LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089293.D
Acq On : 25 Jul 2016 23:12
Operator : UM/SJ
Sample : H4207-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EW-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-BF072016.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	1.701	8	10	30	rVB	938309	1778400	100.00%	13.330%
2	4.696	269	272	280	rBV	35400	69458	3.91%	0.521%
3	5.141	309	311	332	rBV	1056860	1295874	72.87%	9.713%
4	6.216	403	405	413	rBV	826357	1316115	74.01%	9.865%
5	6.330	413	415	433	rVB	1344780	1453856	81.75%	10.898%
6	6.559	433	435	446	rVB	219854	266997	15.01%	2.001%
7	6.719	446	449	451	rBV	1035765	1054172	59.28%	7.902%
8	7.005	471	474	483	rBV	48917	105404	5.93%	0.790%
9	7.130	483	485	503	rVB	592638	813258	45.73%	6.096%
10	7.850	545	548	550	rBV	273036	325796	18.32%	2.442%
11	8.925	639	642	652	rBV	1386497	1375638	77.35%	10.311%
12	9.325	675	677	679	rBV	406895	343154	19.30%	2.572%
13	9.588	698	700	703	rBV	398221	377032	21.20%	2.826%
14	10.376	767	769	778	rBV	778844	781678	43.95%	5.859%
15	10.513	778	781	785	rVV2	25595	54460	3.06%	0.408%
16	11.062	827	829	840	rVB	350289	341664	19.21%	2.561%
17	12.639	965	967	970	rBV	681024	958964	53.92%	7.188%
18	13.554	1045	1047	1054	rBV	36452	55547	3.12%	0.416%
19	13.679	1056	1058	1066	rVV	253293	252278	14.19%	1.891%
20	14.182	1098	1102	1108	rBV	12421	27468	1.54%	0.206%
21	14.777	1153	1154	1159	rVB2	10926	18827	1.06%	0.141%
22	15.017	1173	1175	1178	rBV	175044	206901	11.63%	1.551%
23	15.417	1208	1210	1213	rBV	16193	25751	1.45%	0.193%
24	16.685	1317	1321	1327	rBV3	15445	42446	2.39%	0.318%

Sum of corrected areas: 13341138

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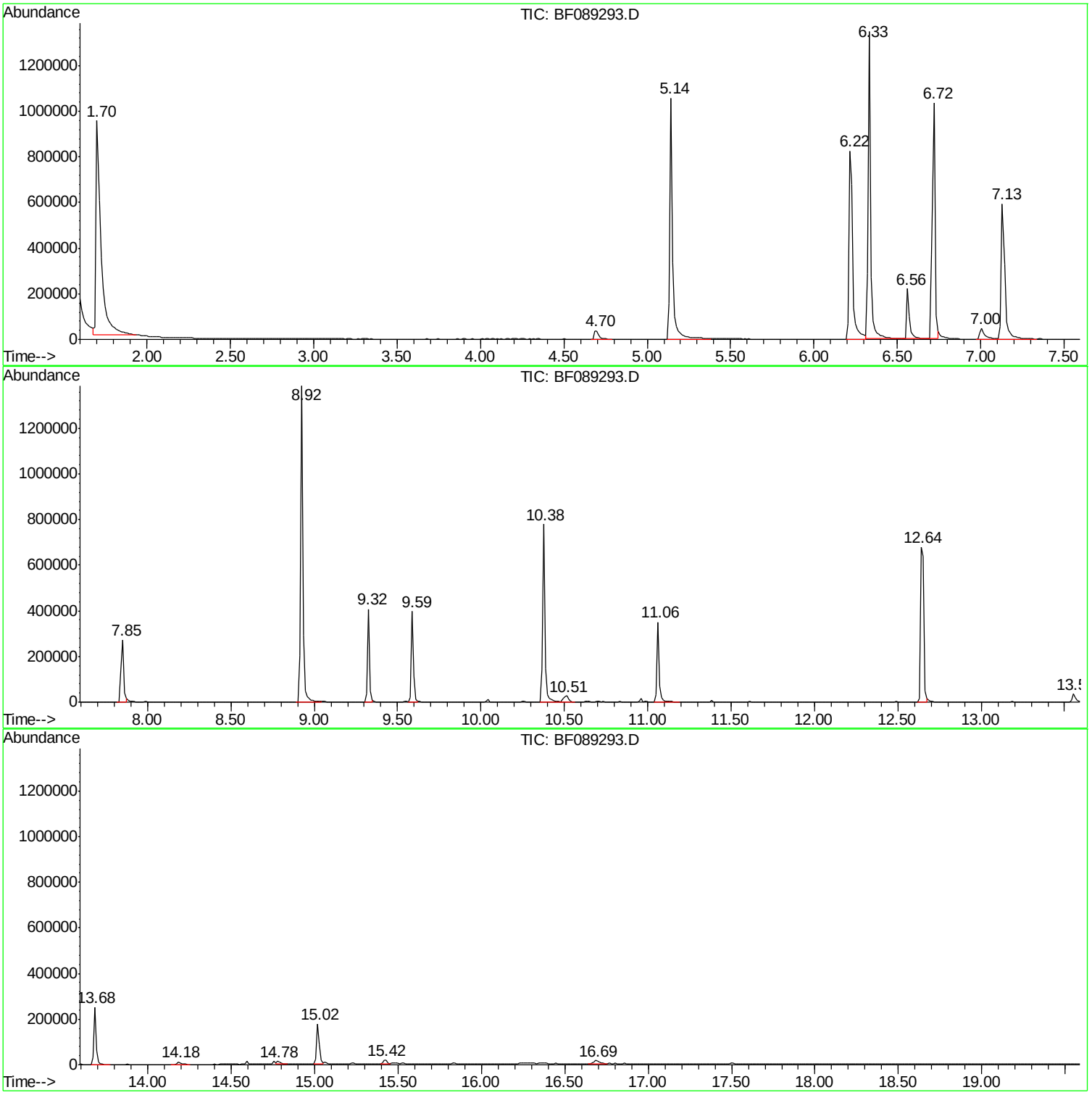
Instrument : BNA_F
ClientSampleId : EW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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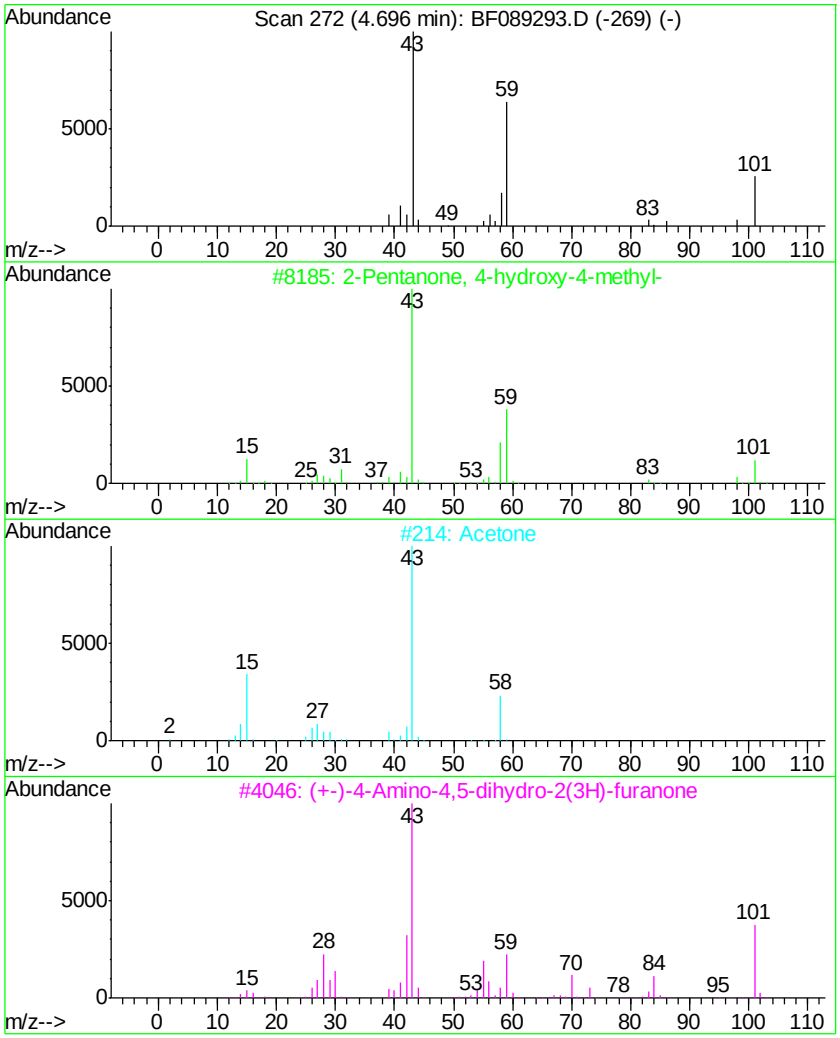
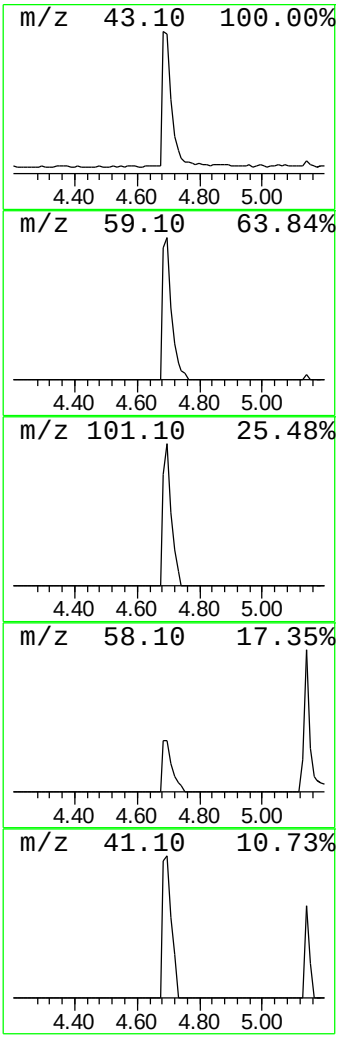
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	5.20 ng	69458	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetone	58	C3H6O	000067-64-1	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Sample : H4207-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

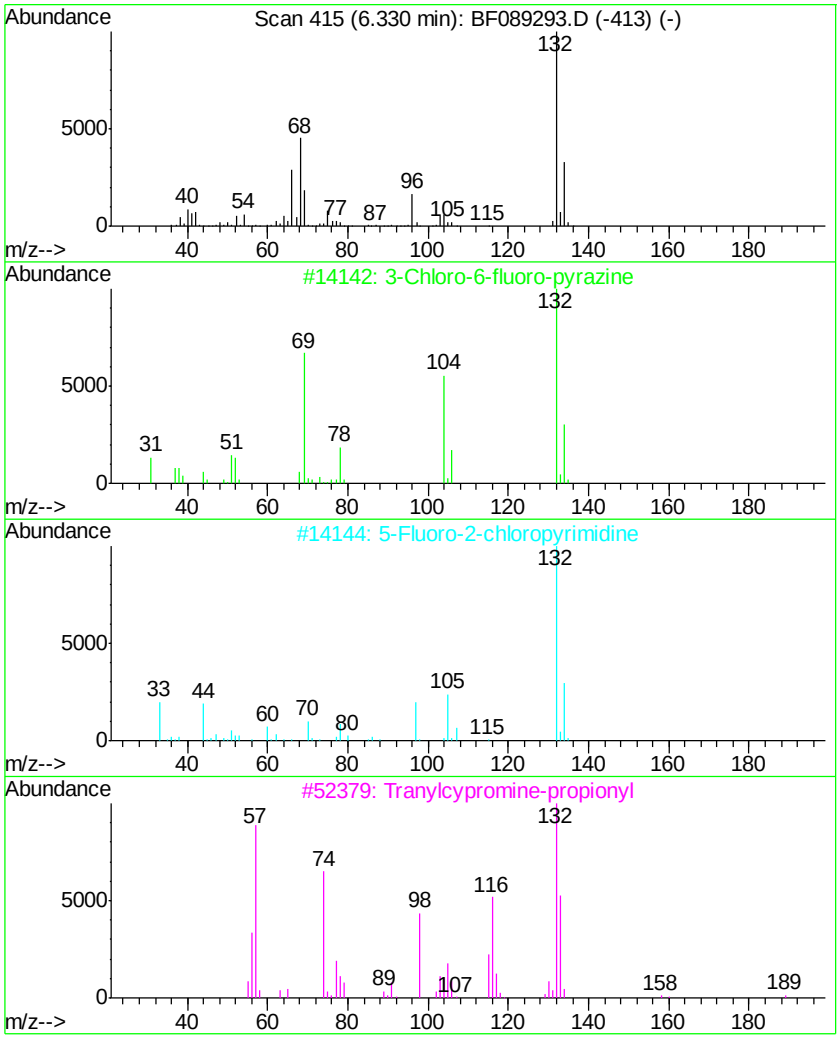
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

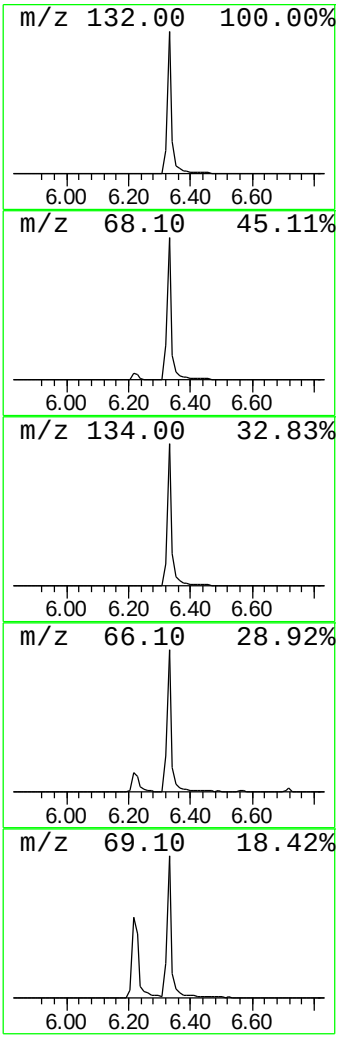
****

Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	108.90 ng	1453860	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H4207-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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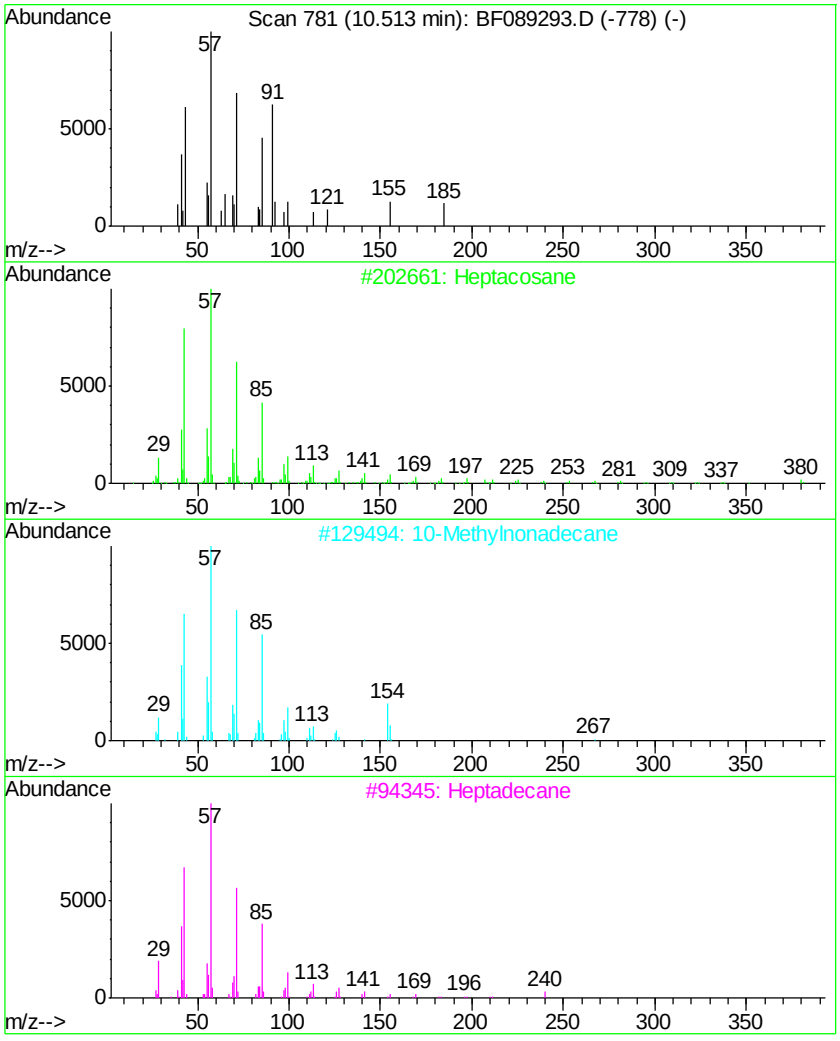
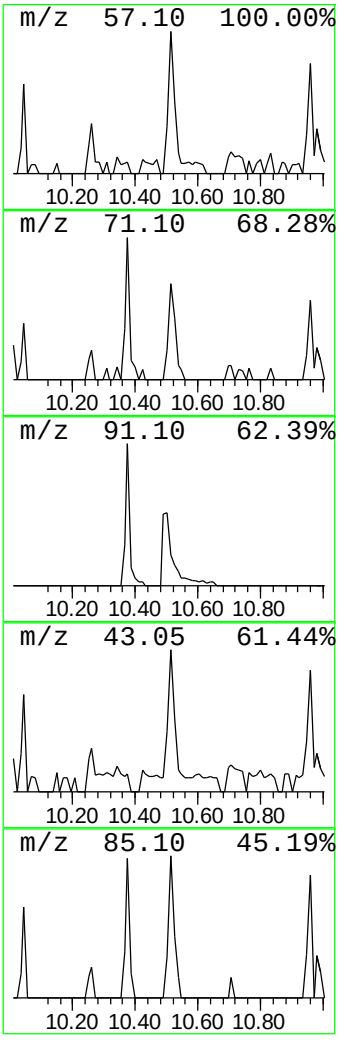
Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	3.19 ng	54460	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	72
2	10-Methylnonadecane	282	C20H42	056862-62-5	72
3	Heptadecane	240	C17H36	000629-78-7	64
4	Hexacosane	366	C26H54	000630-01-3	64
5	Docosane	310	C22H46	000629-97-0	64





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Operator : UM/SJ
Sample : H4207-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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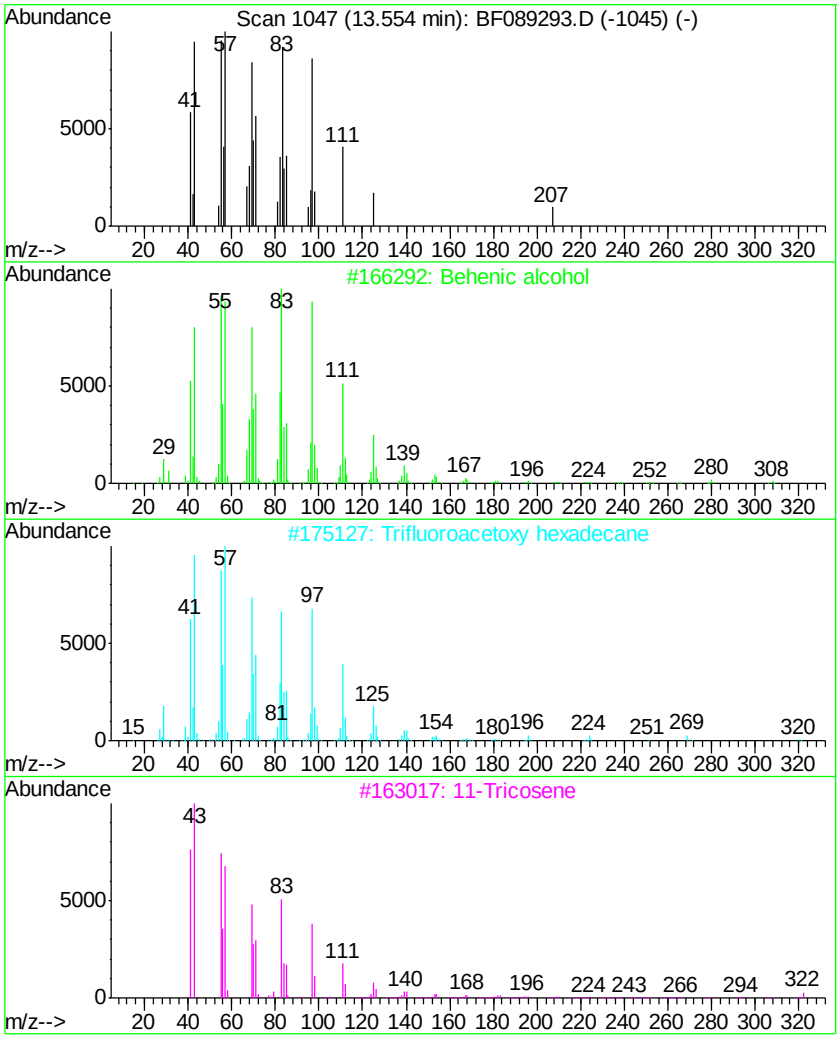
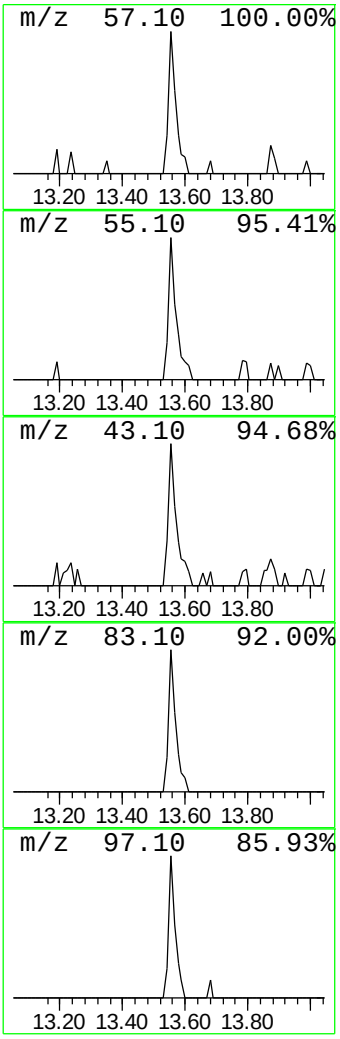
Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.40 ng	55547	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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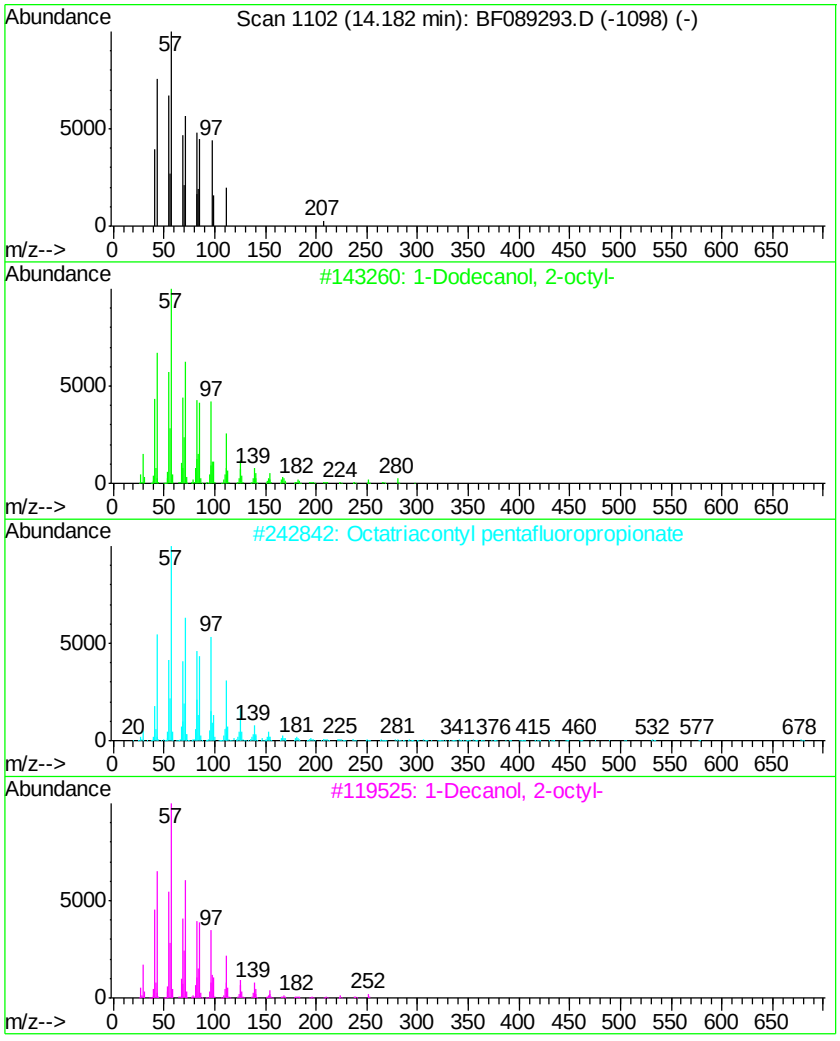
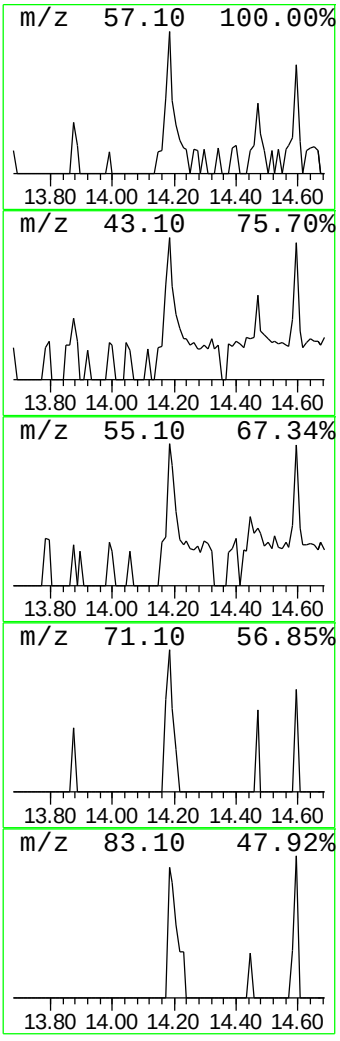
Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	2.18 ng	27468	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	90
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	90
4	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	83
5	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	80





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Instrument : BNA_F
ClientSampleId : EW-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

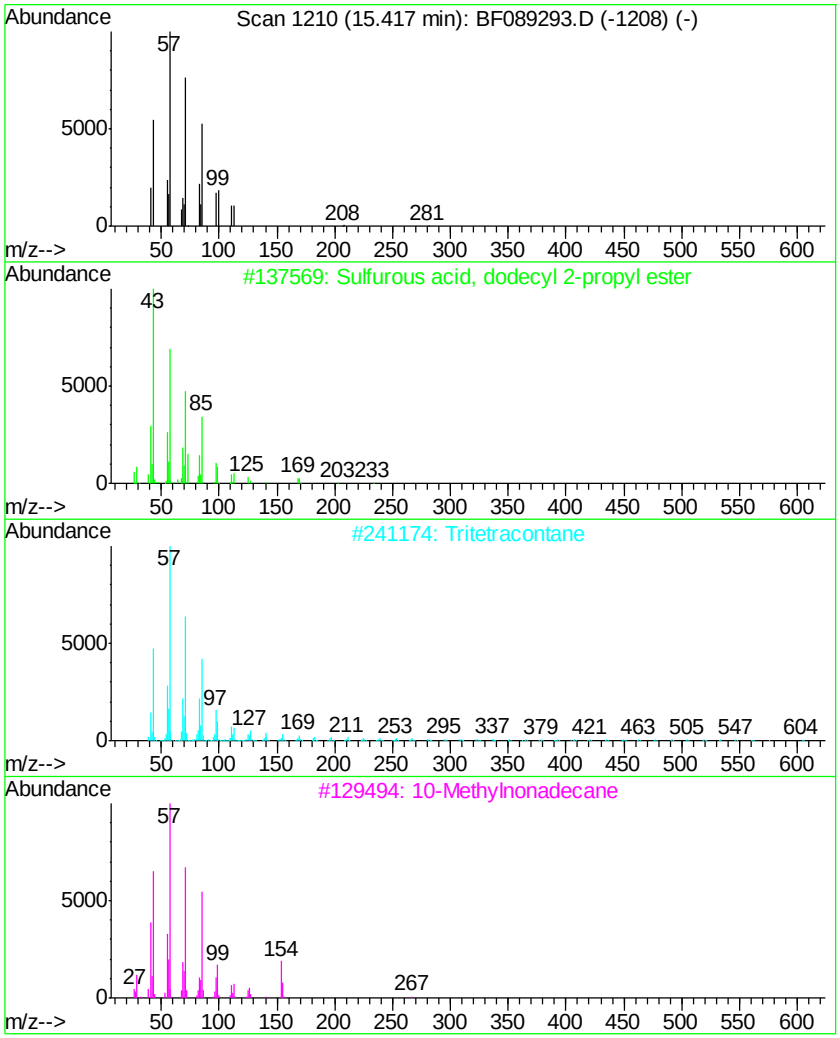
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

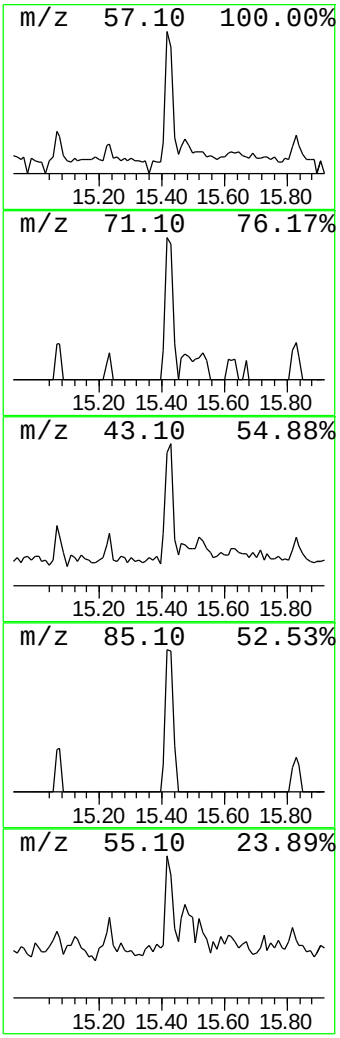
****

Peak Number 8 Sulfurous acid, dodecyl 2-p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	2.49 ng	25751	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90
2	Tritetracontane	605	C43H88	007098-21-7	90
3	10-Methylnonadecane	282	C20H42	056862-62-5	86
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	83
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

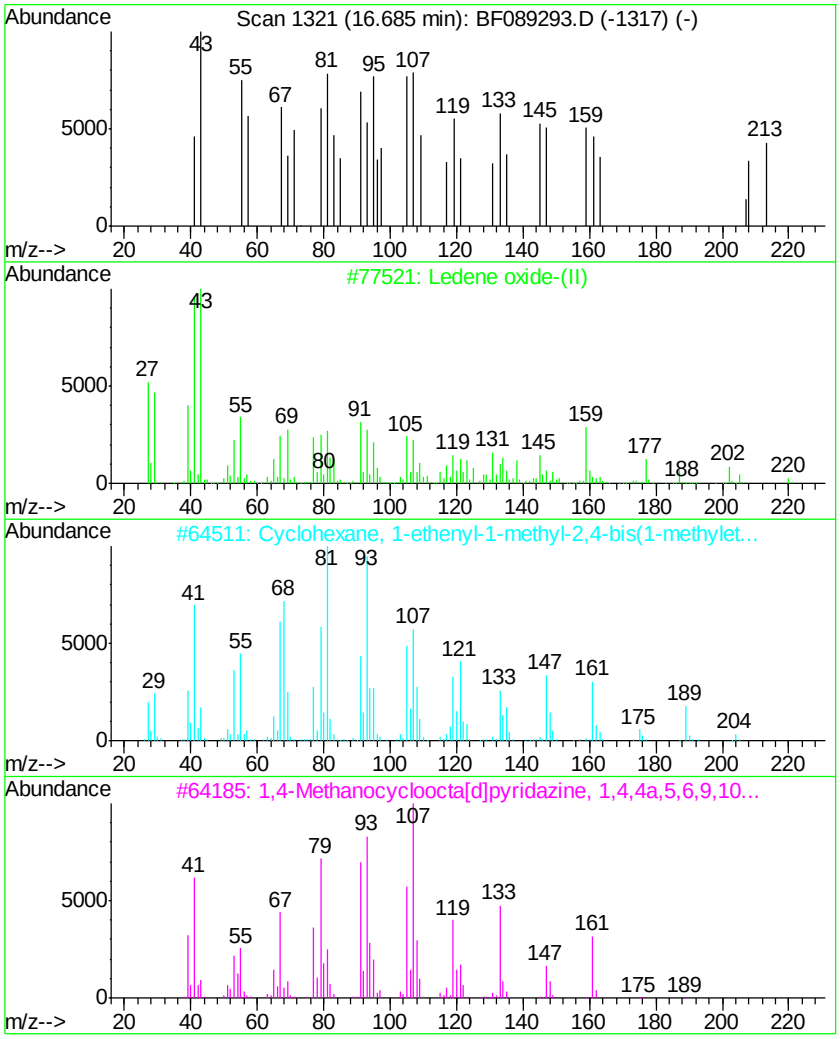
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

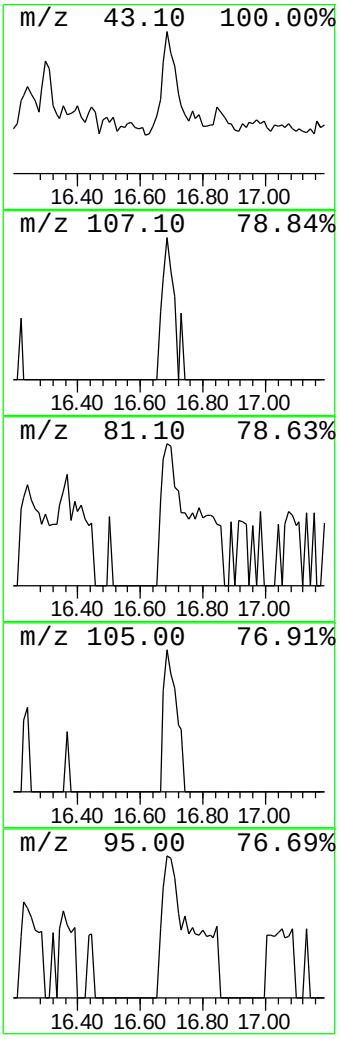
****

Peak Number 9 unknown16.69 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	4.10 ng	42446	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledene oxide-(II)	220	C15H24O	1000159-36-7	37
2	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	32
3	1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	27
4	5,8,11,14,17-Eicosapentaenoic ac...	316	C21H32O2	002734-47-6	27
5	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	27





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.70	5.2	ng	69458	1	6.56	266997	20.0
unknown6.33	6.33	108.9	ng	1453860	1	6.56	266997	20.0
Heptacosane	10.51	3.2	ng	54460	4	11.06	341664	20.0
Behenic alcohol	13.55	4.4	ng	55547	5	13.68	252278	20.0
1-Dodecanol, 2-oc...	14.18	2.2	ng	27468	5	13.68	252278	20.0
Sulfurous acid, d...	15.42	2.5	ng	25751	6	15.02	206901	20.0
unknown16.69	16.69	4.1	ng	42446	6	15.02	206901	20.0