LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080754.D
Acq On : 1 Aug 2015 1:32
Operator : TP/UM
Sample : G3127-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

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-BF073015.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	2.178	4	8	11	rBV2	47001	79645	1.88%	0.193%
2	3.218	97	99	114	rBV2	93364	242263	5.72%	0.587%
3	4.407	200	203	206	rVB	141822	197394	4.66%	0.478%
4	5.059	256	260	262	rBV	2627441	3905400	92.25%	9.461%
5	5.459	292	295	298	rBV	3628139	3813748	90.08%	9.239%
6	5.859	329	330	333	rVB	126733	143733	3.40%	0.348%
7	6.430	377	380	381	rBV	35944	44615	1.05%	0.108%
8	6.476	381	384	387	rVV	2970479	4233594	100.00%	10.257%
9	6.625	394	397	399	rBV	3039996	4163014	98.33%	10.086%
10	6.853	415	417	419	rBV	999232	873709	20.64%	2.117%
11	7.013	428	431	433	rBV	2345434	3017593	71.28%	7.311%
12	7.413	463	466	468	rBV	2798326	2784845	65.78%	6.747%
13	7.493	468	473	475	rVB	58236	72353	1.71%	0.175%
14	8.133	526	529	531	rBV	1189926	1081104	25.54%	2.619%
15	9.208	620	623	626	rBV	3780024	4065000	96.02%	9.848%
16	9.608	655	658	660	rBV	578608	695486	16.43%	1.685%
17	9.882	680	682	685	rVB	1176372	1105521	26.11%	2.678%
18	10.671	748	751	753	rBV	2760586	2739163	64.70%	6.636%
19	10.796	758	762	766	rVV2	48812	64432	1.52%	0.156%
20	11.242	799	801	802	rBV	70844	57711	1.36%	0.140%
21	11.368	809	812	814	rVB	958854	1075109	25.39%	2.605%
22	11.665	832	838	840	rBV	171914	428393	10.12%	1.038%
23	11.894	856	858	867	rVB	128689	184146	4.35%	0.446%
24	12.156	878	881	883	rBV	1904307	1776169	41.95%	4.303%
25	12.831	939	940	944	rVB2	28674	43047	1.02%	0.104%
26	12.945	948	950	953	rBV	2686351	3105272	73.35%	7.523%
27	13.985	1039	1041	1044	rBV	542668	706218	16.68%	1.711%
28	15.403	1162	1165	1168	rBV	445996	578125	13.66%	1.401%

Sum of corrected areas: 41276802

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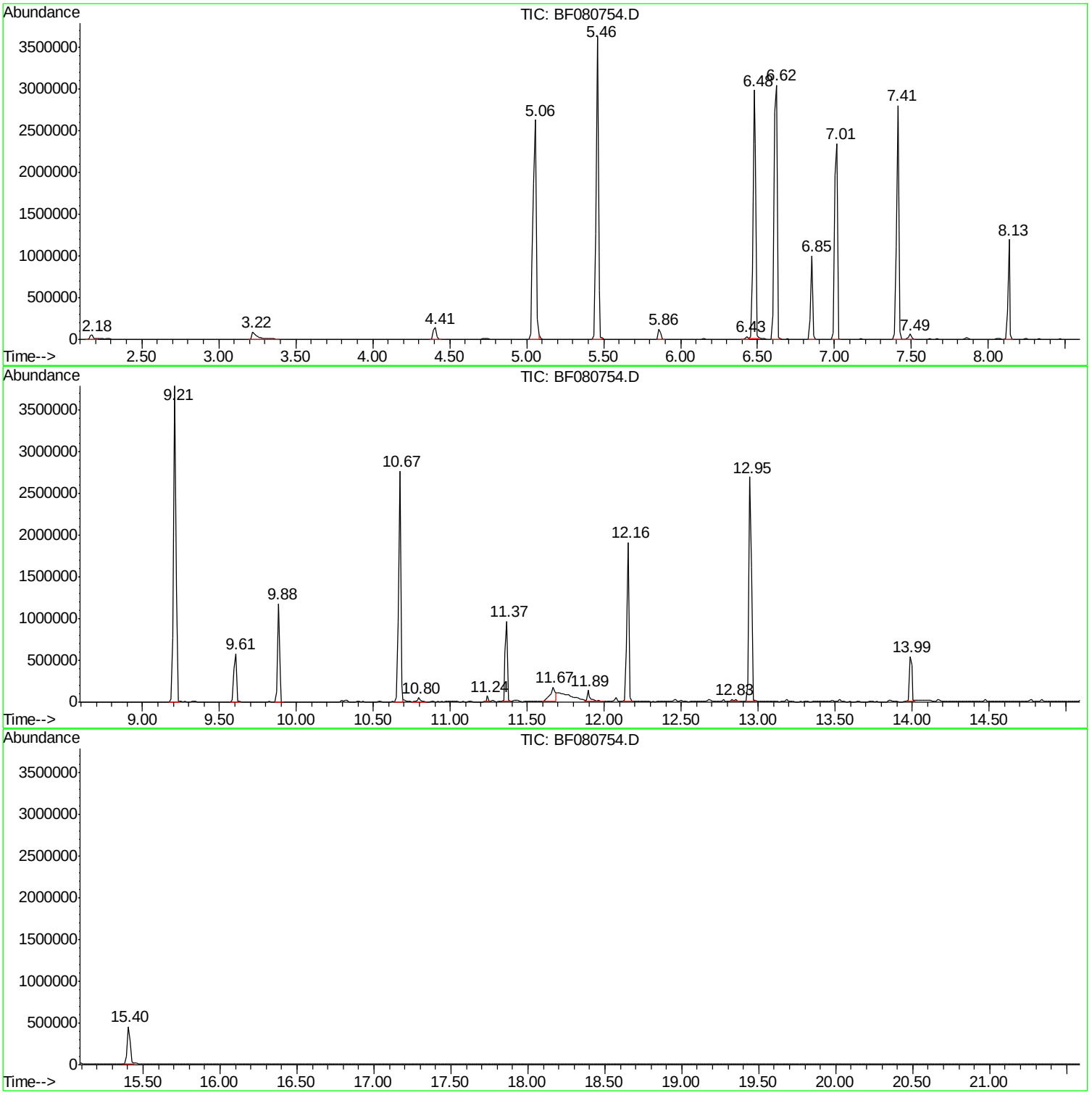
Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 46 Sample Multiplier: 1

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ClientSampleId :

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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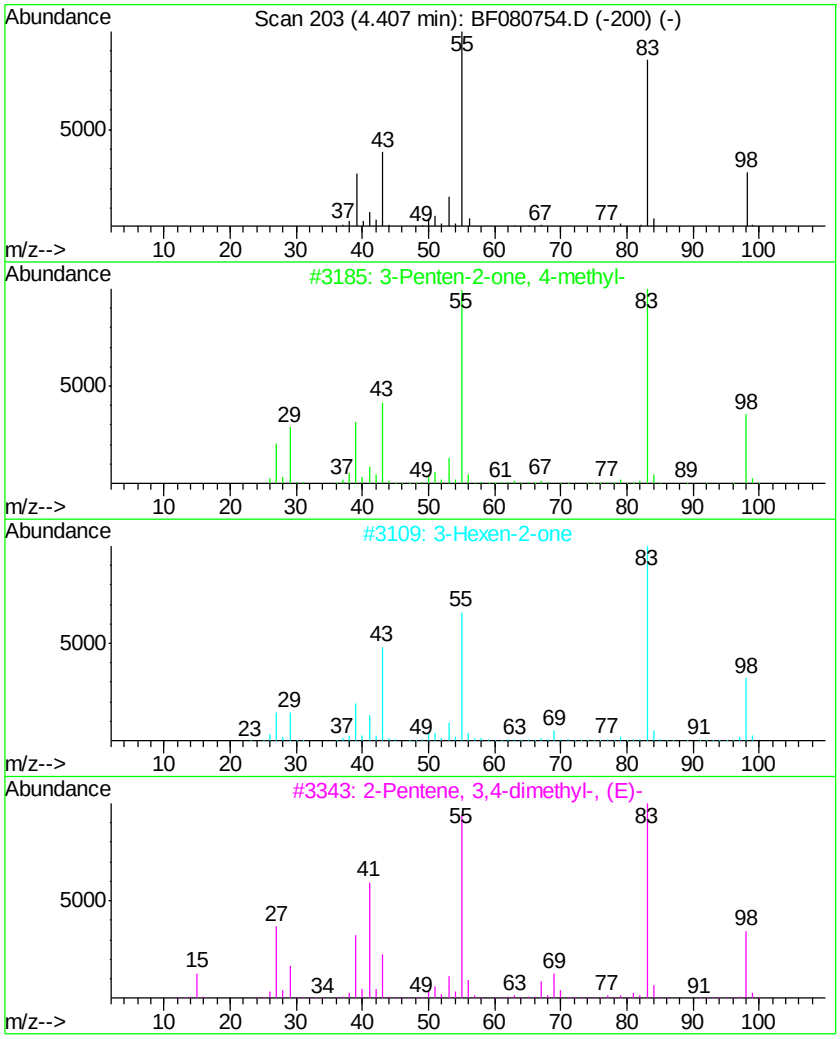
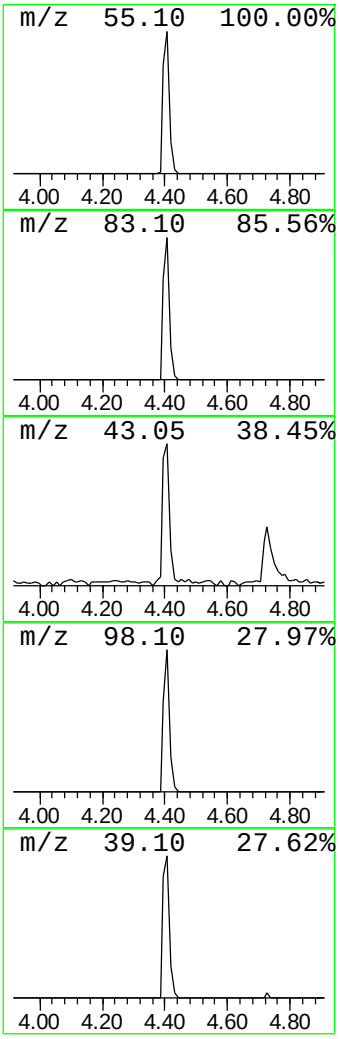
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	4.52 ng	197394	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080754.D
Acq On : 1 Aug 2015 1:32
Operator : TP/UM
Sample : G3127-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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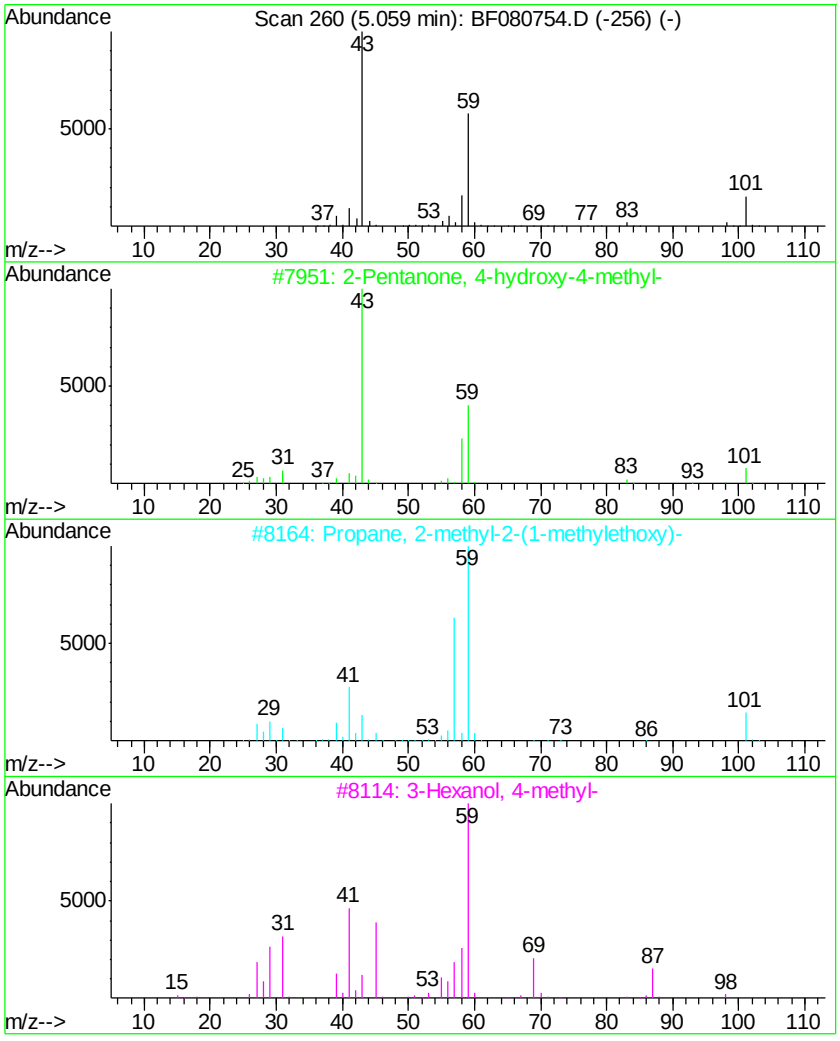
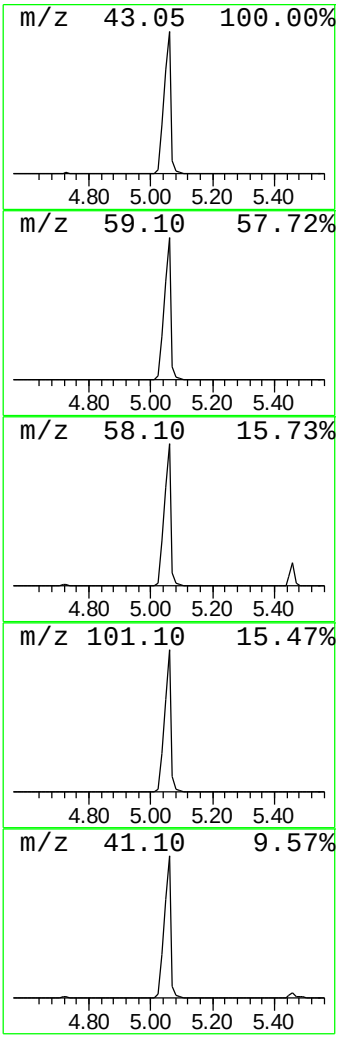
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	89.40 ng	3905400	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080754.D
Acq On : 1 Aug 2015 1:32
Operator : TP/UM
Sample : G3127-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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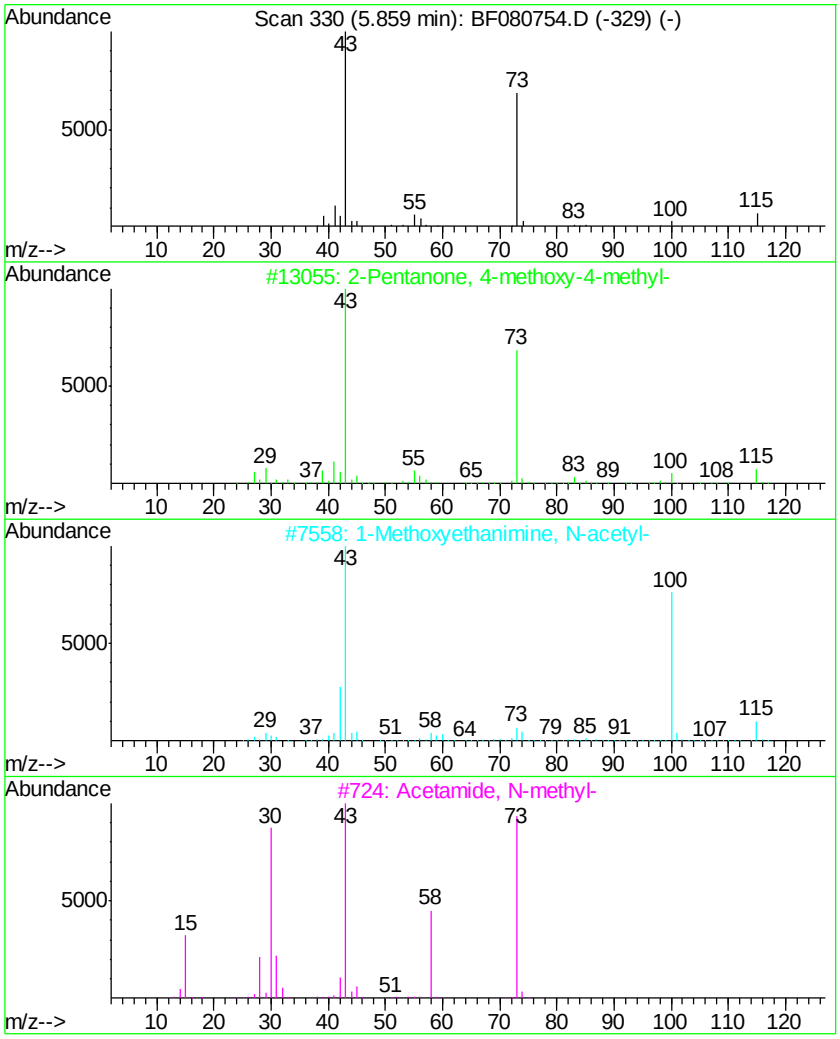
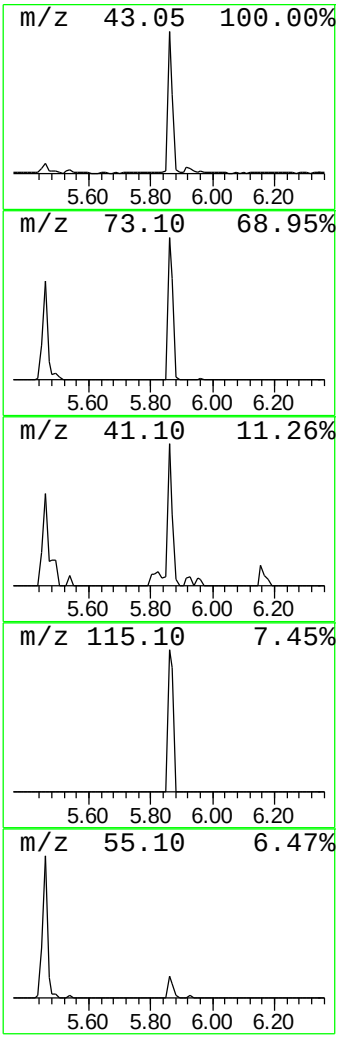
Peak Number 4 unknown5.86 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	3.29 ng	143733	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	38
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	9
5	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	9





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Data File : BF080754.D
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Operator : TP/UM
Sample : G3127-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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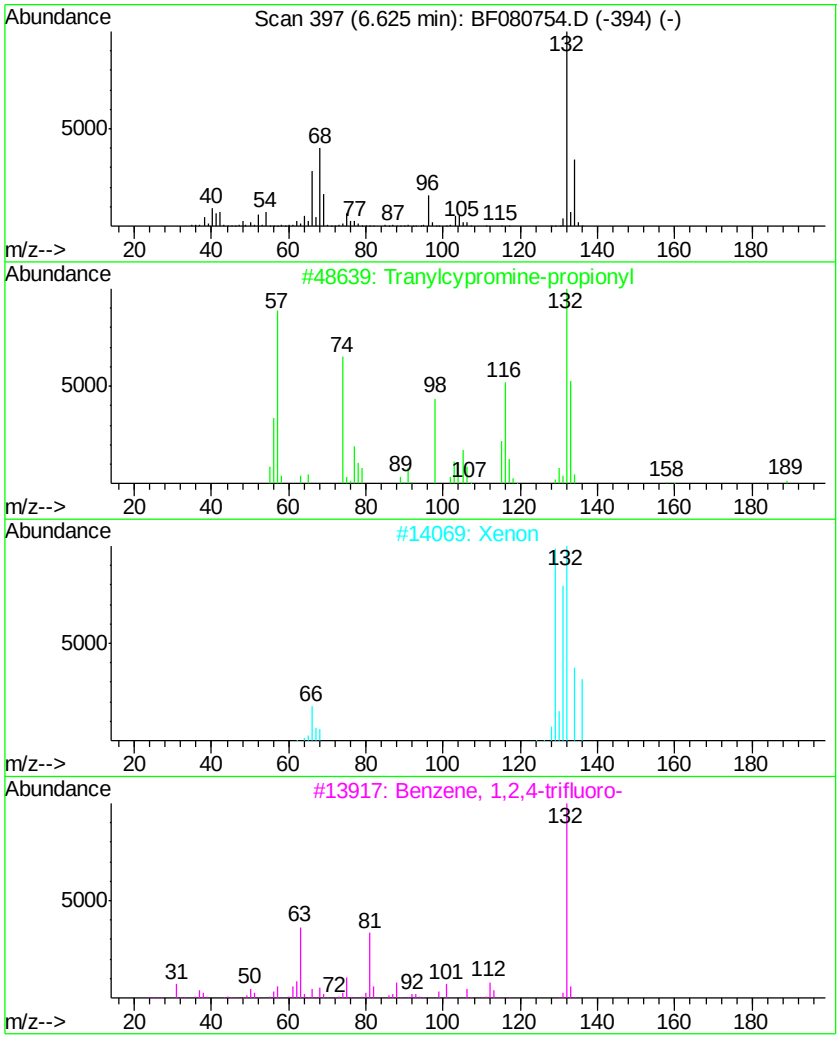
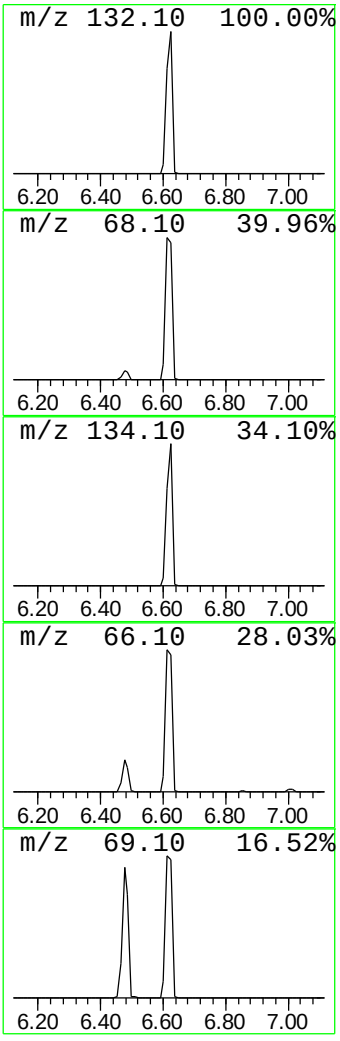
Peak Number 5 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.30 ng	4163010	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	Xenon	132	Xe	007440-63-3	9
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
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Operator : TP/UM
Sample : G3127-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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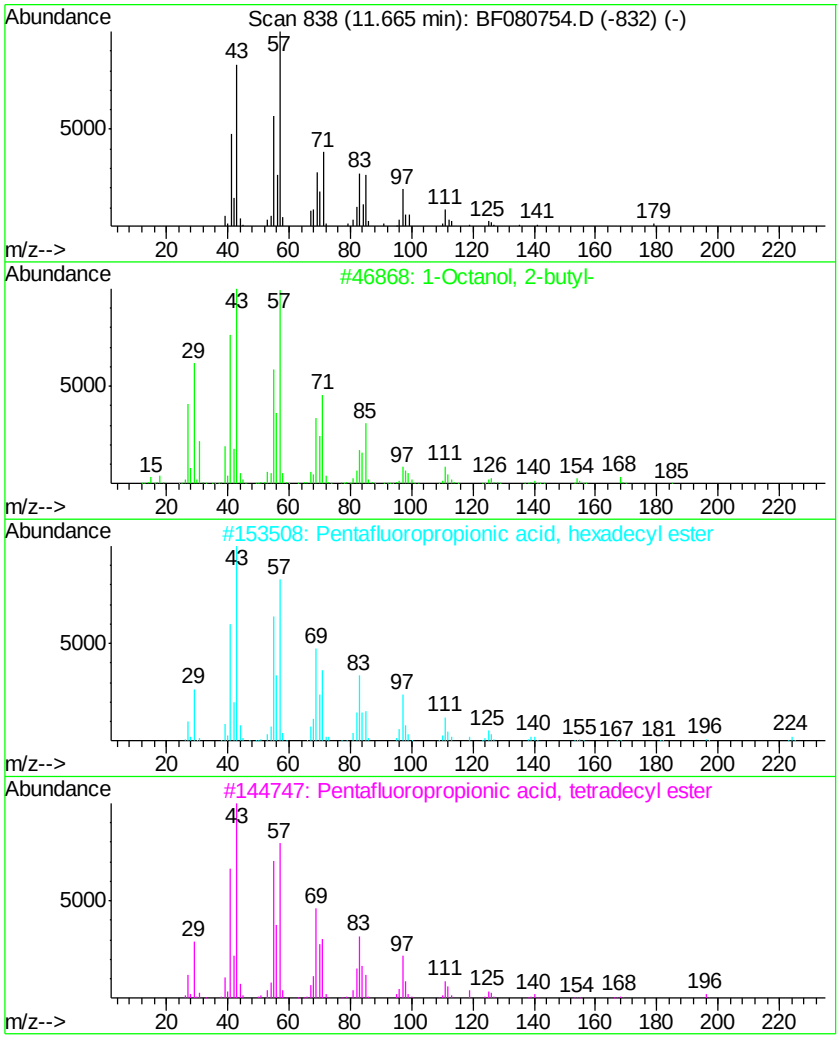
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

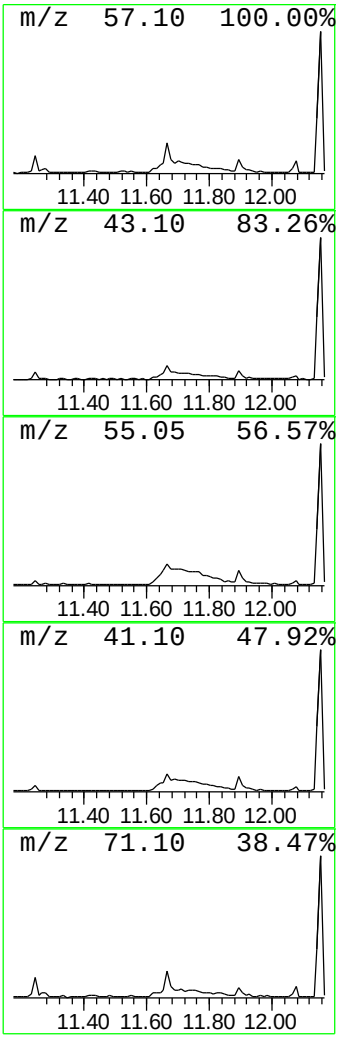
****

Peak Number 7 1-Octanol, 2-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	7.97 ng	428393	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	80
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	70
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	60
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	60
5	Decane	142	C10H22	000124-18-5	58





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Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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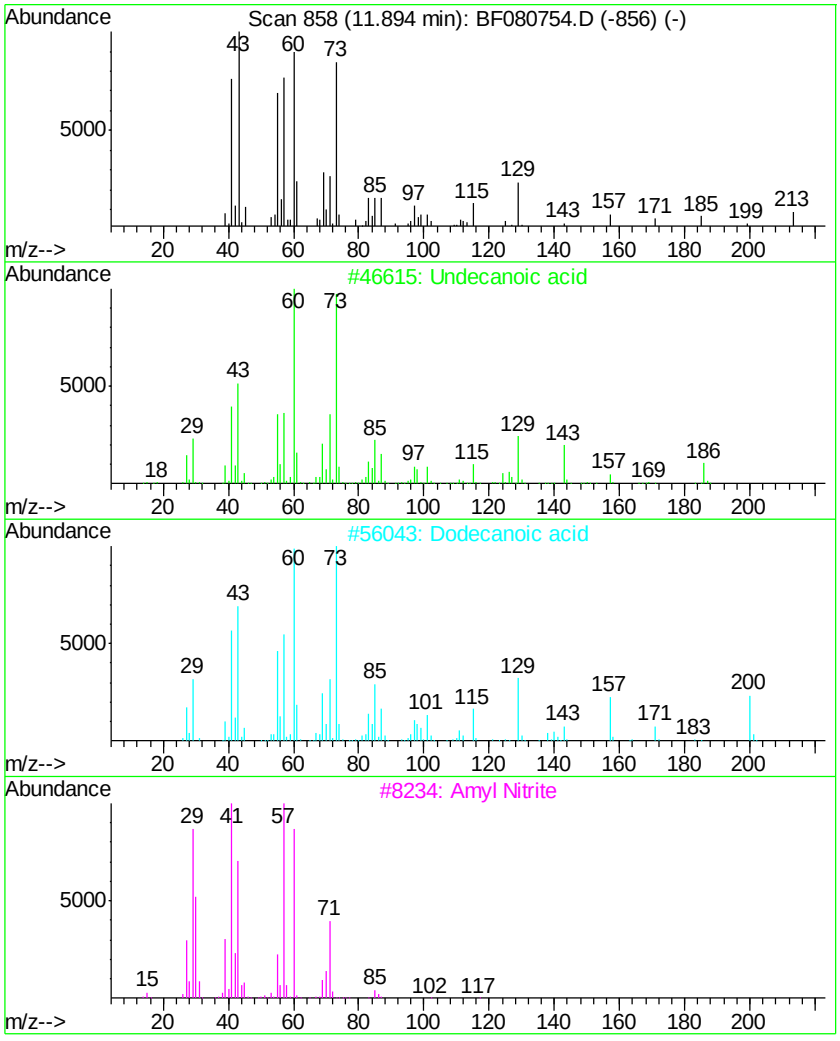
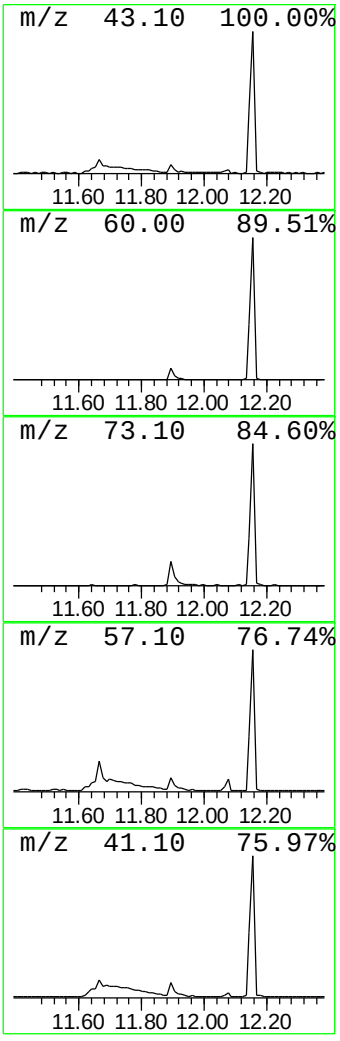
Peak Number 8 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.43 ng	184146	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Amyl Nitrite	117	C5H11NO2	000110-46-3	43
4	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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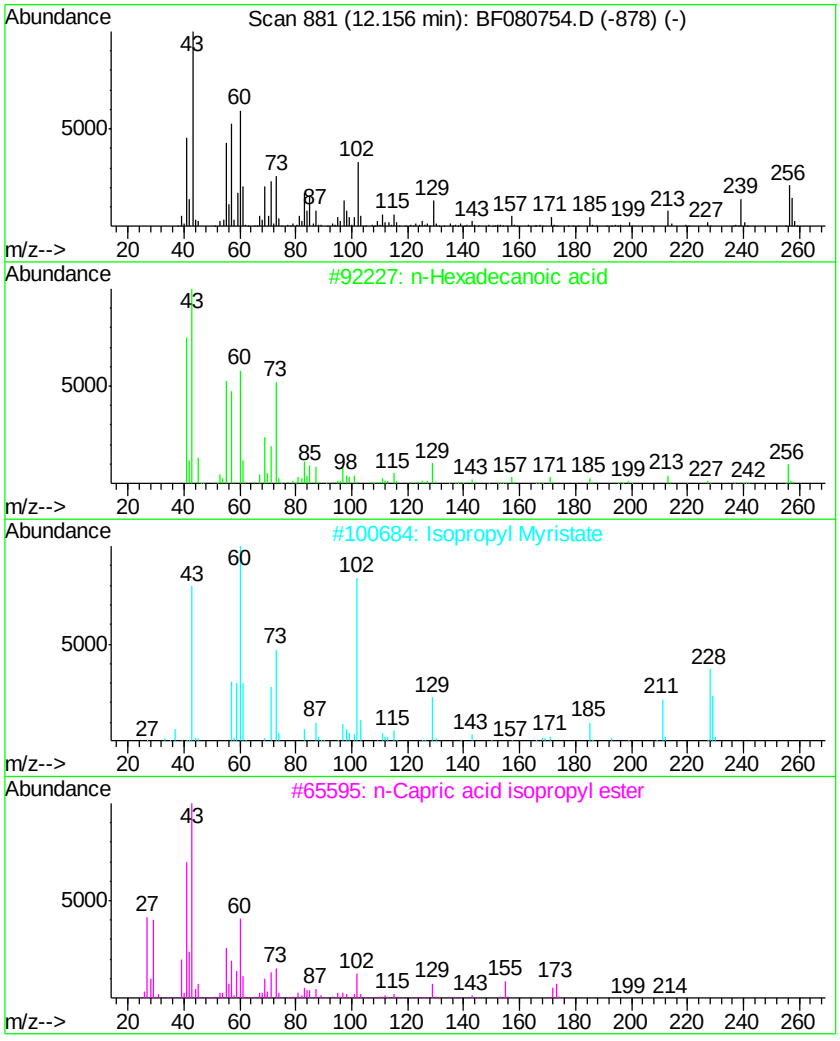
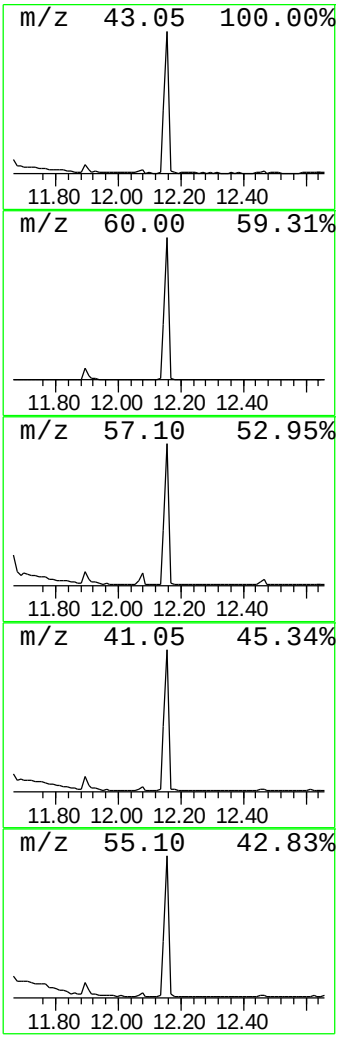
Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	33.04 ng	1776170	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	43
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	37
4	Undecanoic acid	186	C11H22O2	000112-37-8	27
5	Dodecanoic acid	200	C12H24O2	000143-07-7	25





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
3-Penten-2-one, 4...	4.41	4.5	ng	197394	1	6.85	873709	20.0
2-Pentanone, 4-hy...	5.06	89.4	ng	3905400	1	6.85	873709	20.0
unknown5.86	5.86	3.3	ng	143733	1	6.85	873709	20.0
unknown6.62	6.62	95.3	ng	4163010	1	6.85	873709	20.0
1-Octanol, 2-butyl-	11.67	8.0	ng	428393	4	11.37	1075110	20.0
Undecanoic acid	11.89	3.4	ng	184146	4	11.37	1075110	20.0
n-Hexadecanoic acid	12.16	33.0	ng	1776170	4	11.37	1075110	20.0