LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090307.D
Acq On : 30 Sep 2016 1:09
Operator : UM/SJ
Sample : H5015-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-3

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-BF092016.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	1.644	3	5	19	rVB	252623	573769	23.49%	2.762%
2	4.536	255	258	269	rBV	301321	462484	18.94%	2.226%
3	5.016	298	300	303	rBV	1603864	2089338	85.54%	10.058%
4	6.124	393	397	399	rBV	1878264	2442402	100.00%	11.757%
5	6.227	403	406	408	rBV	2452550	2432298	99.59%	11.709%
6	6.456	424	426	429	rBV	769216	756509	30.97%	3.642%
7	6.616	437	440	442	rBV	1802447	1652009	67.64%	7.952%
8	7.027	474	476	479	rBV	959071	1341578	54.93%	6.458%
9	7.747	537	539	542	rBV	1114535	981828	40.20%	4.726%
10	8.833	631	634	636	rBV	2110312	1848964	75.70%	8.901%
11	9.233	667	669	671	rBV	935749	770754	31.56%	3.710%
12	9.496	690	692	694	rBV	1212728	1040213	42.59%	5.007%
13	10.273	758	760	763	rBV2	690660	947090	38.78%	4.559%
14	10.422	772	773	780	rVB	29832	46006	1.88%	0.221%
15	10.959	818	820	823	rBV	615924	741516	30.36%	3.570%
16	12.548	956	959	961	rBV	961638	879810	36.02%	4.235%
17	13.474	1037	1040	1047	rBV	45300	77825	3.19%	0.375%
18	13.577	1047	1049	1058	rVV	684567	672677	27.54%	3.238%
19	14.102	1092	1095	1098	rBV	50937	76921	3.15%	0.370%
20	14.342	1114	1116	1118	rBV	21034	27110	1.11%	0.131%
21	14.514	1129	1131	1133	rBV2	35305	37838	1.55%	0.182%
22	14.674	1142	1145	1149	rBV	106089	137020	5.61%	0.660%
23	14.902	1162	1165	1168	rBV	466524	499943	20.47%	2.407%
24	15.131	1182	1185	1191	rBV	61036	78290	3.21%	0.377%
25	15.314	1199	1201	1203	rBV	49188	68292	2.80%	0.329%
26	15.920	1251	1254	1260	rBV	49051	91100	3.73%	0.439%

Sum of corrected areas: 20773584

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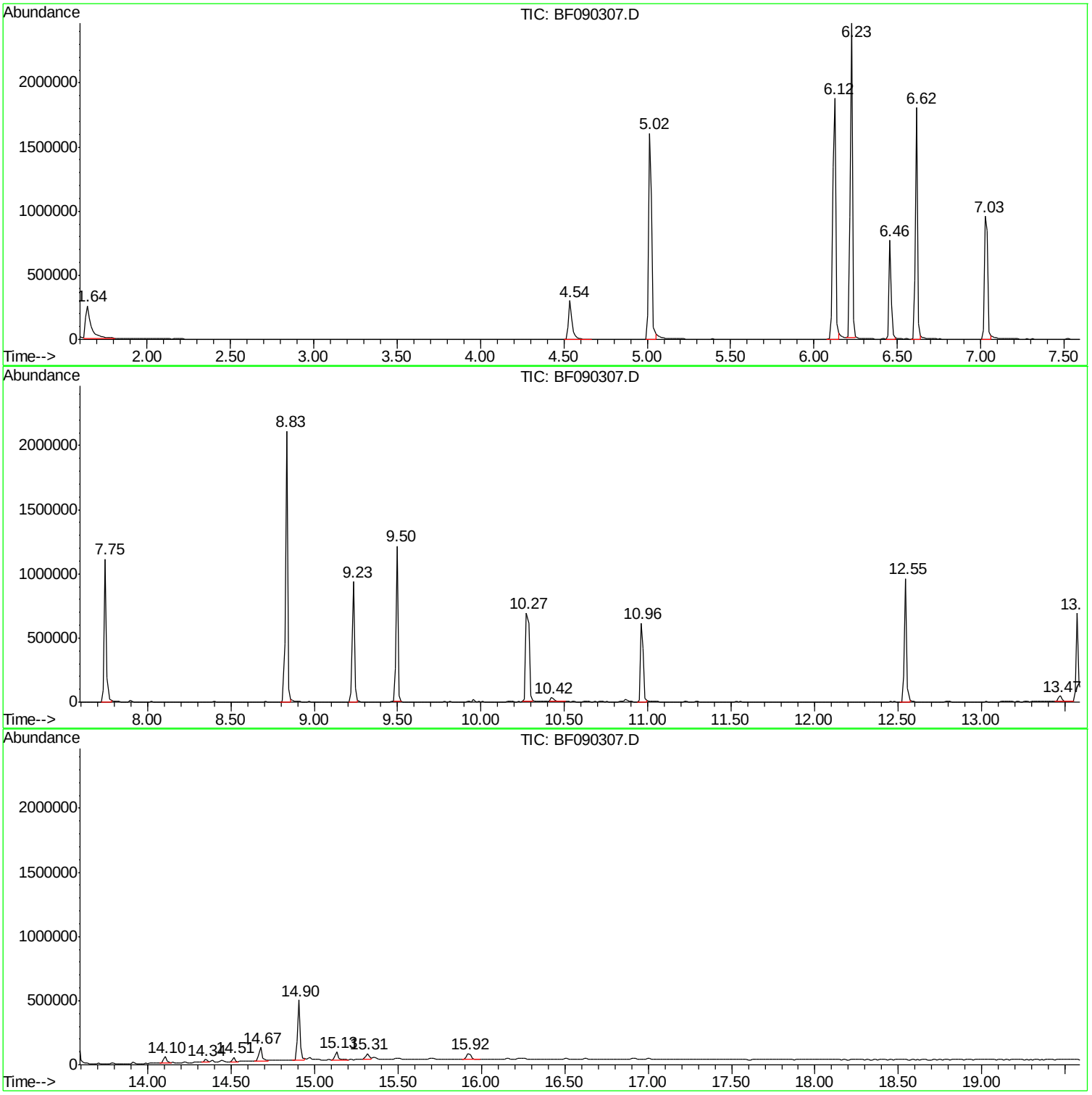
Instrument :
BNA_F
ClientSampleId :
COMPOSITE-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090307.D
Acq On : 30 Sep 2016 1:09
Operator : UM/SJ
Sample : H5015-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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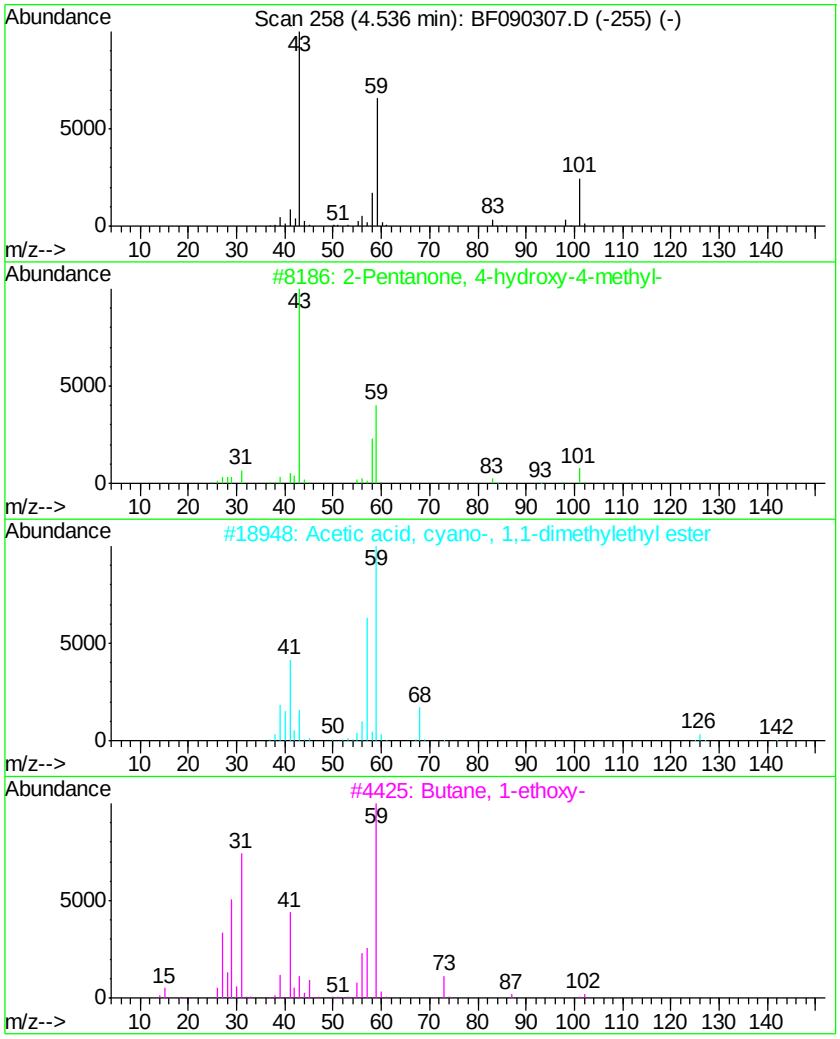
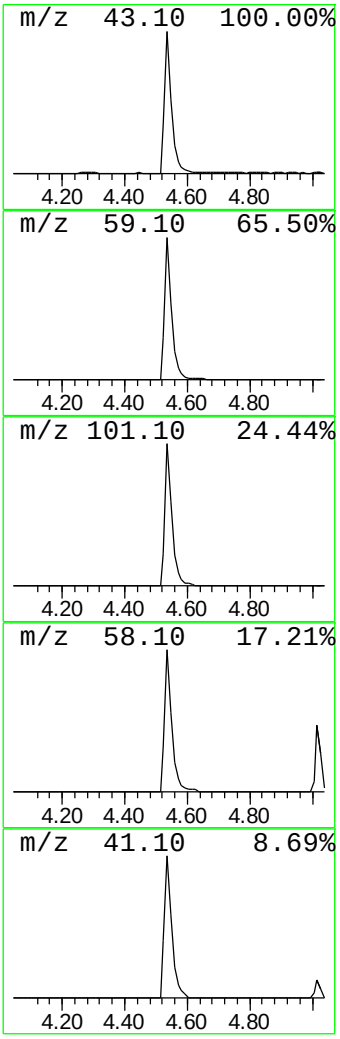
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	12.23 ng	462484	1,4-Dichlorobenzene-d4	6.46

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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Instrument : BNA_F
ClientSampleId : COMPOSITE-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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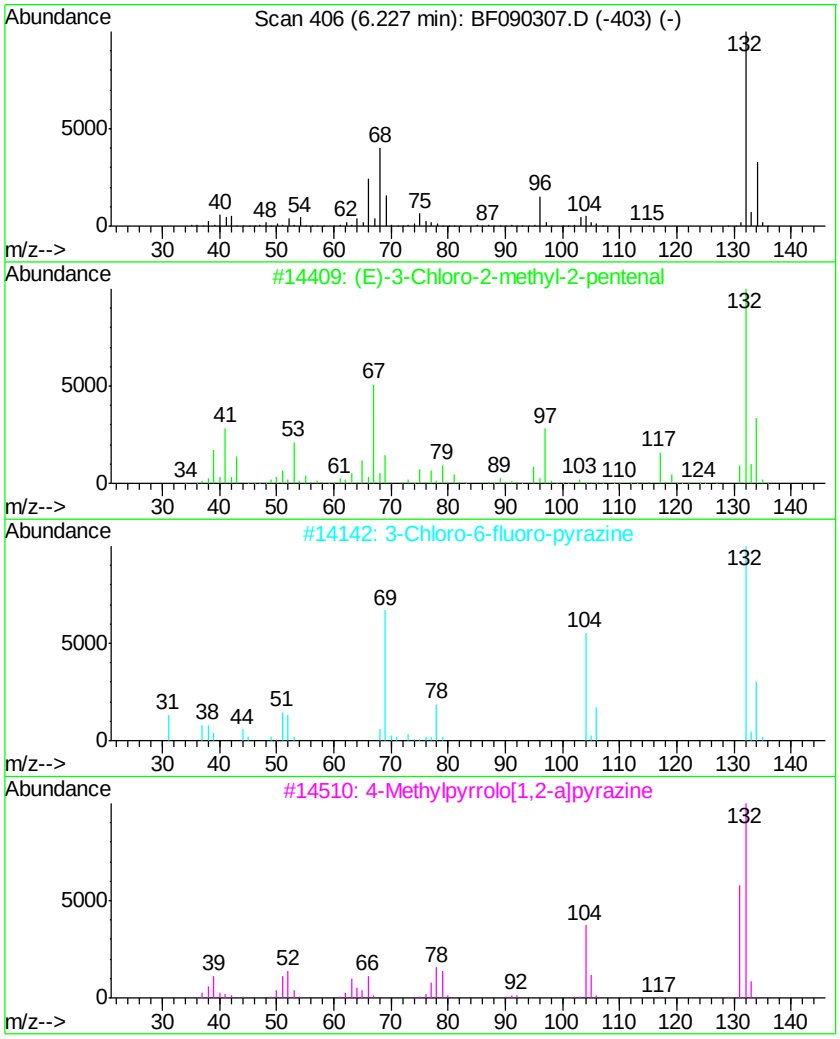
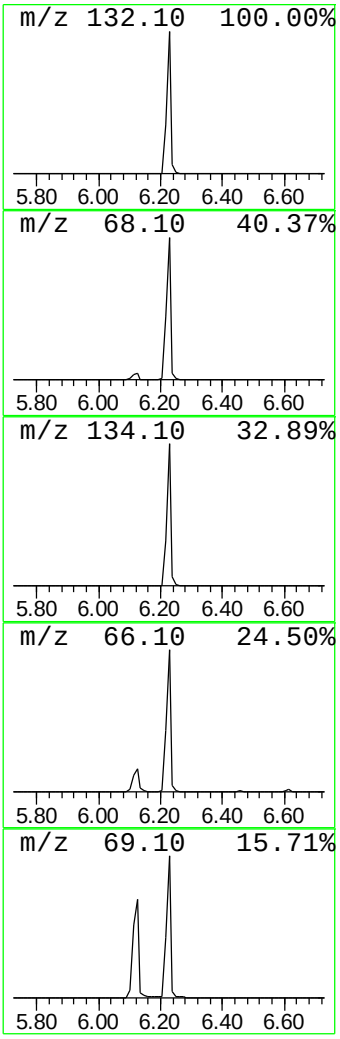
Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	64.30 ng	2432300	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : UM/SJ
Sample : H5015-03
Misc :
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Instrument : BNA_F
ClientSampleId : COMPOSITE-3

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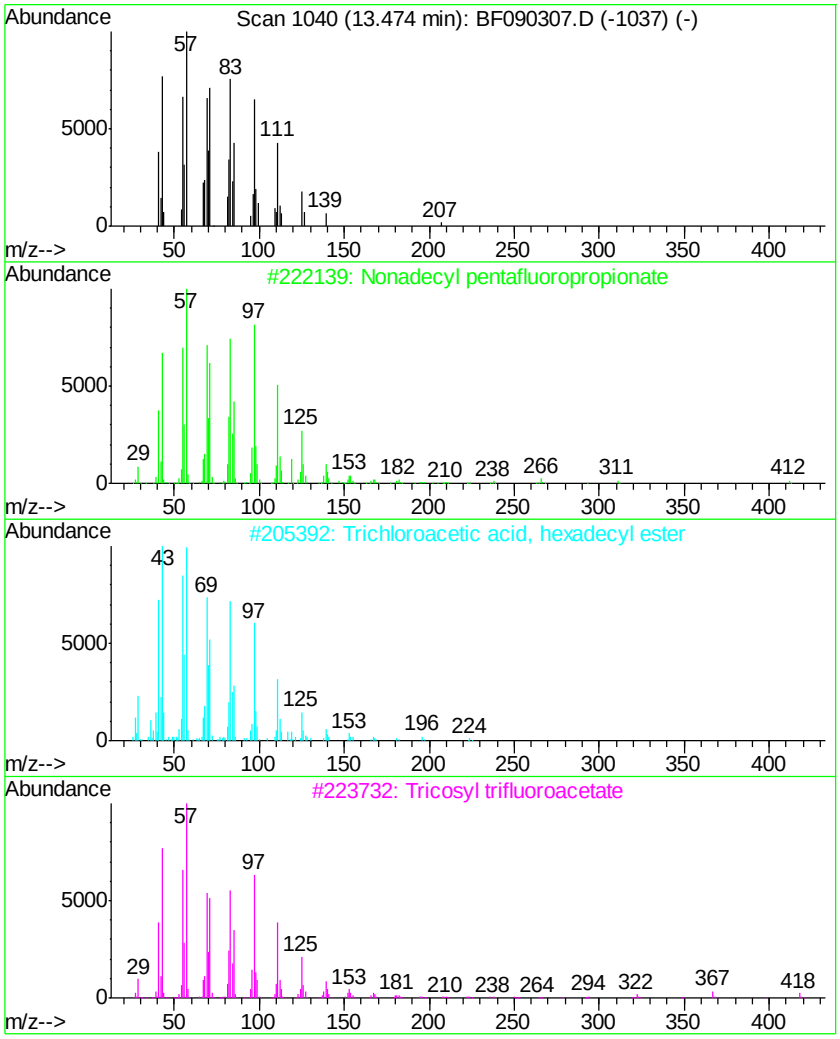
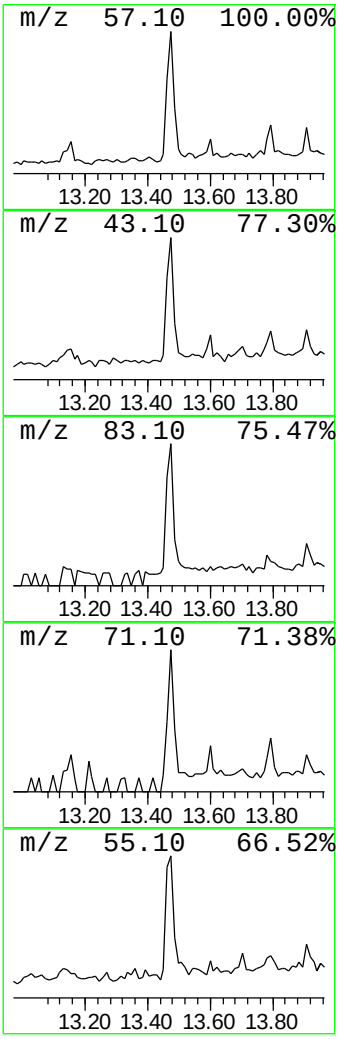
Peak Number 5 Nonadecyl pentafluoropropio... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.31 ng	77825	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	87





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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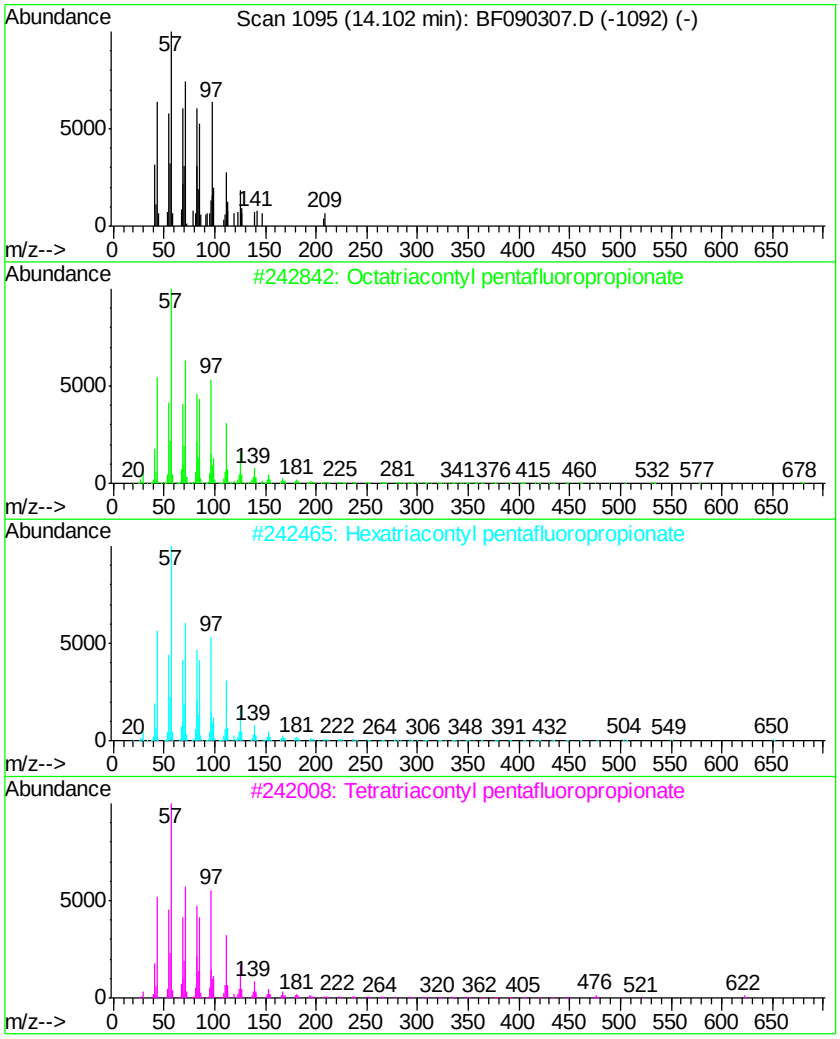
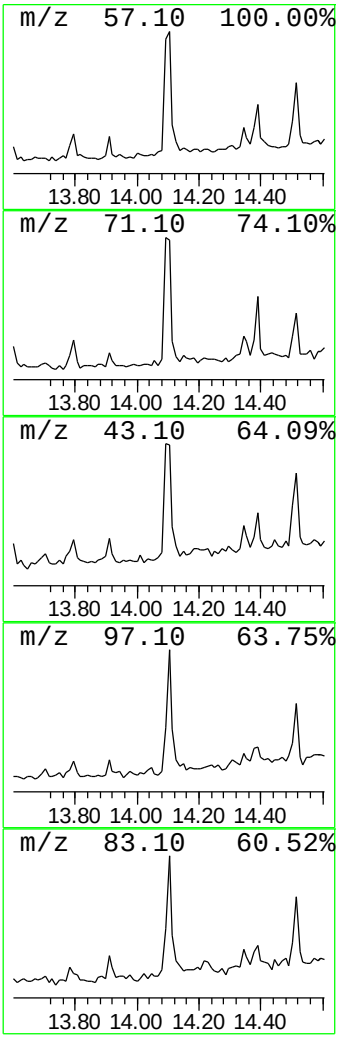
Peak Number 6 Octatriacontyl pentafluorop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.29 ng	76921	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
2	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87
3	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	80
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	60





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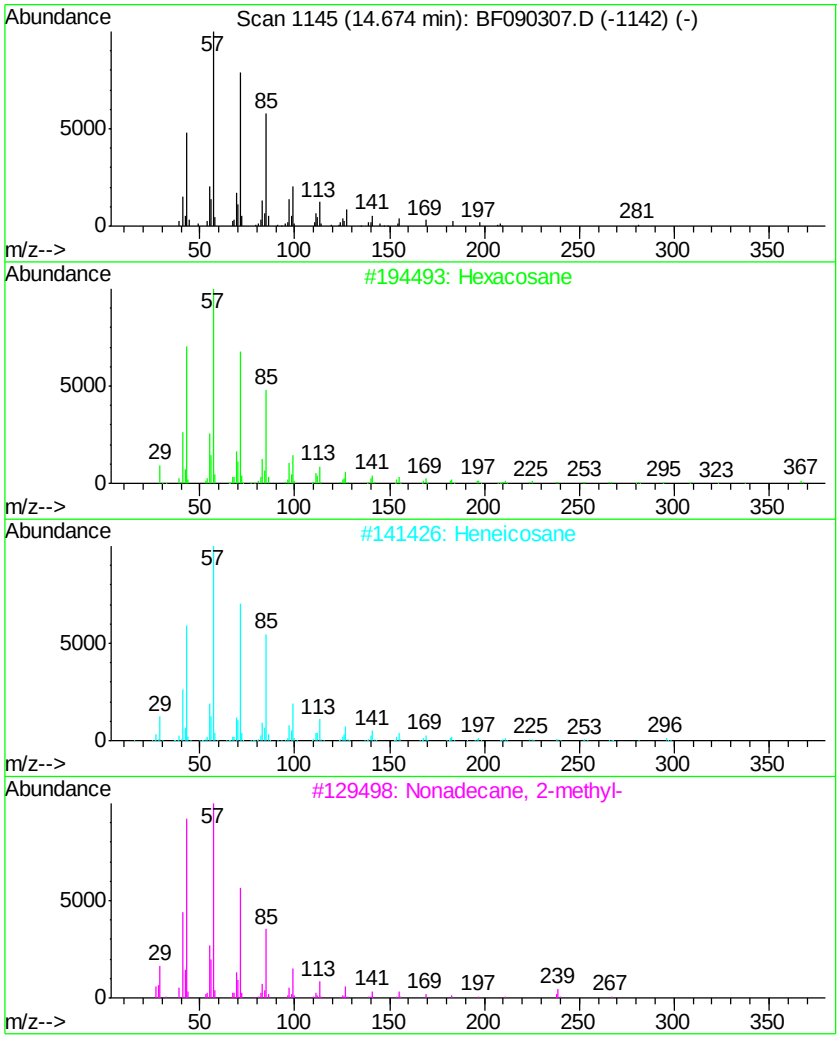
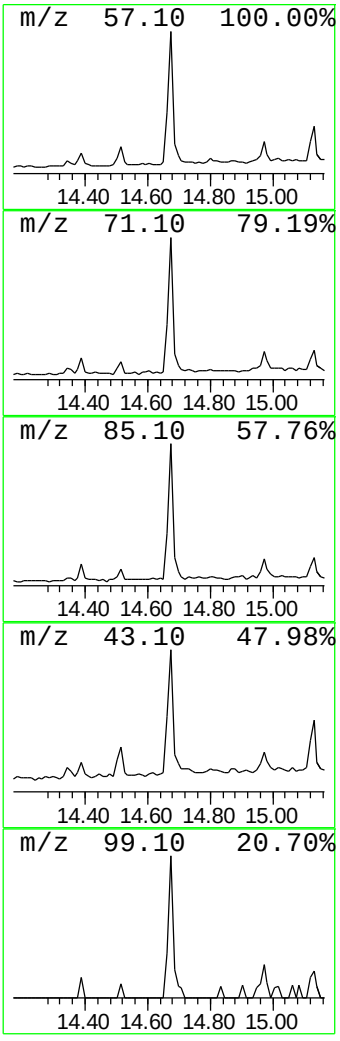
Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	5.48 ng	137020	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octacosane	394	C28H58	000630-02-4	90





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Instrument : BNA_F
ClientSampleId : COMPOSITE-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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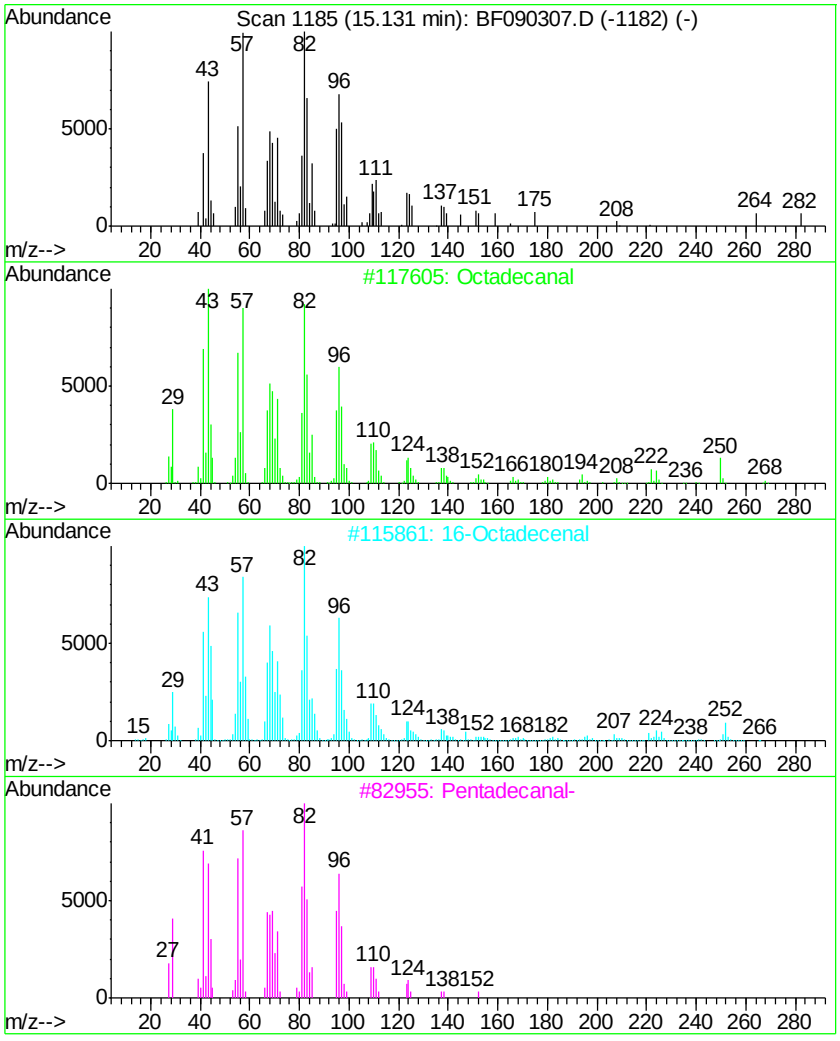
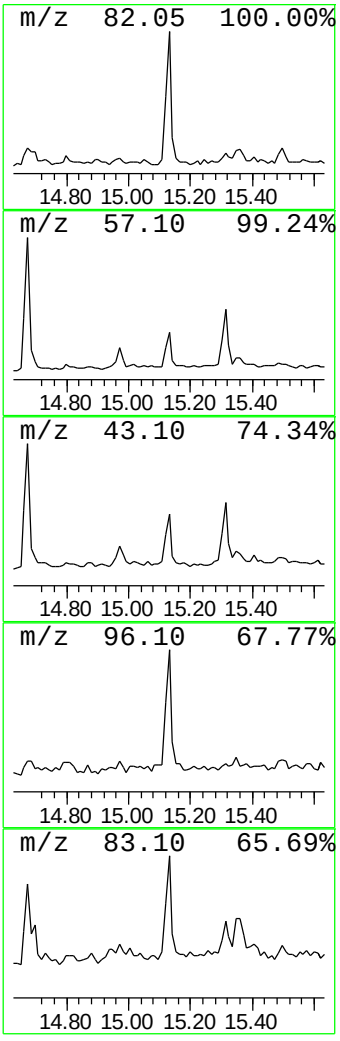
Peak Number 8 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	3.13 ng	78290	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	16-Octadecenal	266	C18H34O	056554-87-1	90
3	Pentadecanal-	226	C15H30O	002765-11-9	87
4	Heptadecanal	254	C17H34O	1000376-70-0	87
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80





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

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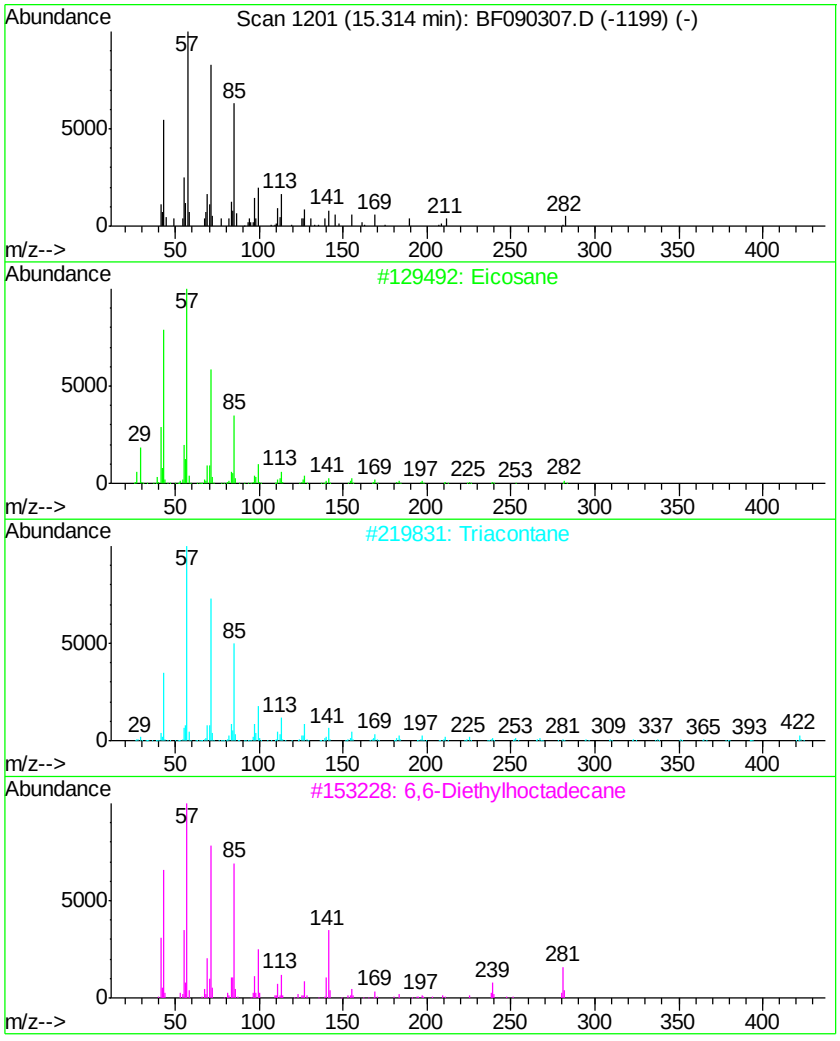
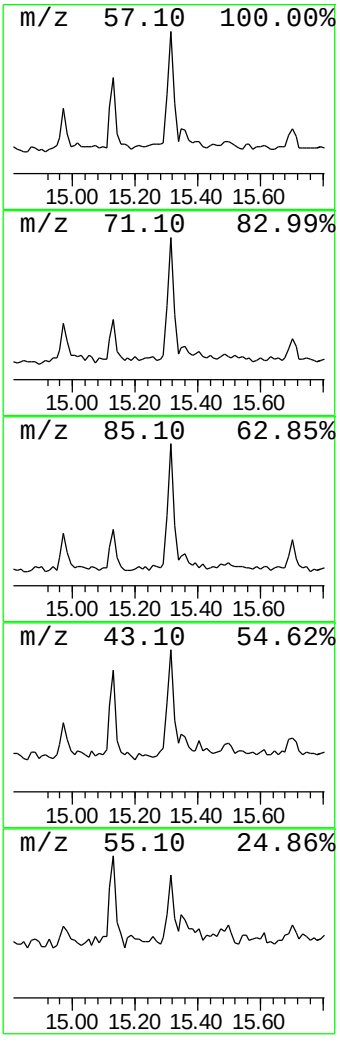
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.73 ng	68292	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Triacontane	422	C30H62	000638-68-6	91
3	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.54	12.2	ng	462484	1	6.46	756509	20.0
unknown6.23	6.23	64.3	ng	2432300	1	6.46	756509	20.0
Nonadecyl pentafl...	13.47	2.3	ng	77825	5	13.58	672677	20.0
Octatriacontyl pe...	14.10	2.3	ng	76921	5	13.58	672677	20.0
Hexacosane	14.67	5.5	ng	137020	6	14.90	499943	20.0
Octadecanal	15.13	3.1	ng	78290	6	14.90	499943	20.0
Eicosane	15.31	2.7	ng	68292	6	14.90	499943	20.0