LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090257.D
Acq On : 27 Sep 2016 17:43
Operator : UM/SJ
Sample : H4933-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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	4	5	52	rVB	2989037	8504743	100.00%	19.797%
2	4.559	257	260	275	rVB	408956	697014	8.20%	1.623%
3	5.039	298	302	304	rBV	2195138	3242863	38.13%	7.549%
4	6.136	394	398	400	rBV	2462271	3559867	41.86%	8.287%
5	6.239	404	407	409	rBV	3117522	3239679	38.09%	7.541%
6	6.467	425	427	430	rBV	878256	807441	9.49%	1.880%
7	6.627	438	441	443	rBV	2813895	2606020	30.64%	6.066%
8	7.039	475	477	480	rBV	1549225	1979510	23.28%	4.608%
9	7.176	487	489	498	rVB	56578	104288	1.23%	0.243%
10	7.759	537	540	542	rBV	1170031	1110080	13.05%	2.584%
11	8.845	632	635	637	rBV	3053105	3815066	44.86%	8.881%
12	9.245	667	670	672	rBV	1158125	1292647	15.20%	3.009%
13	9.496	690	692	695	rVB	1252389	1264146	14.86%	2.943%
14	10.285	758	761	764	rBV	2148997	2360514	27.76%	5.495%
15	10.433	770	774	778	rBV	109599	142069	1.67%	0.331%
16	10.971	818	821	823	rBV	1373562	1374965	16.17%	3.201%
17	11.233	841	844	848	rBV	70840	94005	1.11%	0.219%
18	11.531	868	870	878	rBV3	84022	149624	1.76%	0.348%
19	12.559	957	960	962	rBV	3293001	3640261	42.80%	8.474%
20	13.474	1037	1040	1047	rBV	227317	364958	4.29%	0.850%
21	13.577	1047	1049	1052	rBV	1155483	1329225	15.63%	3.094%
22	14.445	1123	1125	1128	rVB	131632	138710	1.63%	0.323%
23	14.902	1162	1165	1167	rBV	1020379	1141059	13.42%	2.656%

Sum of corrected areas: 42958754

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
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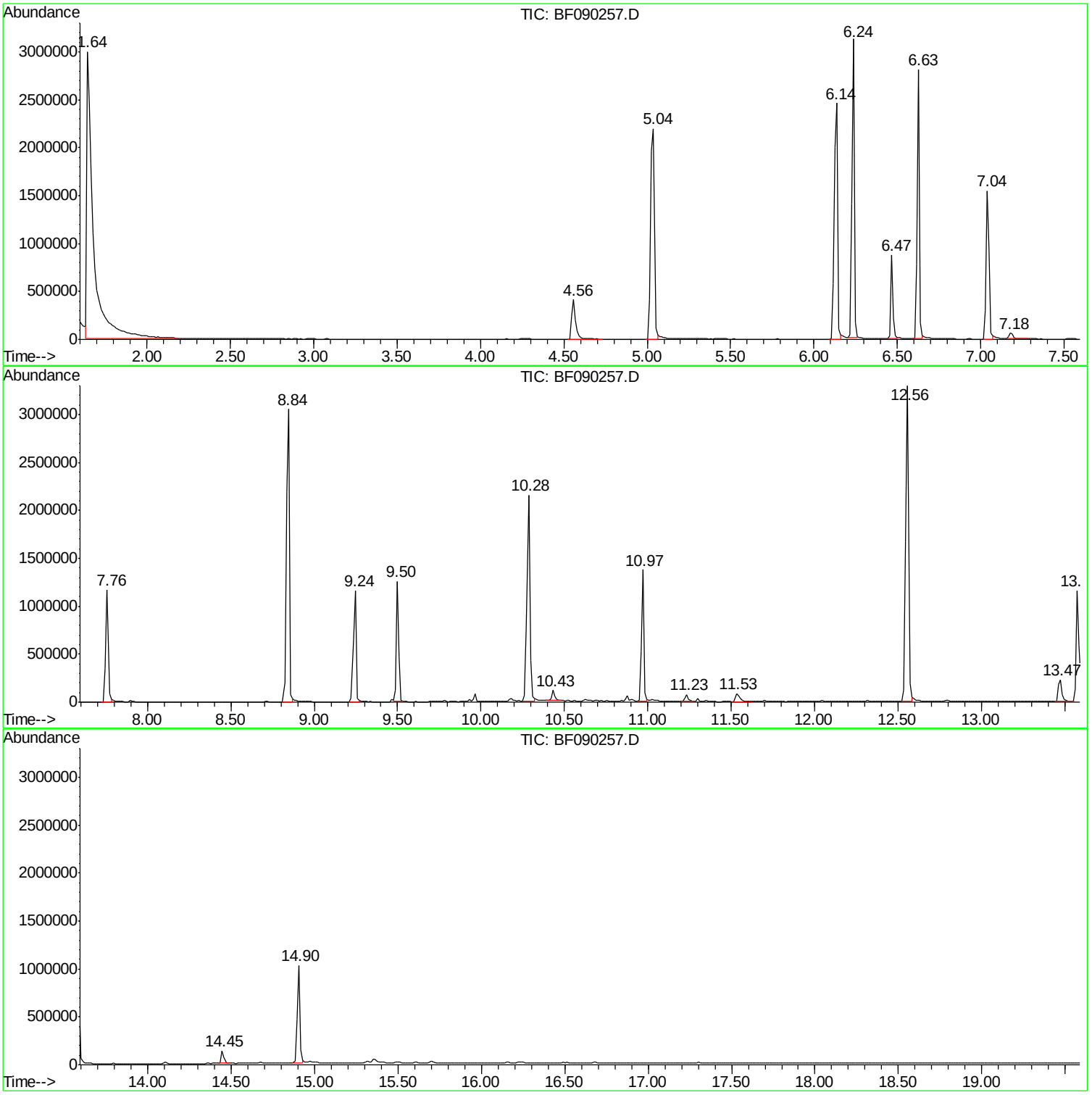
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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\BF092716\
Data File : BF090257.D
Acq On : 27 Sep 2016 17:43
Operator : UM/SJ
Sample : H4933-07
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ClientSampleId : B6-9.5-10

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

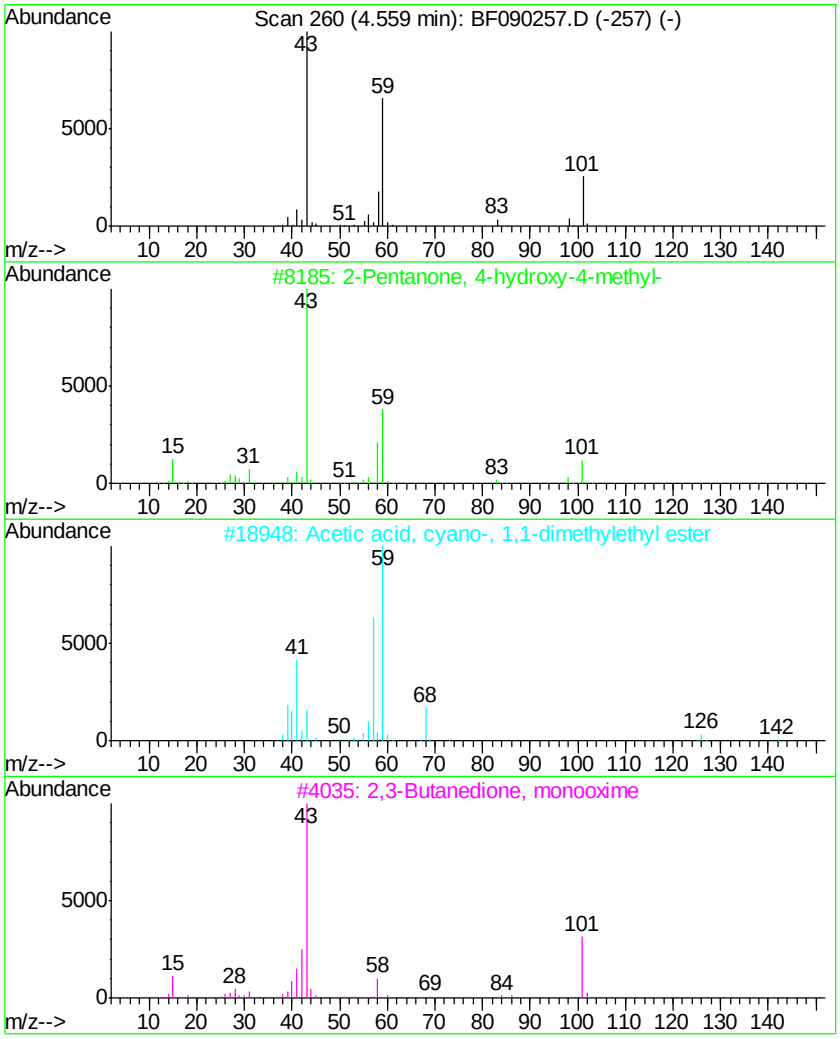
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

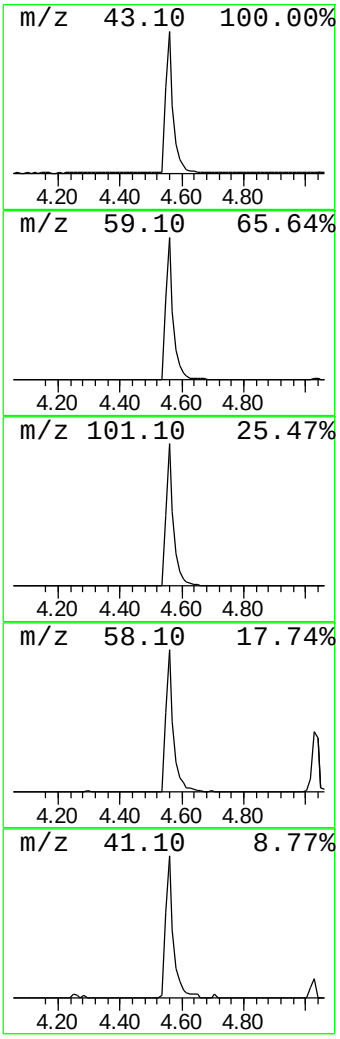
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	17.26 ng	697014	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090257.D
Acq On : 27 Sep 2016 17:43
Operator : UM/SJ
Sample : H4933-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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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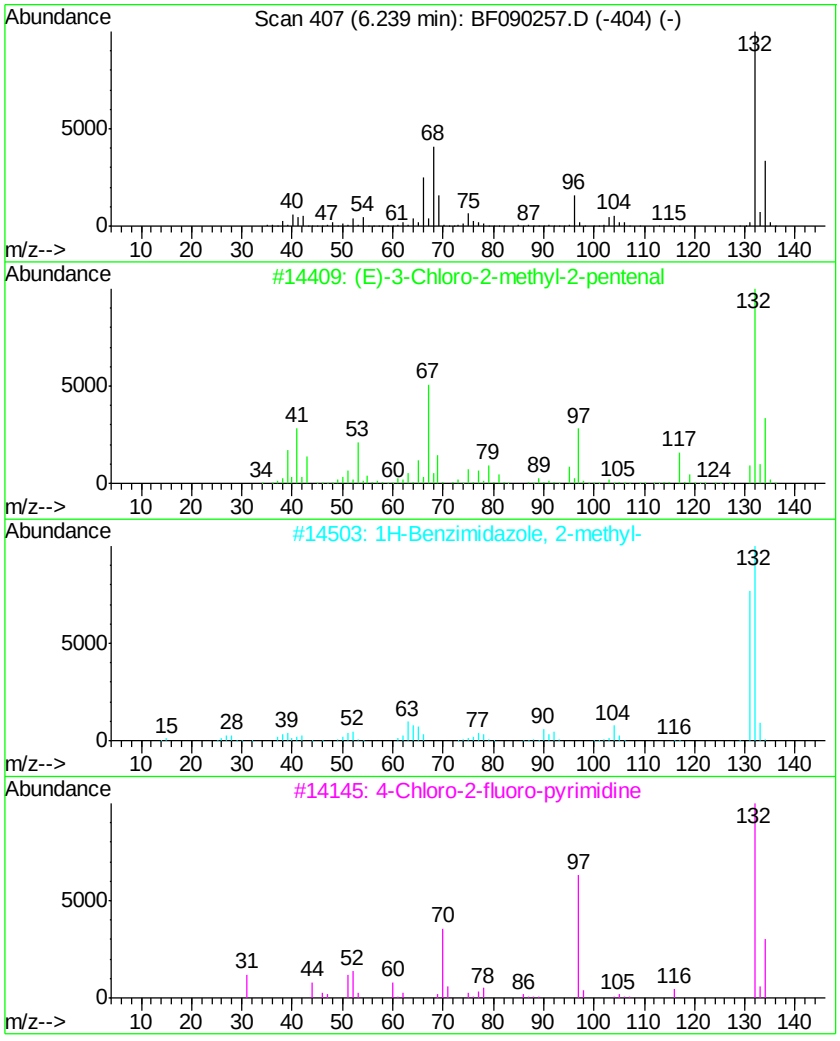
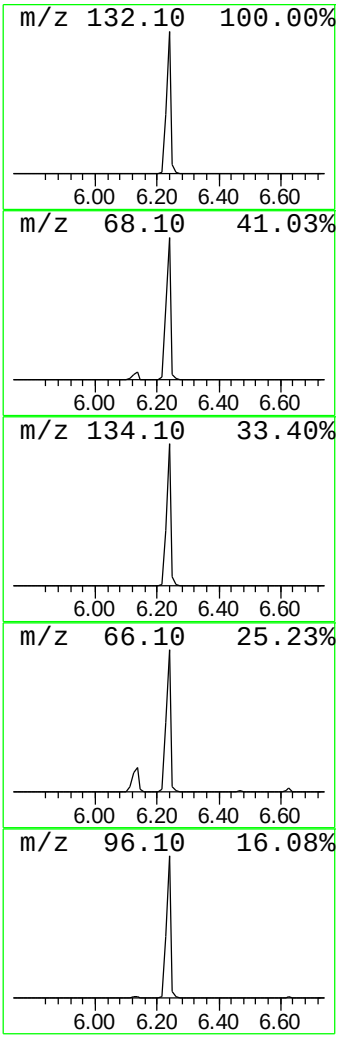
Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	80.25 ng	3239680	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090257.D
Acq On : 27 Sep 2016 17:43
Operator : UM/SJ
Sample : H4933-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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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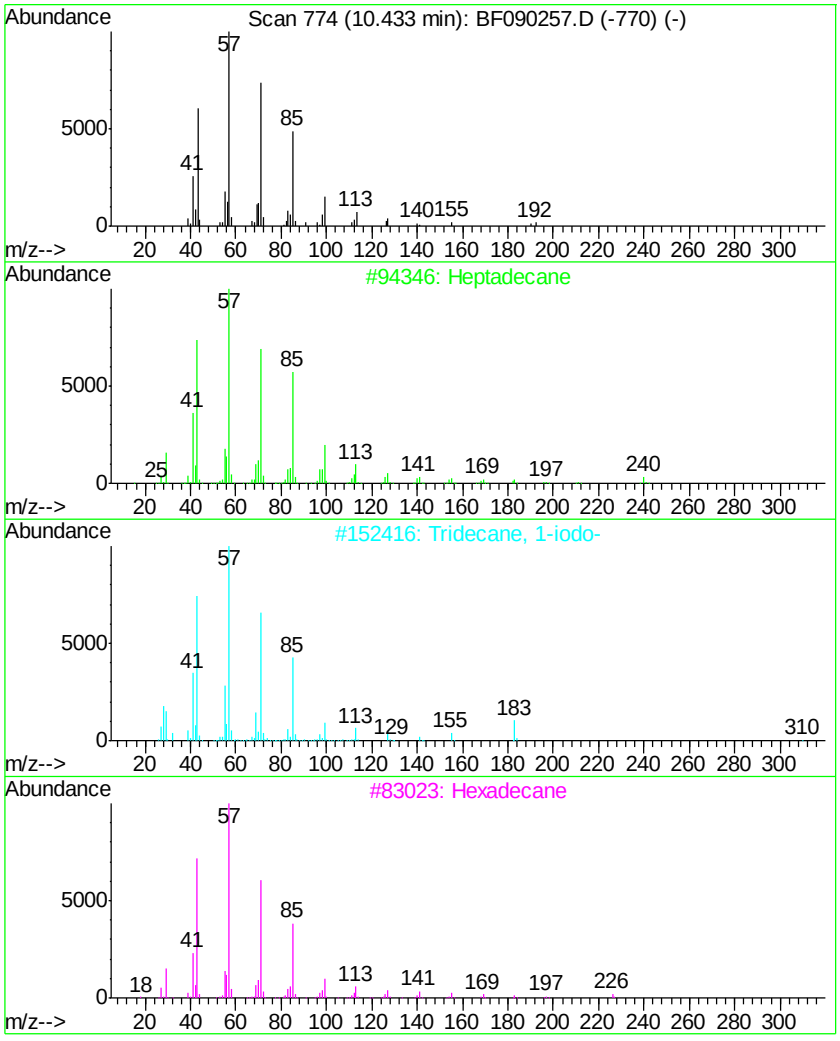
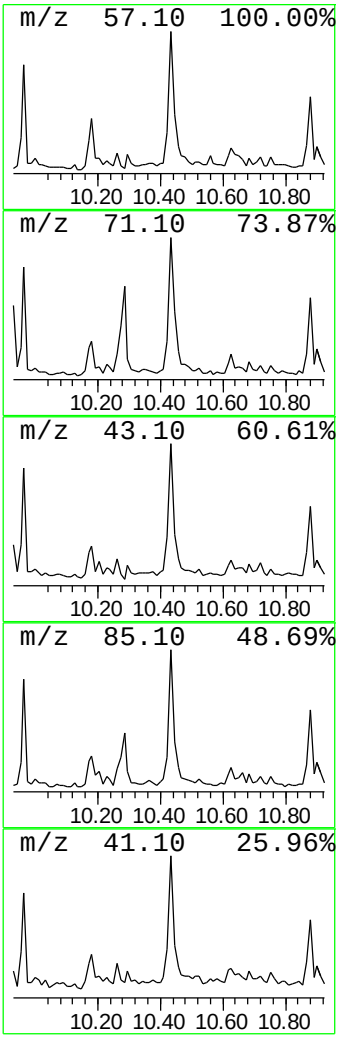
****

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.07 ng	142069	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
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Operator : UM/SJ
Sample : H4933-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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

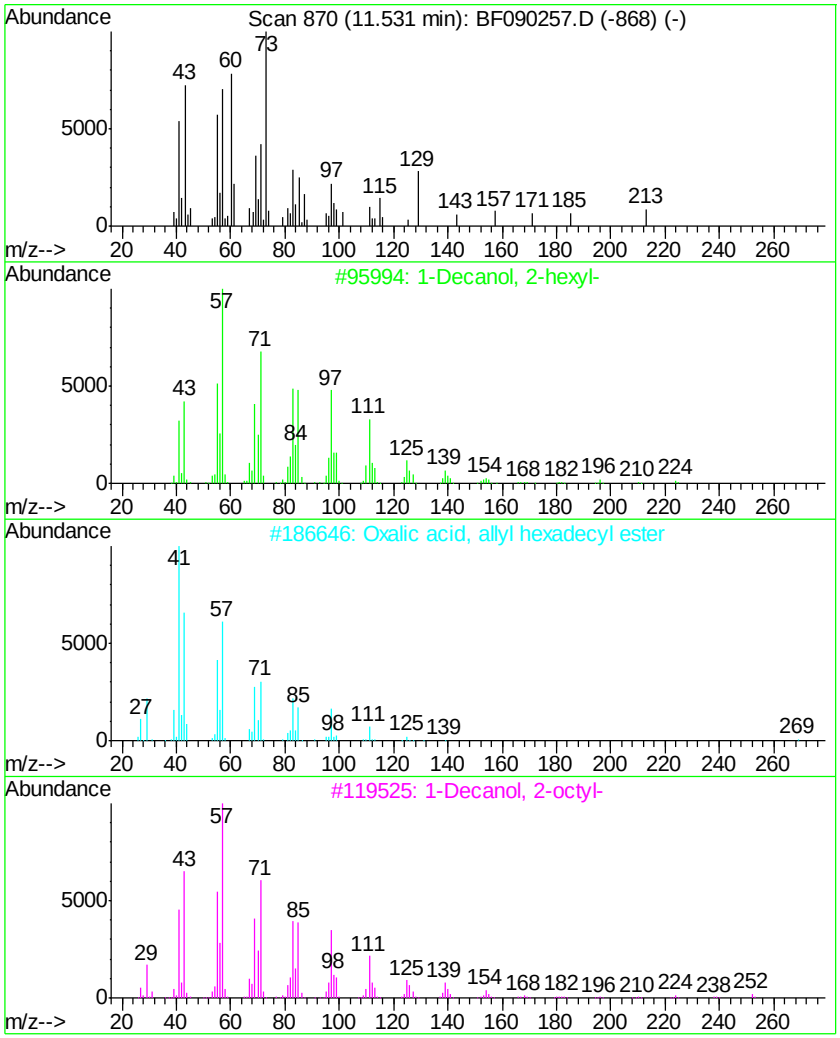
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

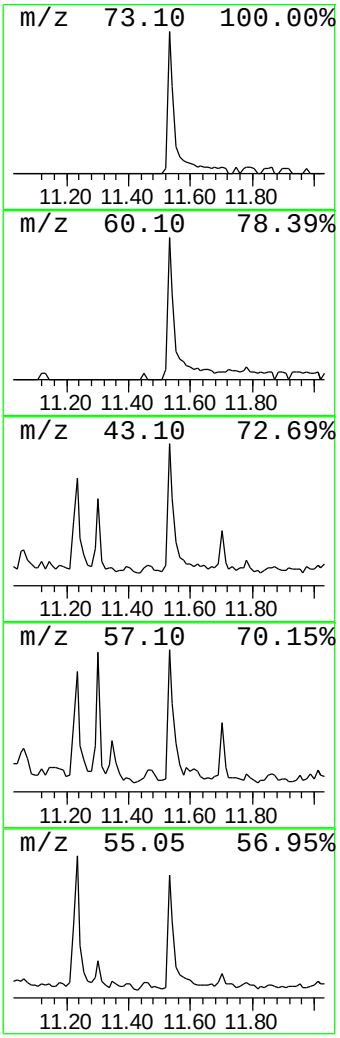
****

Peak Number 6 unknown11.53 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.18 ng	149624	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	30
4	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	30
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090257.D
Acq On : 27 Sep 2016 17:43
Operator : UM/SJ
Sample : H4933-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B6-9.5-10

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

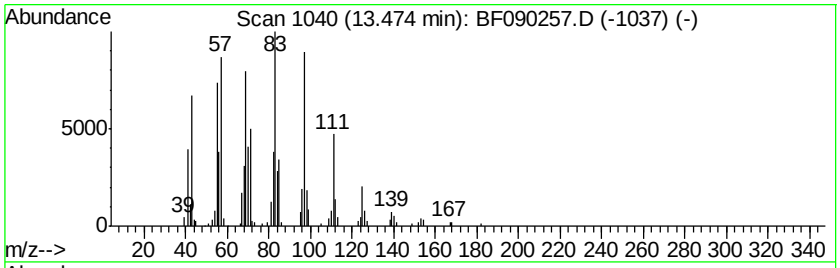
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

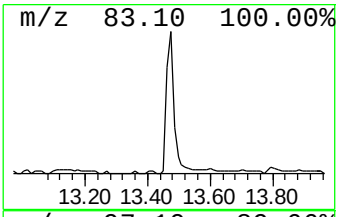
****

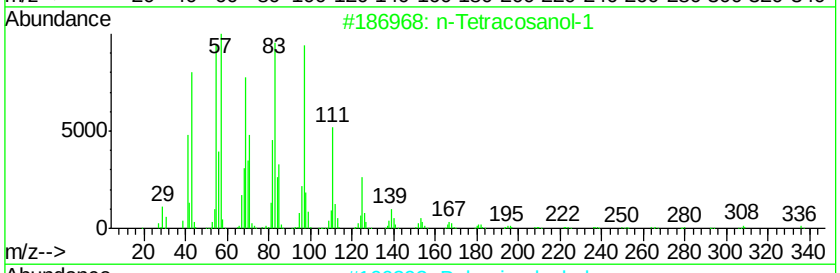
Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

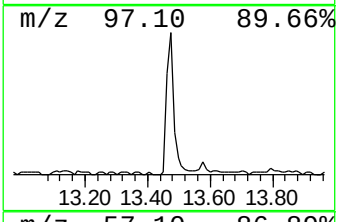
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.49 ng	364958	Chrysene-d12	13.58

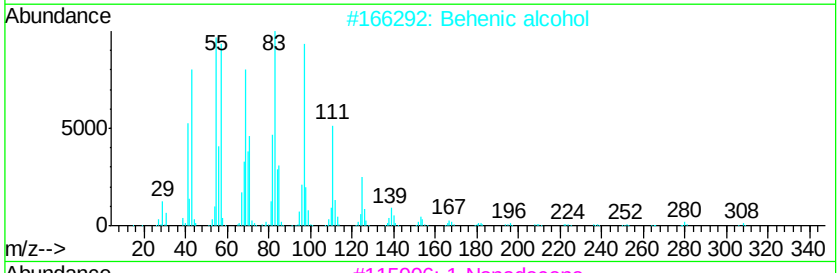
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93

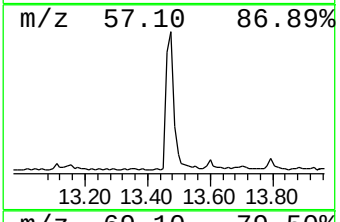


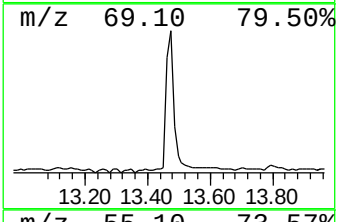


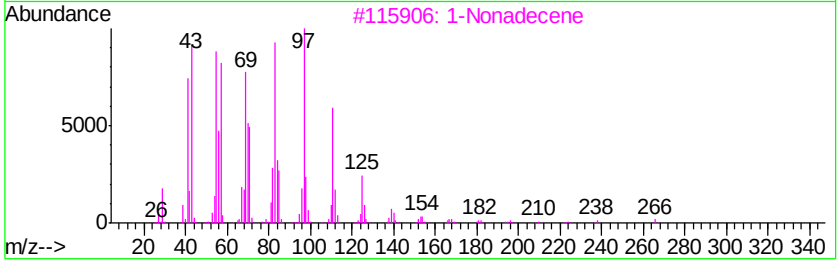


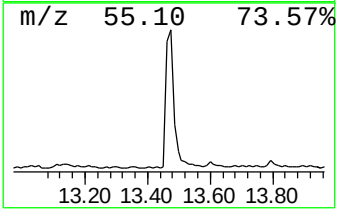












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

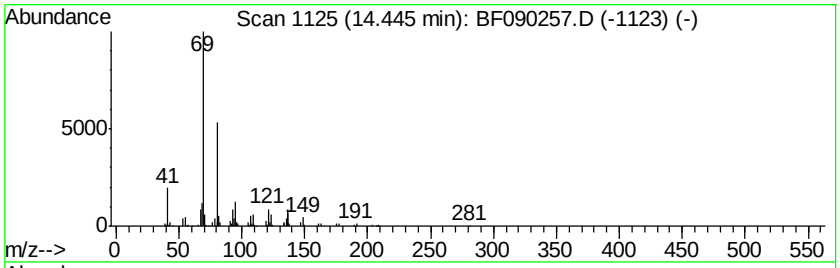
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

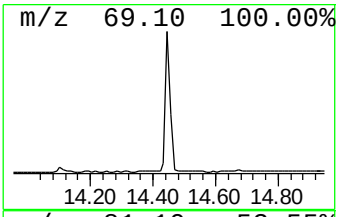
****

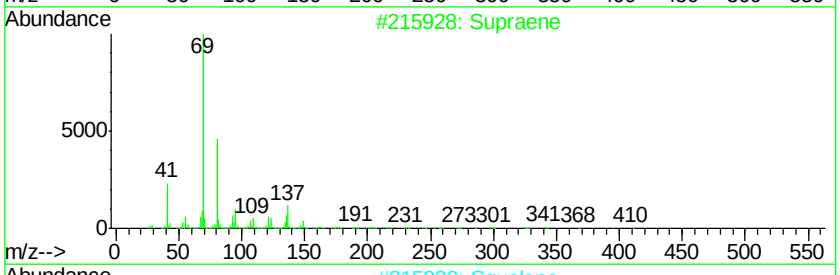
Peak Number 8 Supraene Concentration Rank 6

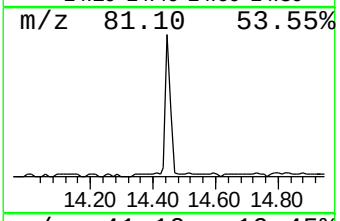
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.43 ng	138710	Perylene-d12	14.90

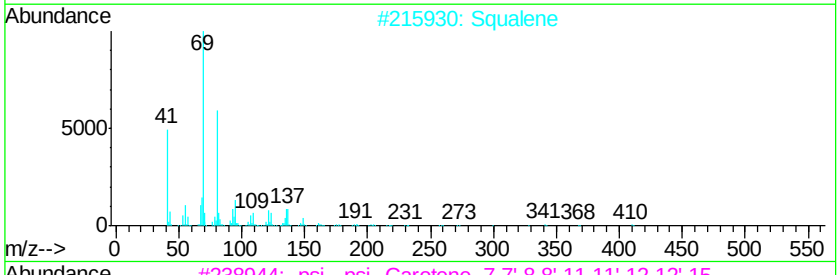
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53

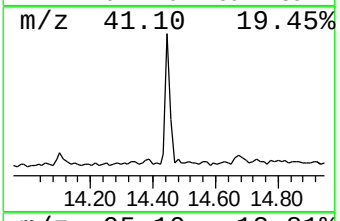


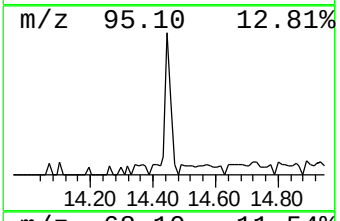


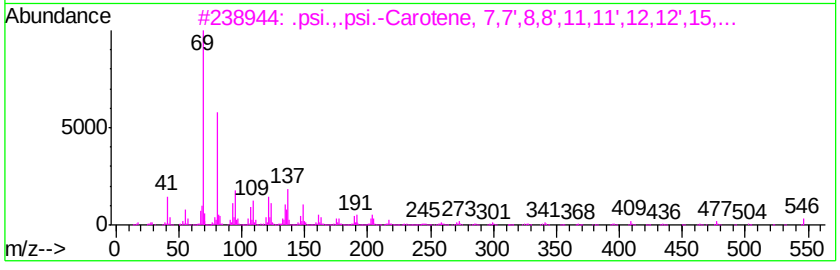


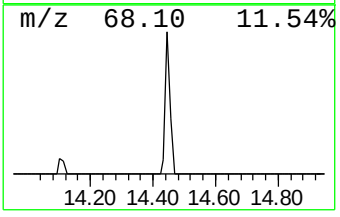












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090257.D
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Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : B6-9.5-10

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	17.3	ng	697014	1	6.47	807441	20.0
unknown6.24	6.24	80.3	ng	3239680	1	6.47	807441	20.0
Heptadecane	10.43	2.1	ng	142069	4	10.97	1374970	20.0
unknown11.53	11.53	2.2	ng	149624	4	10.97	1374970	20.0
n-Tetracosanol-1	13.47	5.5	ng	364958	5	13.58	1329230	20.0
Supraene	14.45	2.4	ng	138710	6	14.90	1141060	20.0