LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092016\
Data File : BF090145.D
Acq On : 20 Sep 2016 20:29
Operator : UM/SJ
Sample : H4854-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-01-A1A

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	1.678	6	8	53	rVB	3442450	11557261	100.00%	27.383%
2	2.215	53	55	70	rVB	79678	174113	1.51%	0.413%
3	4.616	262	265	276	rBV	439406	697915	6.04%	1.654%
4	5.084	303	306	320	rBV	2556396	2860061	24.75%	6.776%
5	6.170	398	401	403	rBV	2810893	3000787	25.96%	7.110%
6	6.284	408	411	413	rBV	3010485	3153126	27.28%	7.471%
7	6.513	429	431	438	rBV	831238	878802	7.60%	2.082%
8	6.673	442	445	447	rBV	2573757	2462609	21.31%	5.835%
9	7.084	478	481	484	rBV	1674870	1762098	15.25%	4.175%
10	7.805	541	544	546	rBV	1305668	1209452	10.46%	2.866%
11	8.890	636	639	641	rBV	3235197	3765631	32.58%	8.922%
12	9.290	671	674	676	rBV	1037000	1112874	9.63%	2.637%
13	9.553	694	697	699	rBV	1108714	1414901	12.24%	3.352%
14	10.331	762	765	768	rBV	1657003	1630091	14.10%	3.862%
15	11.016	822	825	828	rBV	1545747	1397963	12.10%	3.312%
16	12.605	961	964	966	rBV	2901261	3183008	27.54%	7.542%
17	13.519	1041	1044	1051	rBV	120722	203454	1.76%	0.482%
18	13.622	1051	1053	1056	rBV	775761	1033285	8.94%	2.448%
19	14.948	1167	1169	1172	rBV	572233	708615	6.13%	1.679%

Sum of corrected areas: 42206046

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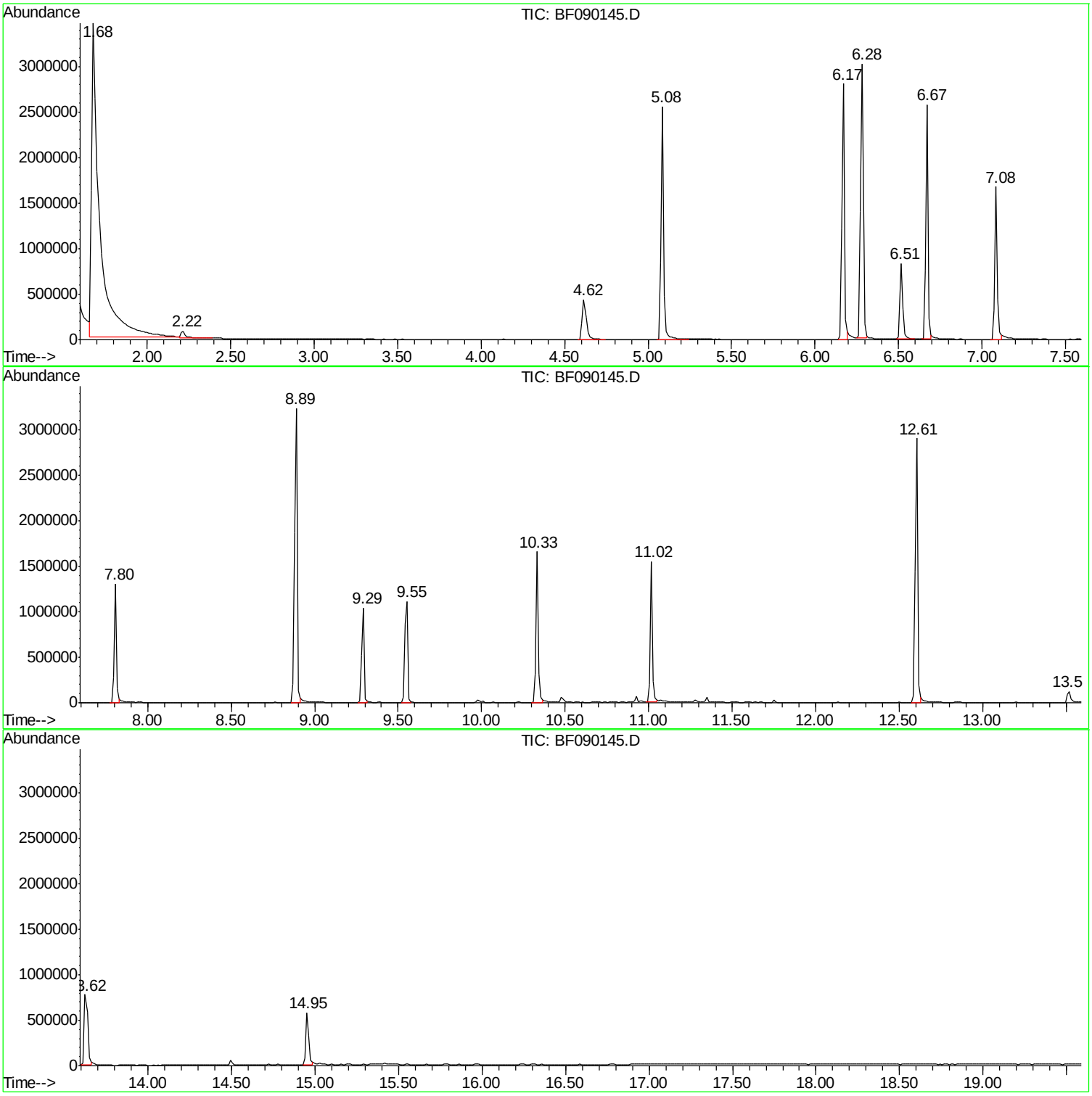
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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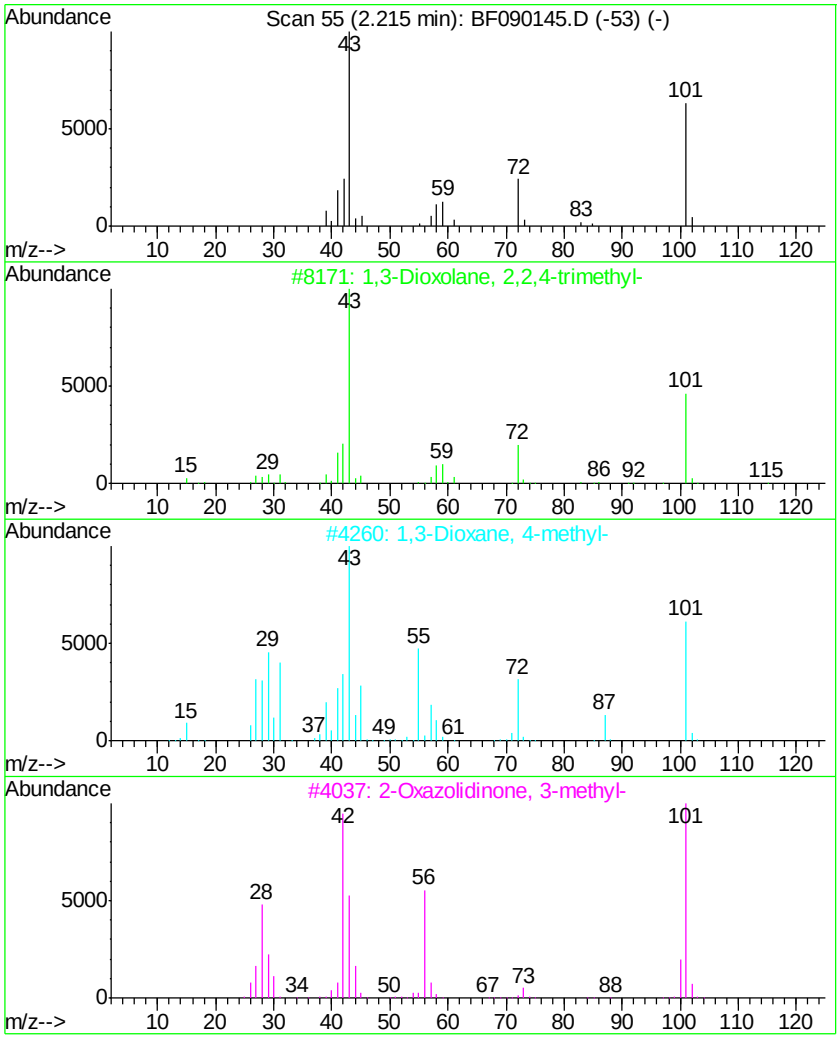
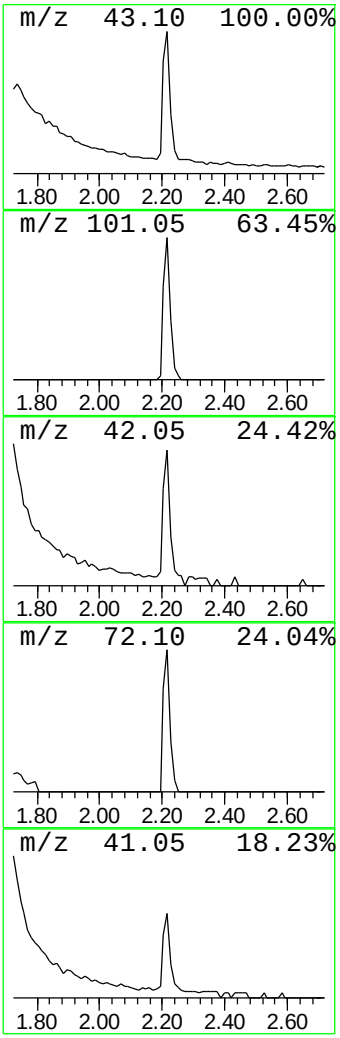
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.96 ng	174113	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	72
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	10
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5	Butane	58	C4H10	000106-97-8	9





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BNA_F
ClientSampleId :
FK-BPM-01-A1A

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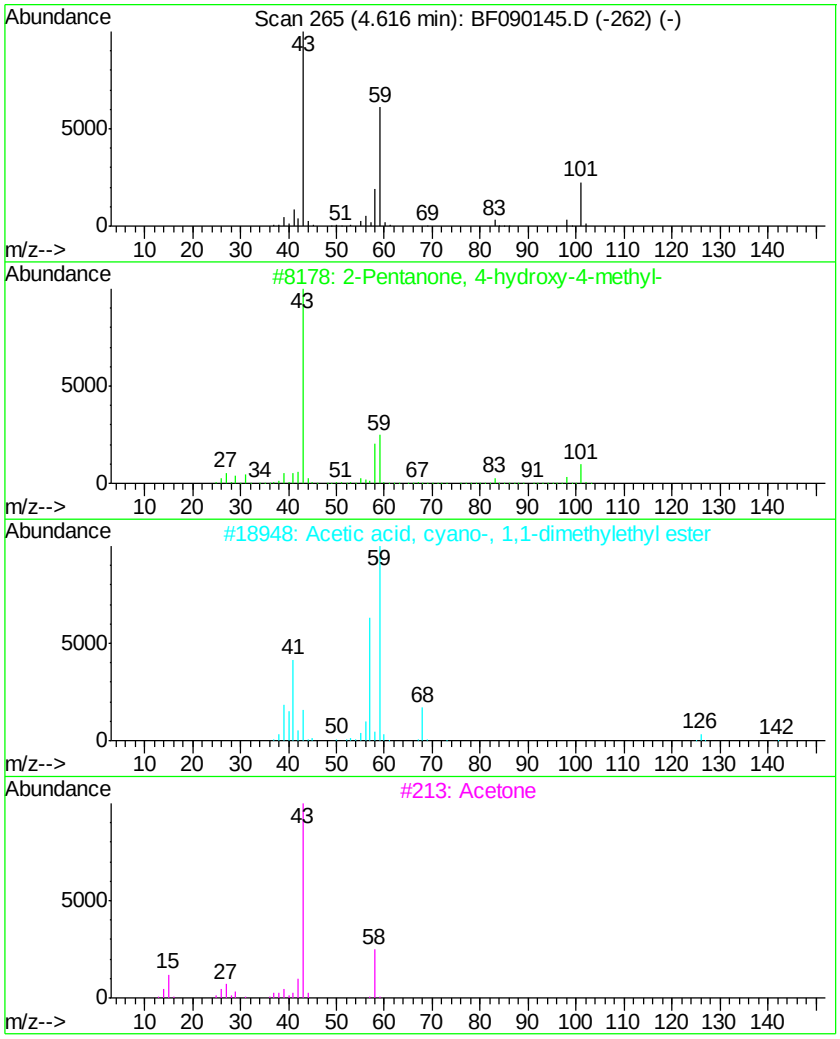
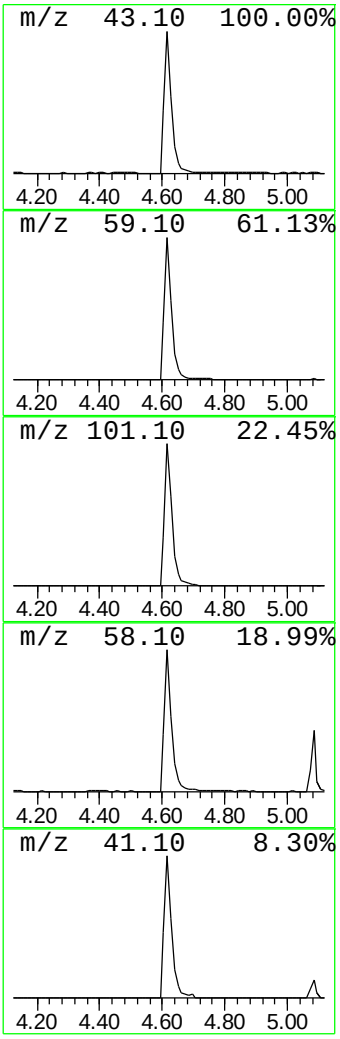
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	15.88 ng	697915	1,4-Dichlorobenzene-d4	6.51

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	17
3	Acetone	58	C3H6O	000067-64-1	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Sample : H4854-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-01-A1A

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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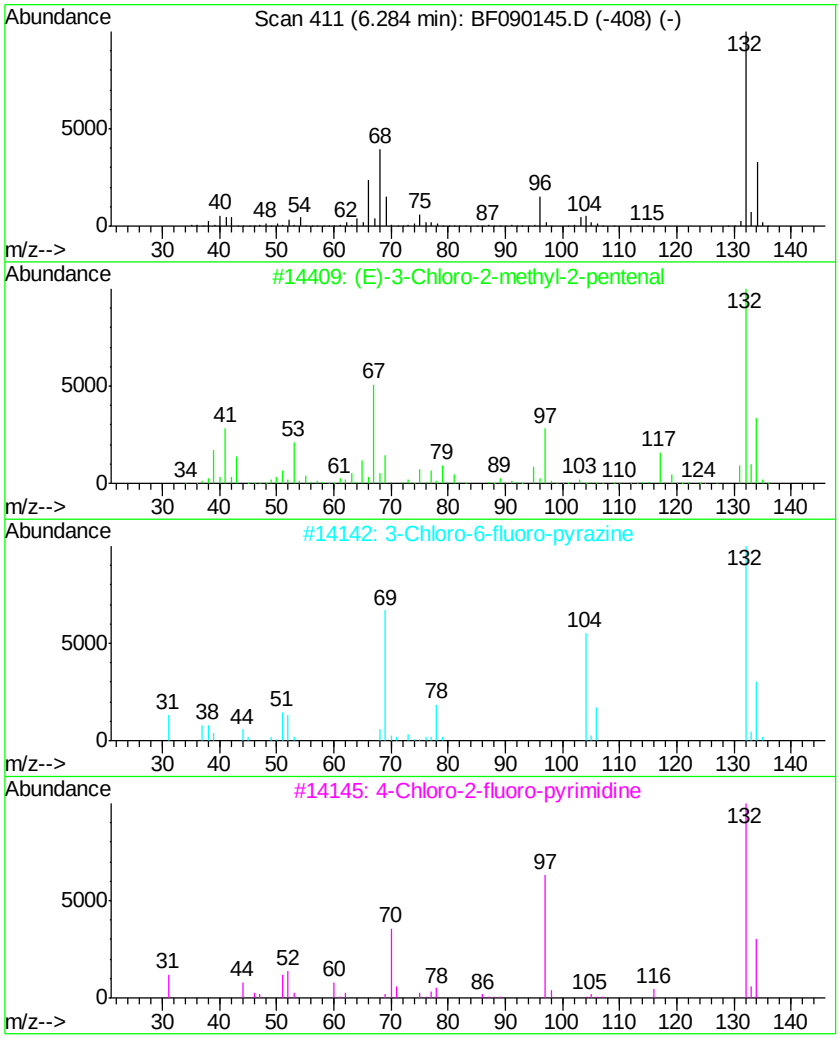
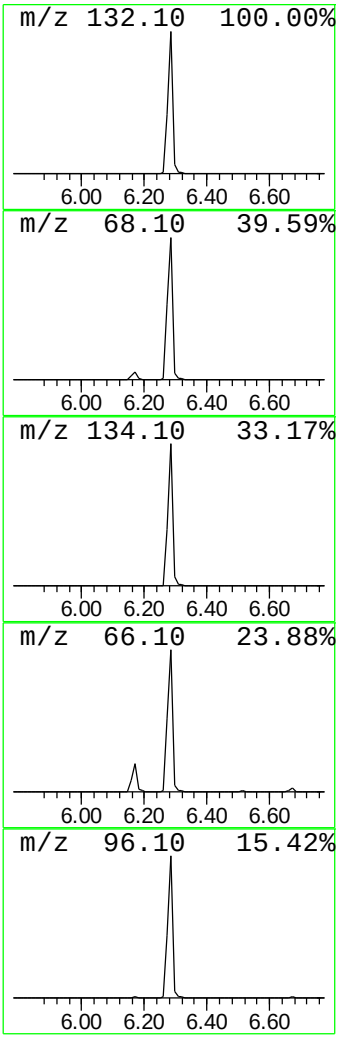
Peak Number 4 unknown6.28 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.28	71.76 ng	3153130	1,4-Dichlorobenzene-d4	6.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : H4854-05
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-01-A1A

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
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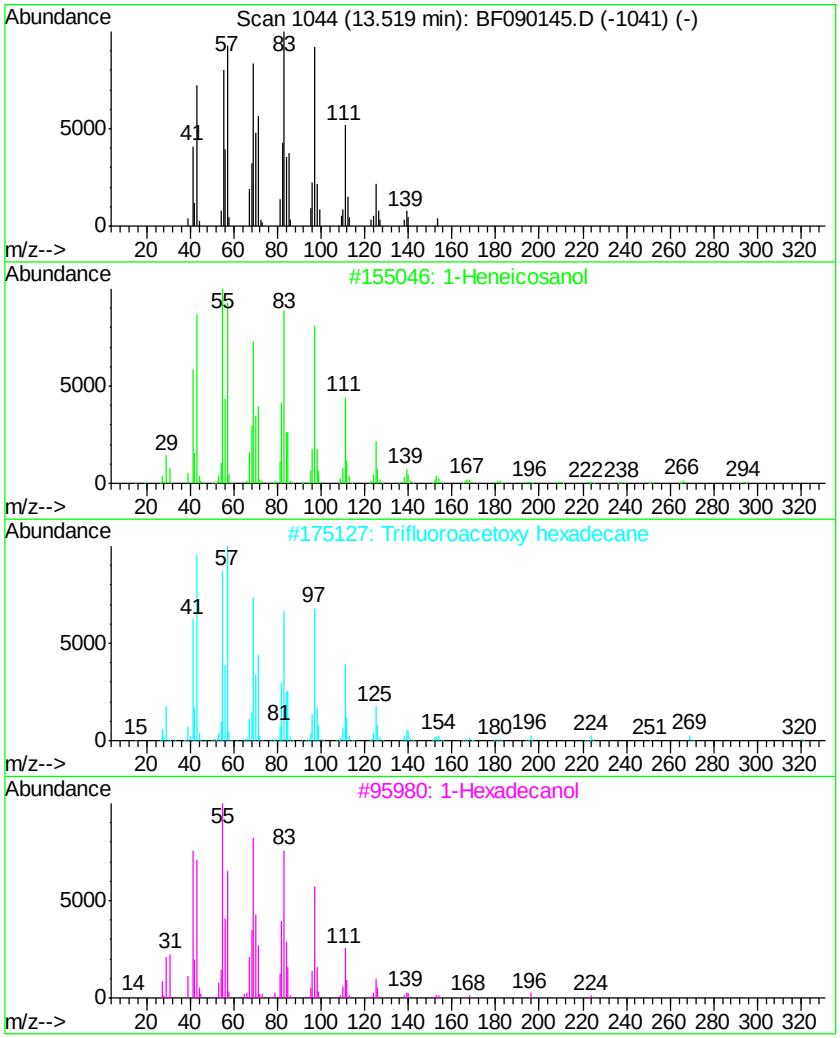
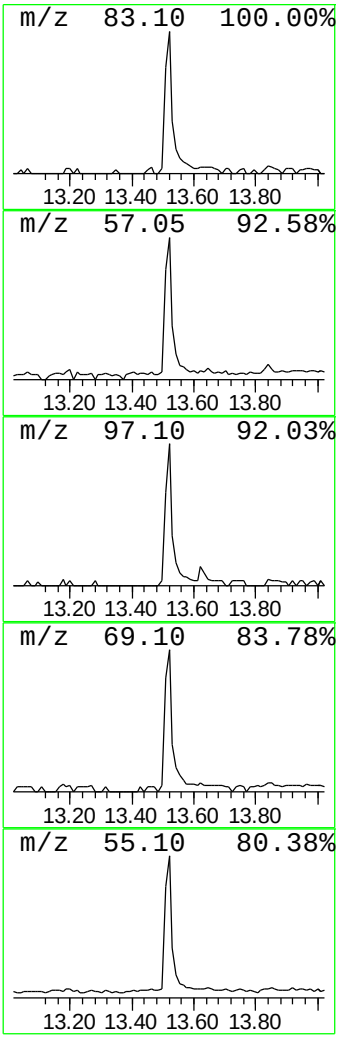
Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	3.94 ng	203454	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90





Tentatively Identified Compound (LSC) summary

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-BPM-01-A1A

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
1,3-Dioxolane, 2,...	2.22	4.0	ng	174113	1	6.51	878802	20.0
2-Pentanone, 4-hy...	4.62	15.9	ng	697915	1	6.51	878802	20.0
unknown6.28	6.28	71.8	ng	3153130	1	6.51	878802	20.0
1-Heneicosanol	13.52	3.9	ng	203454	5	13.62	1033290	20.0