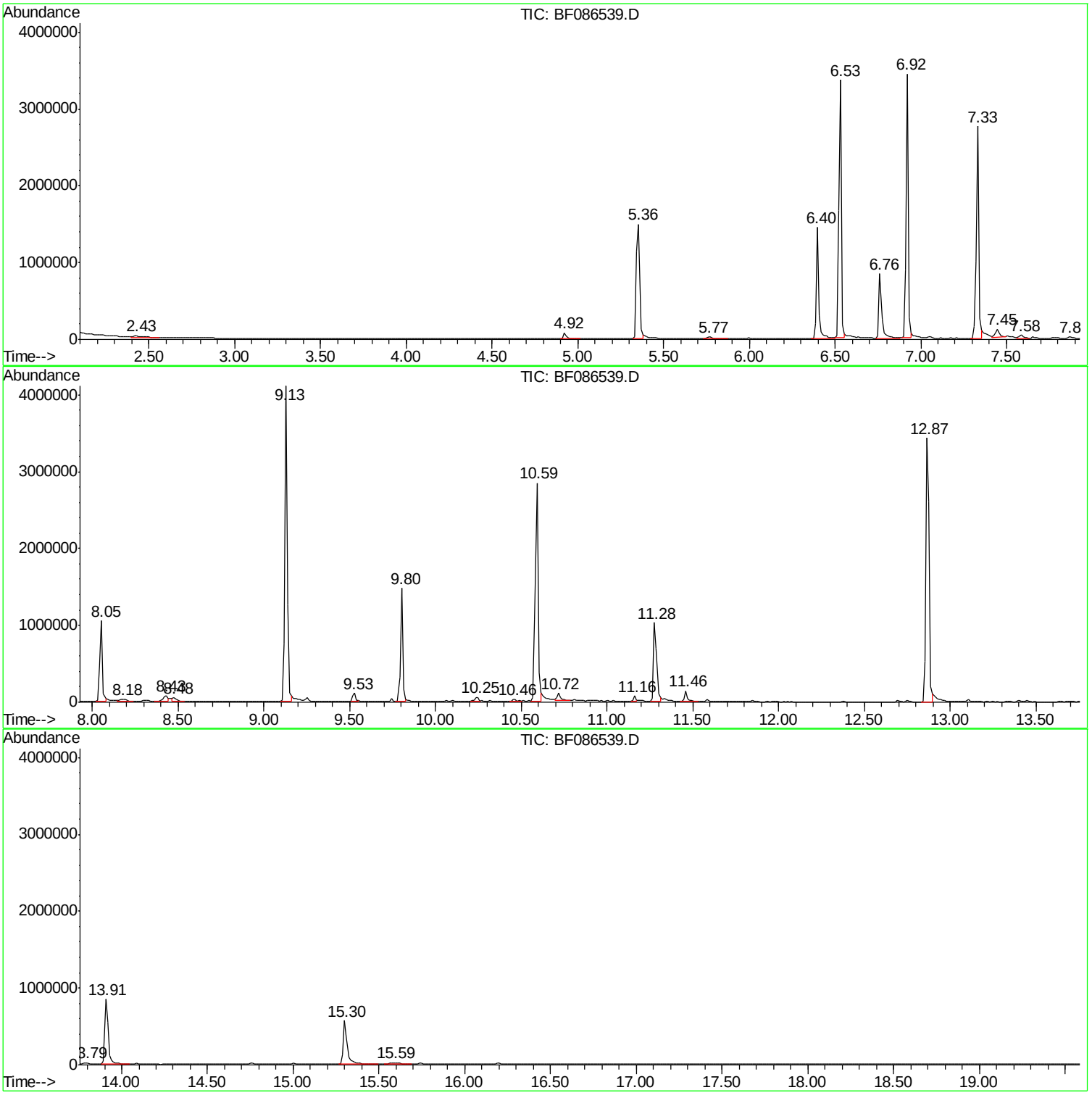
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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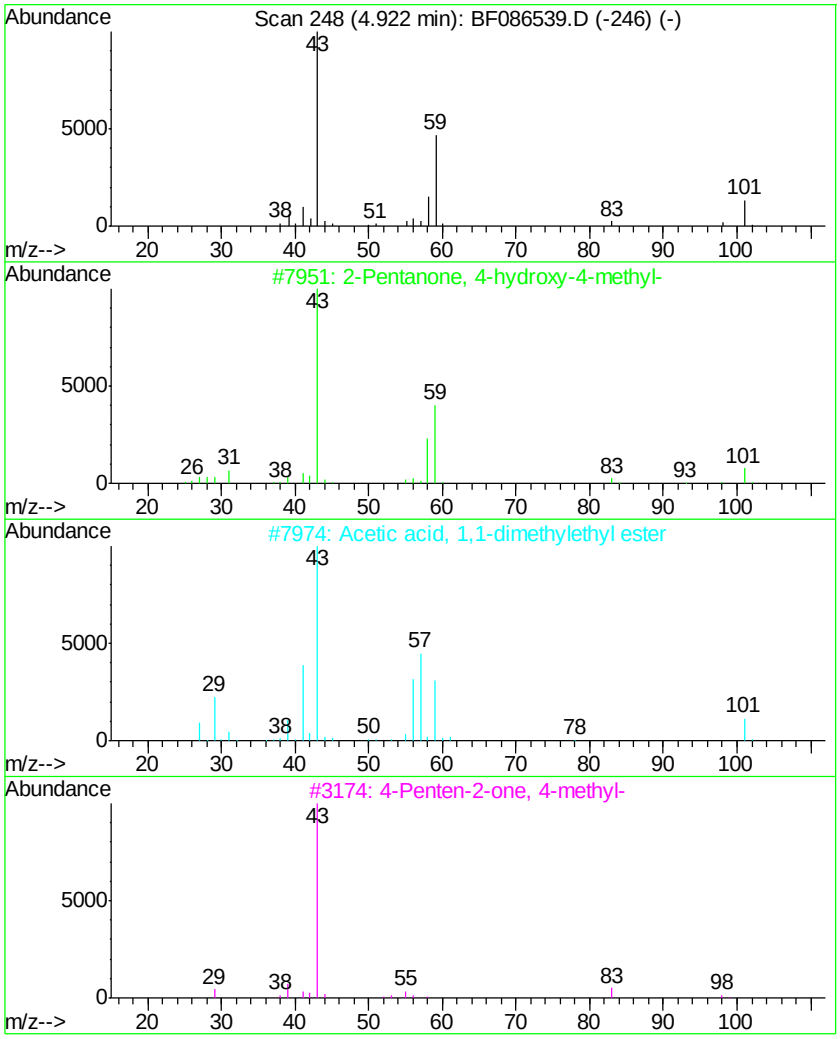
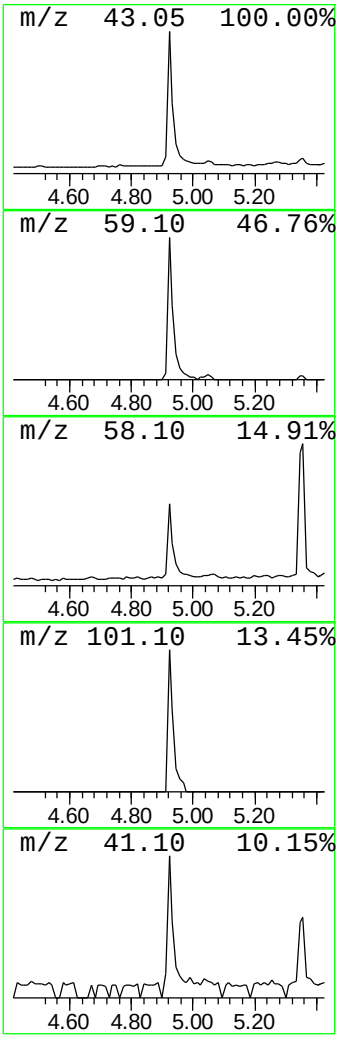
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.34 ng	107676	1,4-Dichlorobenzene-d4	6.76

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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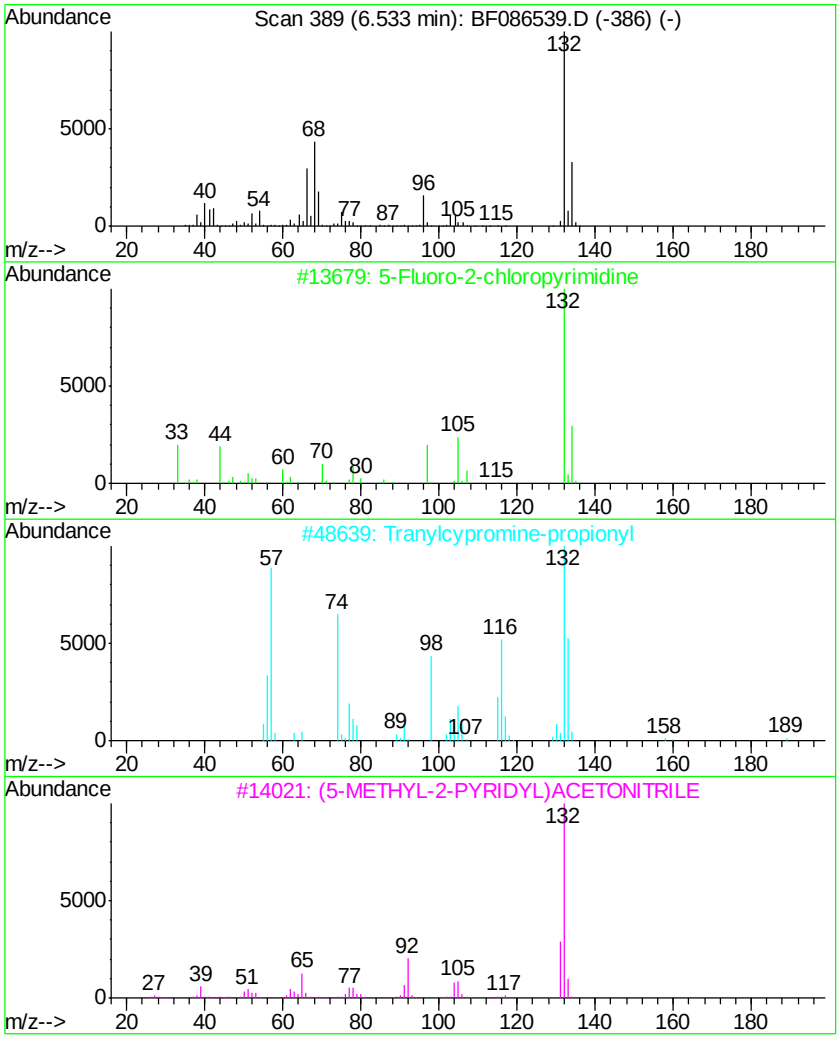
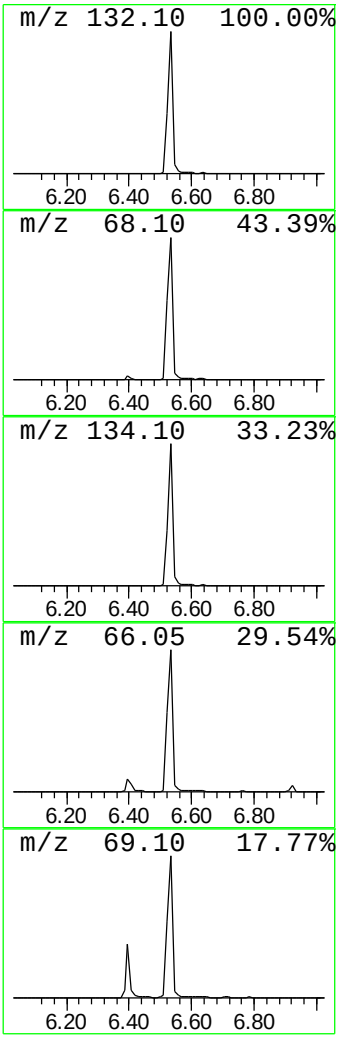
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	77.88 ng	3590630	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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ClientSampleId : CF-1

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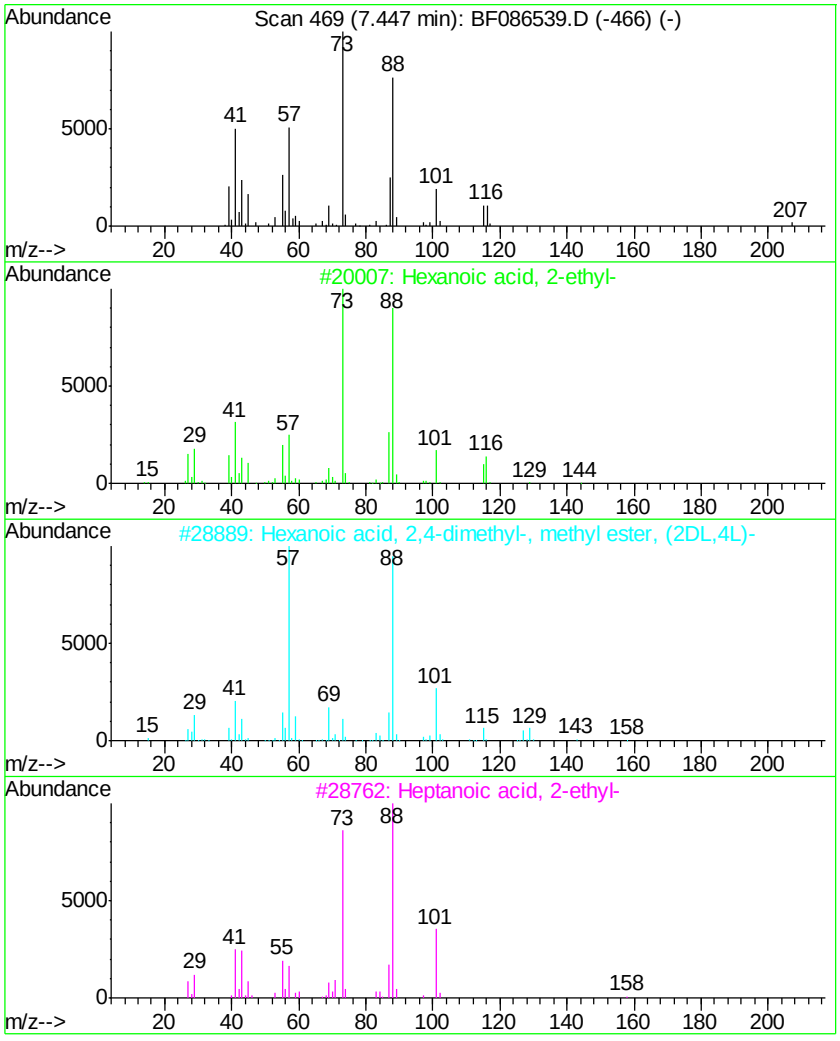
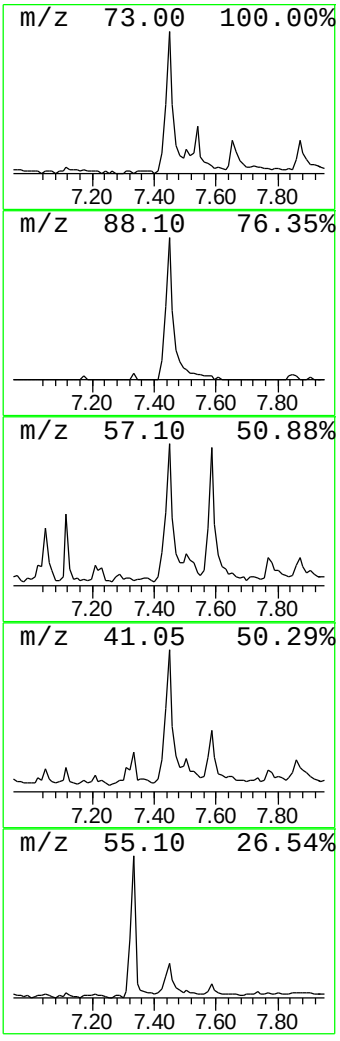
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	3.18 ng	178331	Naphthalene-d8	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	53
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	50
5	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	50





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Sample : H2740-01
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Instrument : BNA_F
ClientSampleId : CF-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
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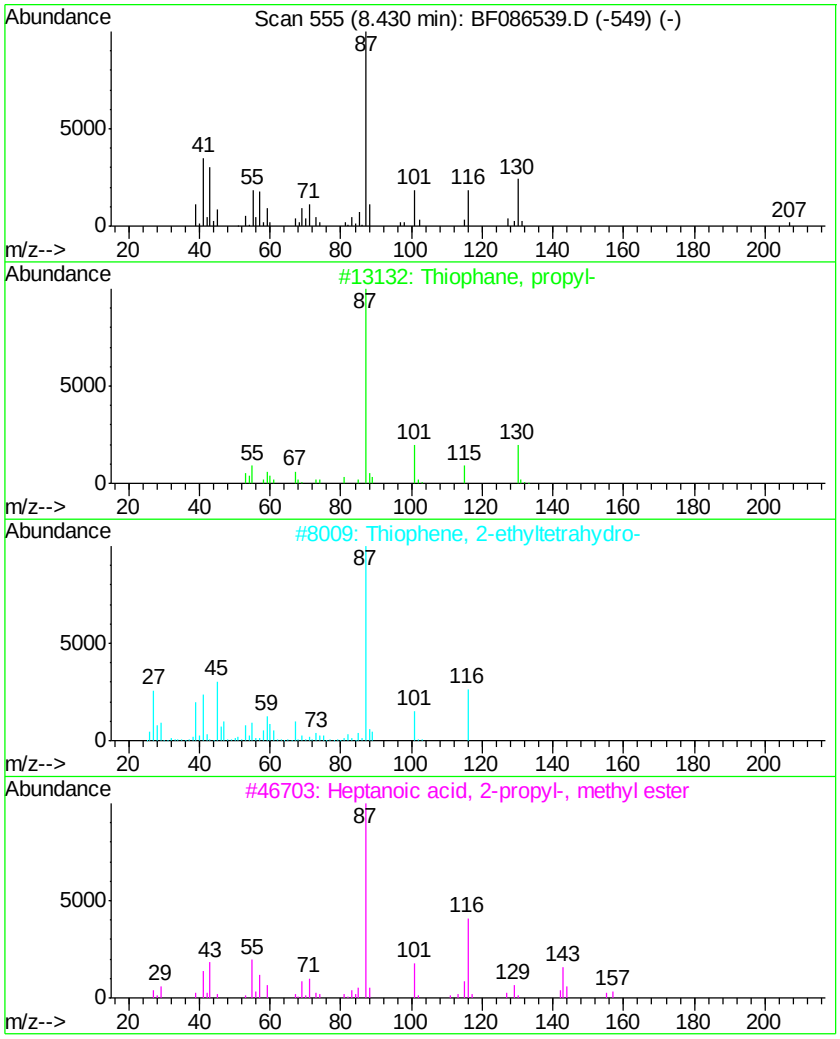
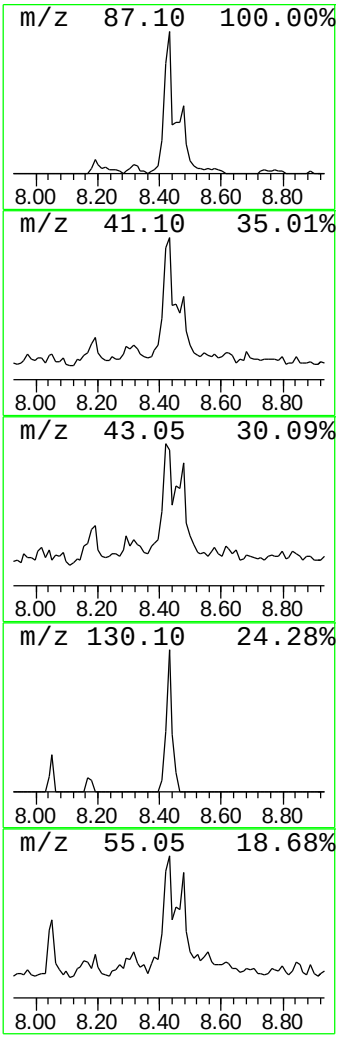
Peak Number 5 Thiophane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	2.52 ng	141293	Naphthalene-d8	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophane, propyl-	130	C7H14S	001551-34-4	64
2	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	64
3	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	59
4	1,3-Dioxolane-2-propanol, 2-meth...	188	C9H16O4	029021-95-2	47
5	.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	45





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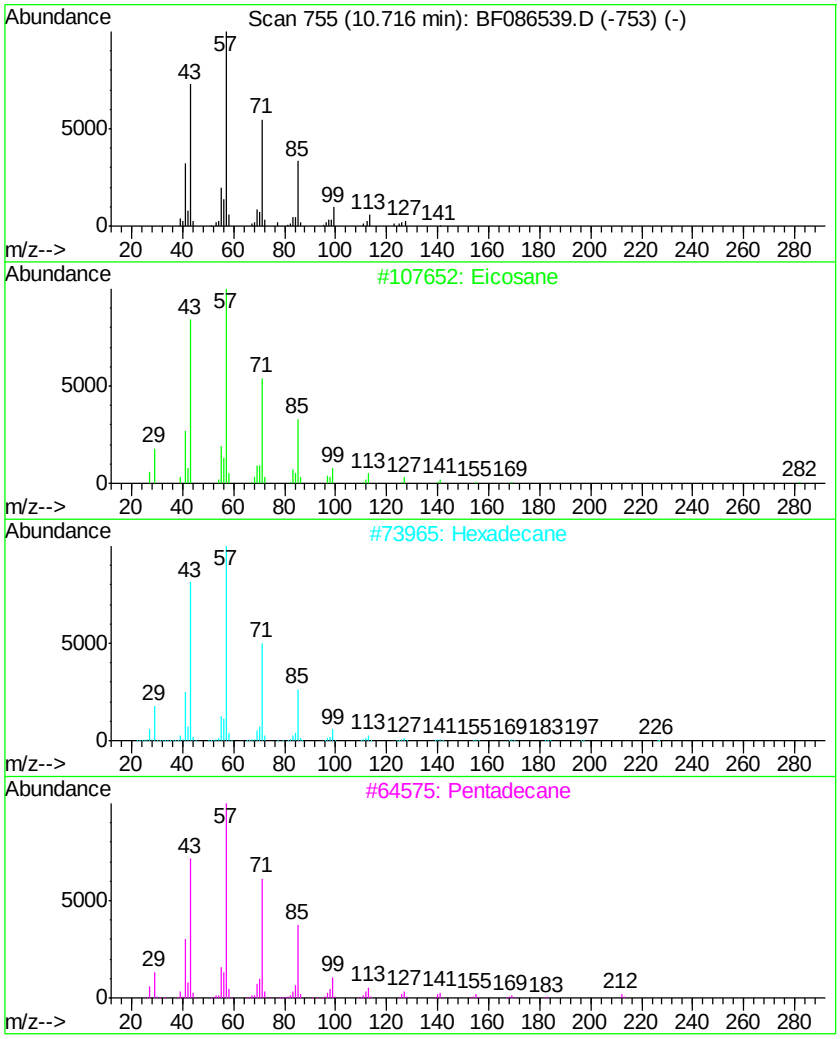
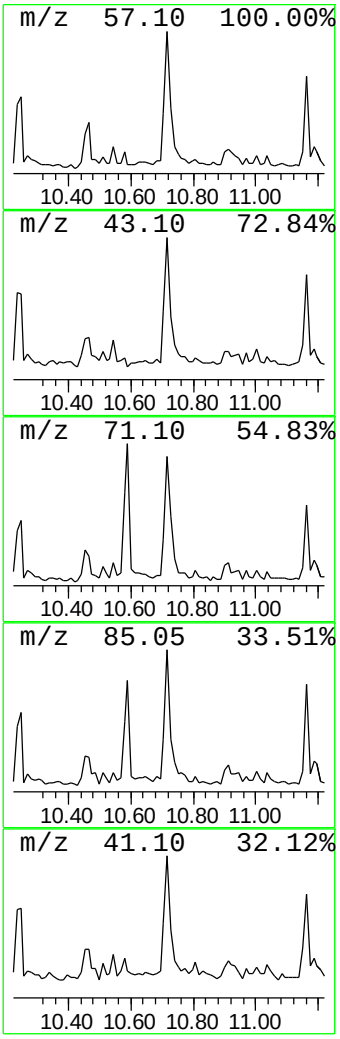
Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.16 ng	138624	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80





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TIC Library : C:\DATABASE\NIST02.L
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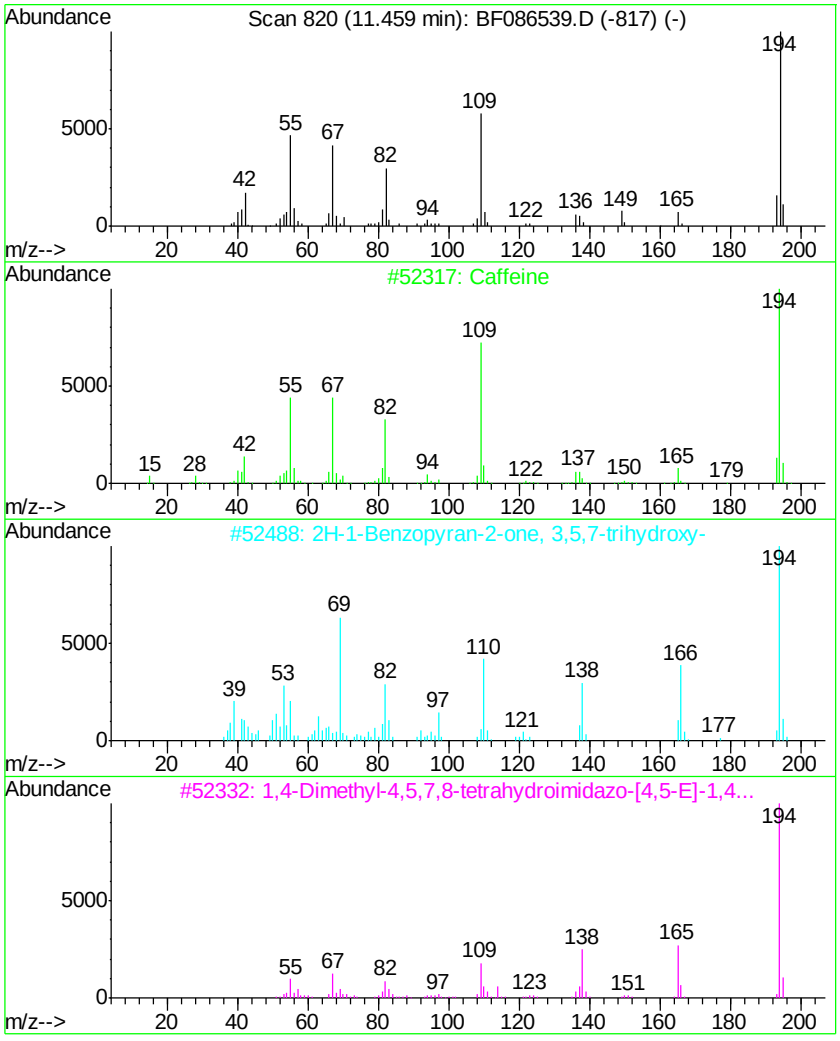
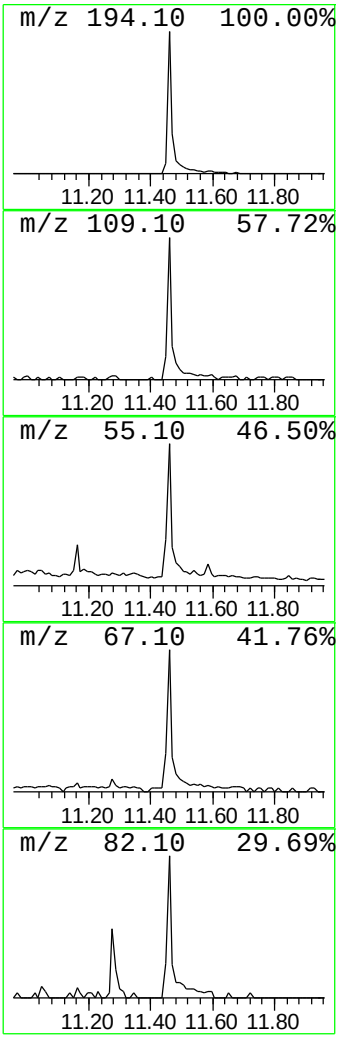
Peak Number 7 Caffeine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	2.31 ng	148464	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	97
2	2H-1-Benzopyran-2-one, 3,5,7-tri...	194	C9H6O5	022065-07-2	43
3	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	43
4	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	40
5	2,5-Dimethoxy-4-ethylbenzaldehyde	194	C11H14O3	050505-61-8	35





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	2.3	ng	107676	1	6.76	922078	20.0
unknown6.53	6.53	77.9	ng	3590630	1	6.76	922078	20.0
Hexanoic acid, 2-...	7.45	3.2	ng	178331	2	8.05	1121720	20.0
Thiophane, propyl-	8.43	2.5	ng	141293	2	8.05	1121720	20.0
Eicosane	10.72	2.2	ng	138624	4	11.28	1284840	20.0
Caffeine	11.46	2.3	ng	148464	4	11.28	1284840	20.0