LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092755.D
Acq On : 3 Feb 2017 00:27
Operator : SJ/MA
Sample : I1650-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37-COMP

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-BF013017.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	4.796	236	237	246	rBV	27128	56651	1.15%	0.146%
2	5.127	263	266	278	rBV	1801289	2556802	51.87%	6.586%
3	5.550	300	303	305	rBV	4651240	4929323	100.00%	12.697%
4	6.579	390	393	396	rBV	3541893	4285949	86.95%	11.040%
5	6.704	401	404	407	rBV	3646412	4113947	83.46%	10.597%
6	6.933	422	424	427	rBV	1053037	880265	17.86%	2.267%
7	7.093	435	438	440	rBV	3526636	3242942	65.79%	8.353%
8	7.505	471	474	476	rBV	2740029	2792737	56.66%	7.193%
9	8.225	534	537	539	rBV	1334137	1148522	23.30%	2.958%
10	9.299	628	631	634	rBV	3991080	4086908	82.91%	10.527%
11	9.688	663	665	668	rBV	583215	627406	12.73%	1.616%
12	9.973	688	690	693	rBV	1128761	1126927	22.86%	2.903%
13	10.396	724	727	729	rVB2	43533	86024	1.75%	0.222%
14	10.762	757	759	762	rBV2	1686169	2151240	43.64%	5.541%
15	10.876	767	769	774	rVB	91542	117156	2.38%	0.302%
16	11.322	806	808	809	rBV	91191	77994	1.58%	0.201%
17	11.459	818	820	823	rBV	1171318	1010774	20.51%	2.604%
18	11.745	843	845	848	rBV	73849	64805	1.31%	0.167%
19	13.048	956	959	961	rBV	3101124	3160823	64.12%	8.142%
20	13.940	1035	1037	1046	rBV	51478	115403	2.34%	0.297%
21	14.100	1048	1051	1053	rVB	758098	819894	16.63%	2.112%
22	15.197	1144	1147	1150	rBV	38171	51173	1.04%	0.132%
23	15.563	1175	1179	1184	rBV	602816	939079	19.05%	2.419%
24	16.008	1215	1218	1222	rBV	49653	78104	1.58%	0.201%
25	16.511	1259	1262	1266	rVB	44287	83952	1.70%	0.216%
26	17.094	1308	1313	1319	rBV	34525	82847	1.68%	0.213%
27	17.791	1370	1374	1381	rVB3	29846	79501	1.61%	0.205%
28	18.614	1442	1446	1451	rBV4	20466	56098	1.14%	0.144%

Sum of corrected areas: 38823246

LSC Report - Integrated Chromatogram

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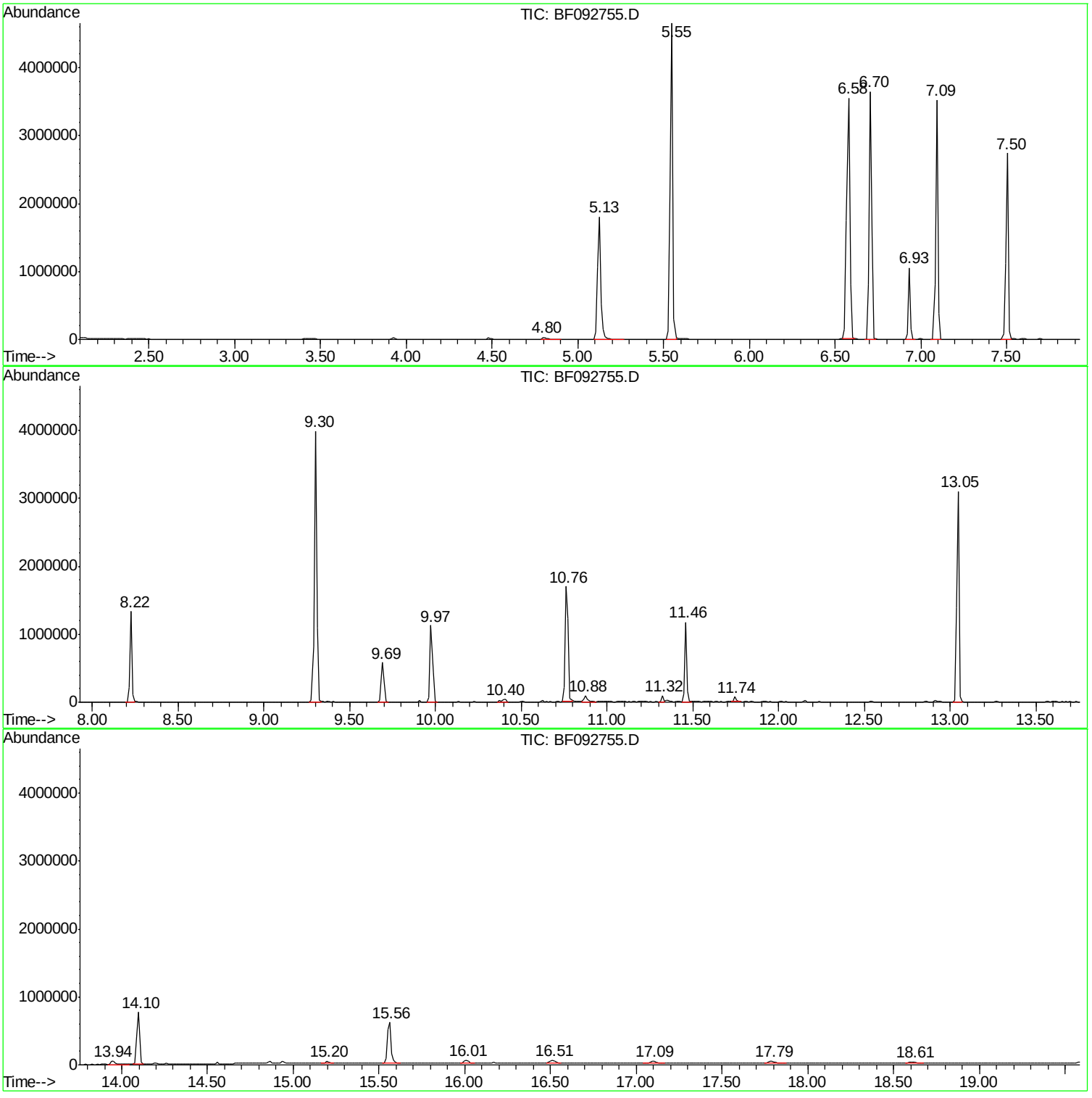
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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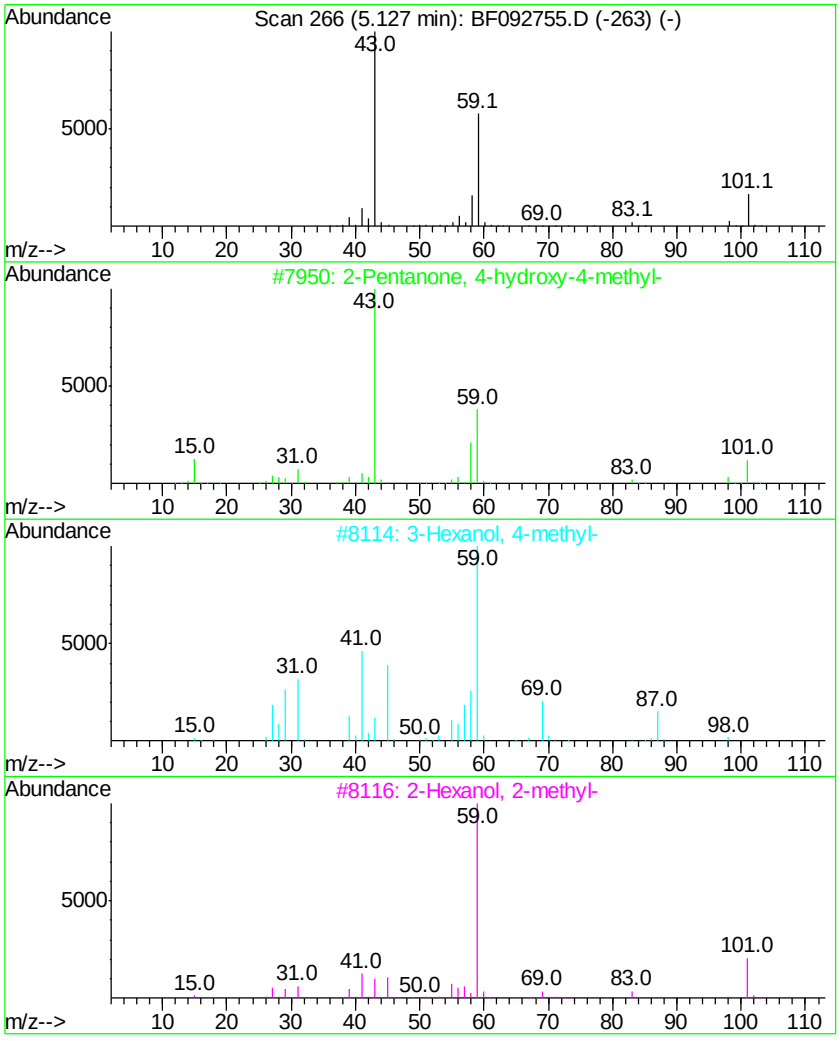
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	58.09 ng	2556800	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



m/z 43.05 100.00%
m/z 59.10 57.73%
m/z 101.10 16.81%
m/z 58.10 15.67%
m/z 41.10 9.27%

Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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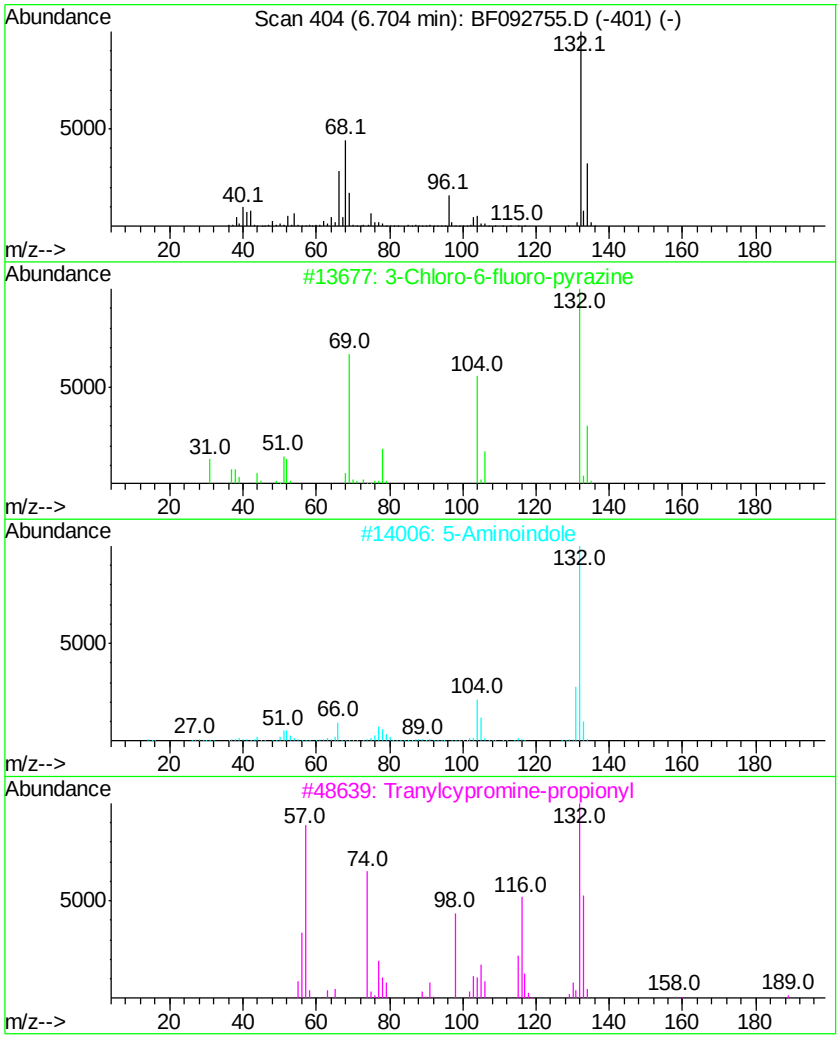
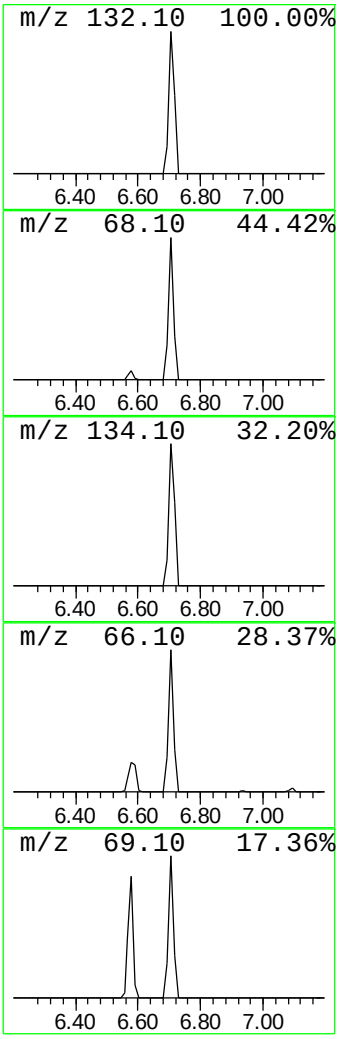
Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	93.47 ng	4113950	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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ClientSampleId : SB-37-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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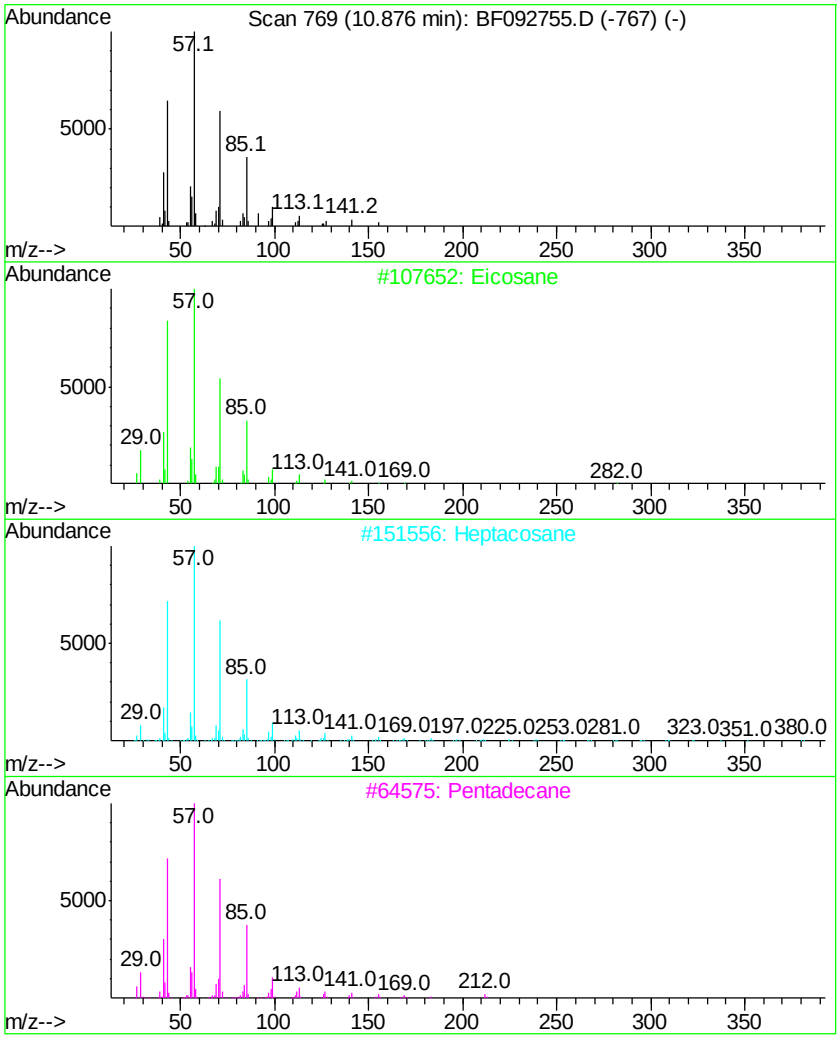
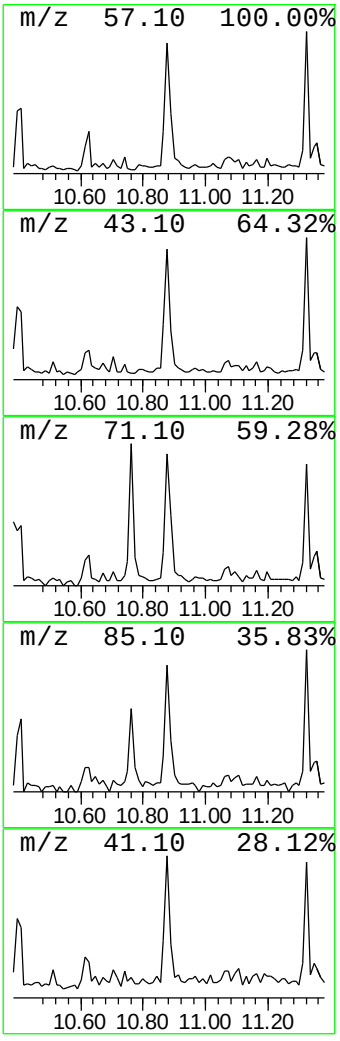
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.32 ng	117156	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Octacosane	394	C28H58	000630-02-4	86





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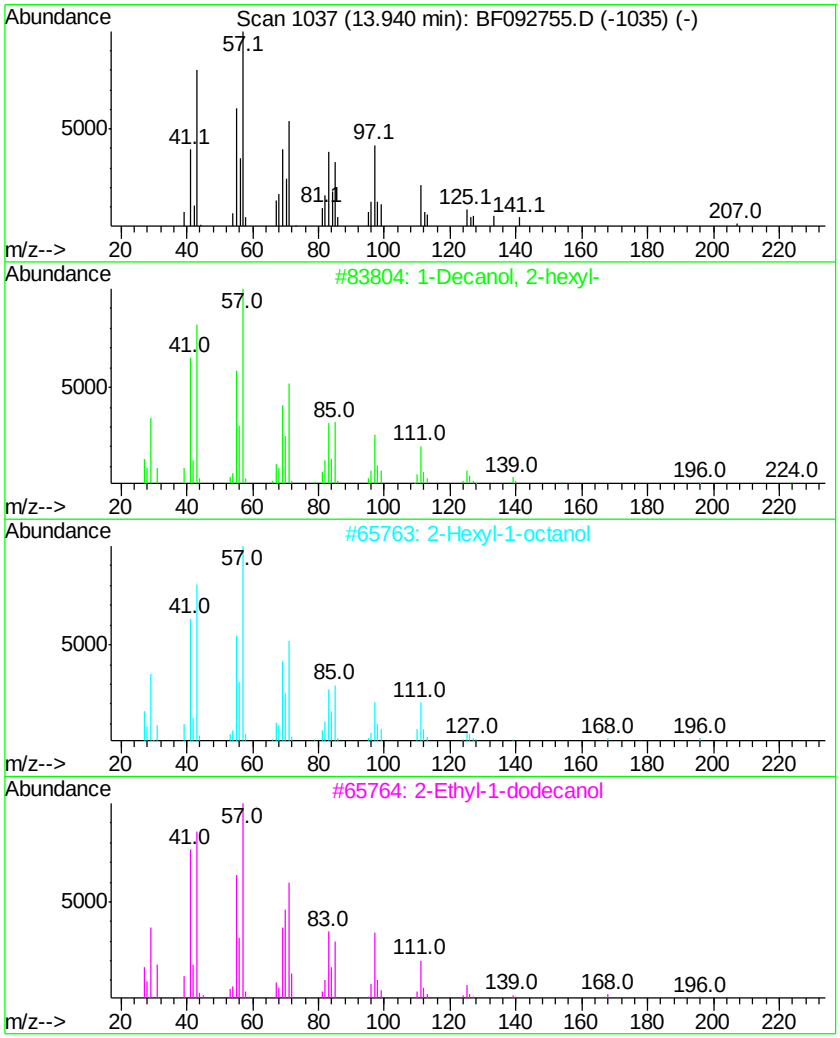
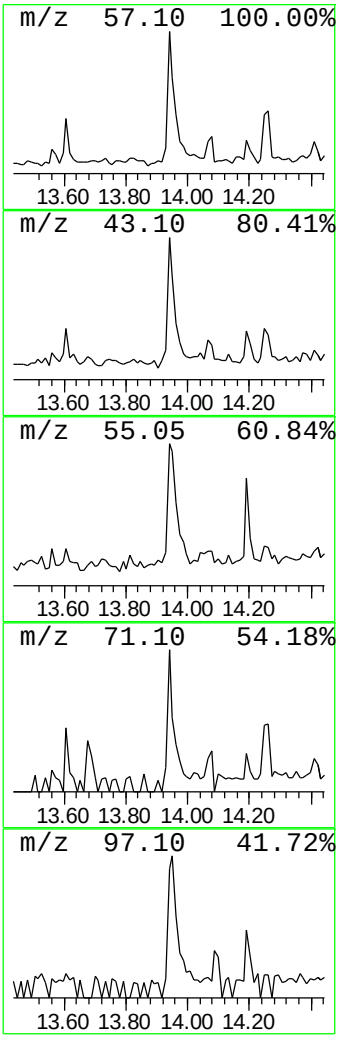
Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.82 ng	115403	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
2	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	83
3	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	80
4	1-Octadecene	252	C18H36	000112-88-9	74
5	1-Docosene	308	C22H44	001599-67-3	72





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
2-Pentanone, 4-hy...	5.13	58.1	ng	2556800	1	6.93	880265	20.0
unknown6.70	6.70	93.5	ng	4113950	1	6.93	880265	20.0
Eicosane	10.88	2.3	ng	117156	4	11.46	1010770	20.0
1-Decanol, 2-hexyl-	13.94	2.8	ng	115403	5	14.10	819894	20.0