LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102016\
Data File : BF090683.D
Acq On : 20 Oct 2016 15:42
Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

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-BF101316.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	5.068	236	239	247	rBV	1035762	1596230	22.50%	2.424%
2	5.491	273	276	278	rBV	5732690	6360788	89.67%	9.659%
3	6.520	362	366	368	rBV	5341141	6719896	94.73%	10.204%
4	6.646	374	377	380	rBV	5336941	6178610	87.10%	9.382%
5	6.874	395	397	408	rBV	1398574	1652903	23.30%	2.510%
6	7.034	408	411	413	rBV	5176344	4860215	68.51%	7.380%
7	7.446	444	447	449	rBV	3515838	4177610	58.89%	6.344%
8	7.549	453	456	463	rVB	162792	352040	4.96%	0.535%
9	8.166	507	510	512	rBV	2209092	2281543	32.16%	3.465%
10	9.240	601	604	607	rBV	5658729	6729077	94.86%	10.218%
11	9.355	612	614	617	rVB	57496	81753	1.15%	0.124%
12	9.640	636	639	641	rBV	1403891	1564318	22.05%	2.375%
13	9.915	661	663	666	rBV	1845075	2505631	35.32%	3.805%
14	10.349	697	701	703	rBV3	56954	121924	1.72%	0.185%
15	10.715	730	733	735	rBV	3844114	4609520	64.98%	7.000%
16	10.829	741	743	750	rVB	124016	181169	2.55%	0.275%
17	11.275	780	782	783	rBV	99803	87364	1.23%	0.133%
18	11.412	791	794	796	rBV	1696192	2389299	33.68%	3.628%
19	11.629	811	813	818	rBV	455015	609867	8.60%	0.926%
20	12.452	883	885	894	rBV	955602	1094107	15.42%	1.661%
21	12.898	919	924	926	rVB2	59445	95603	1.35%	0.145%
22	13.001	930	933	935	rBV	6627040	7093864	100.00%	10.772%
23	13.469	972	974	977	rVB	426304	578436	8.15%	0.878%
24	13.892	1009	1011	1022	rBV	203041	306761	4.32%	0.466%
25	14.052	1022	1025	1027	rBV	1338798	1952757	27.53%	2.965%
26	15.492	1148	1151	1166	rBV	1113325	1515972	21.37%	2.302%
27	16.441	1230	1234	1240	rVB2	38140	85082	1.20%	0.129%
28	17.698	1340	1344	1353	rVB2	20961	71428	1.01%	0.108%

Sum of corrected areas: 65853767

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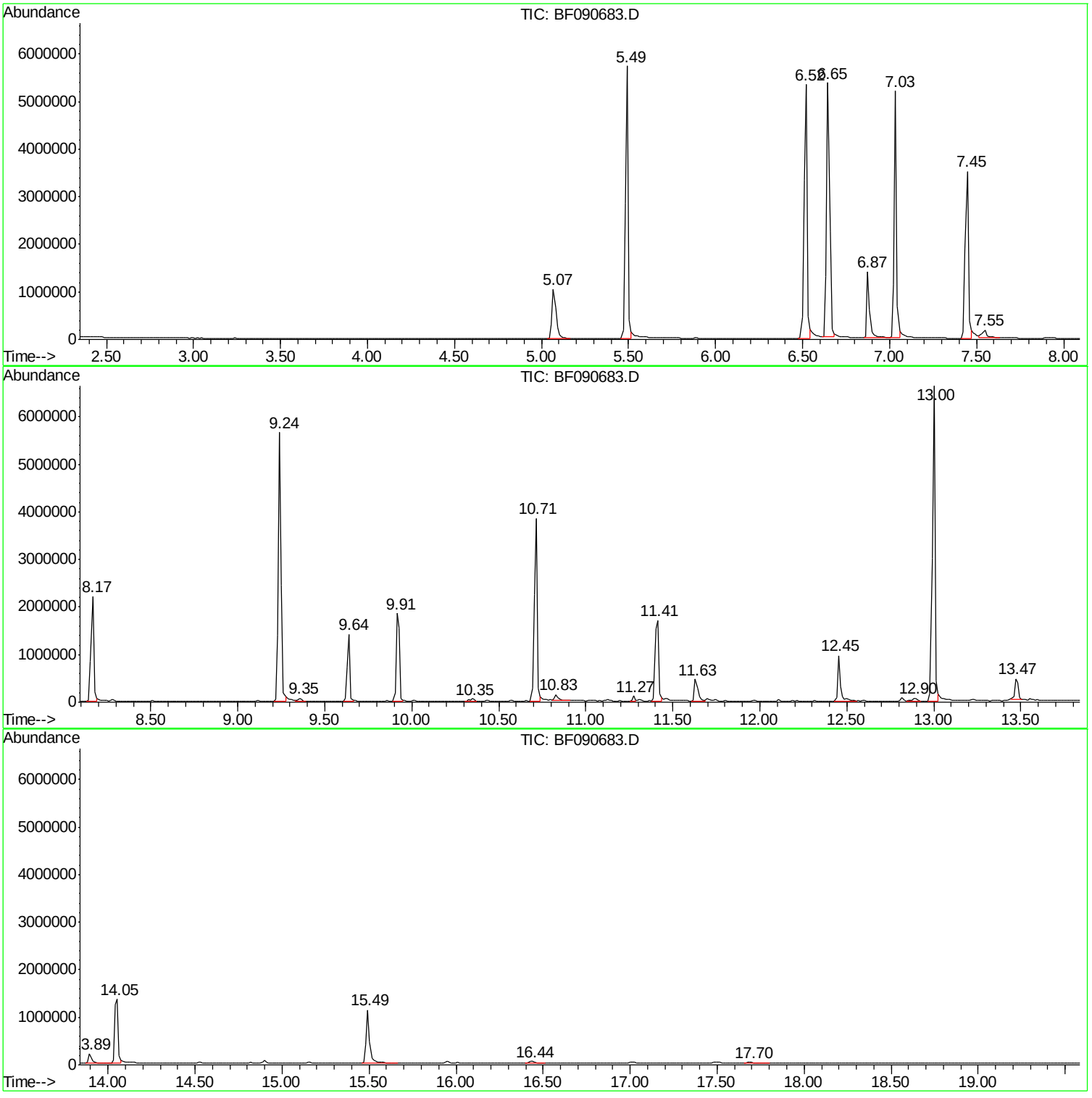
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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\BF102016\
Data File : BF090683.D
Acq On : 20 Oct 2016 15:42
Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

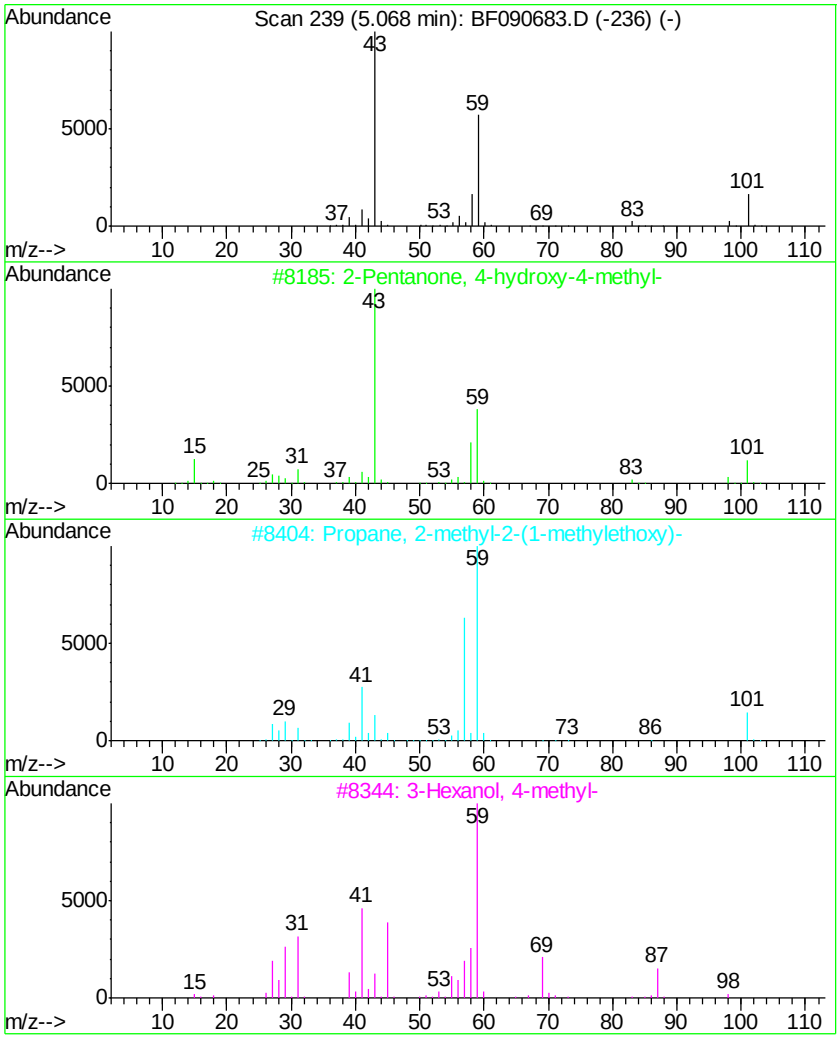
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

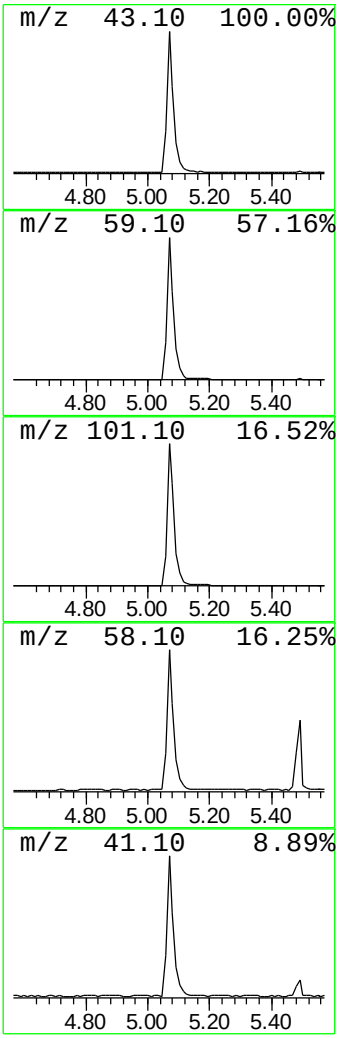
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	19.31 ng	1596230	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BF090683.D
Acq On : 20 Oct 2016 15:42
Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

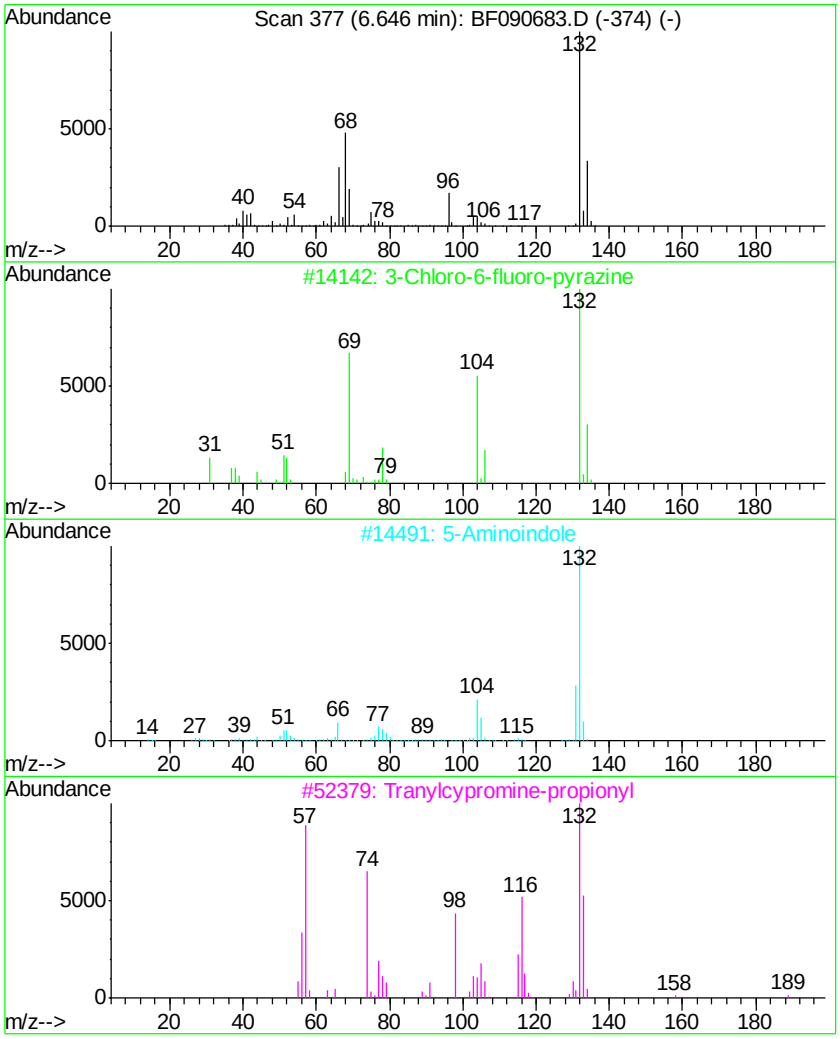
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

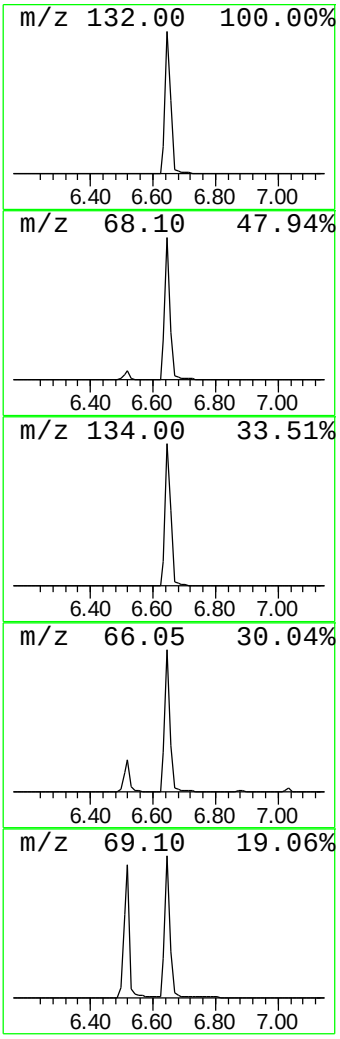
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	74.76 ng	6178610	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
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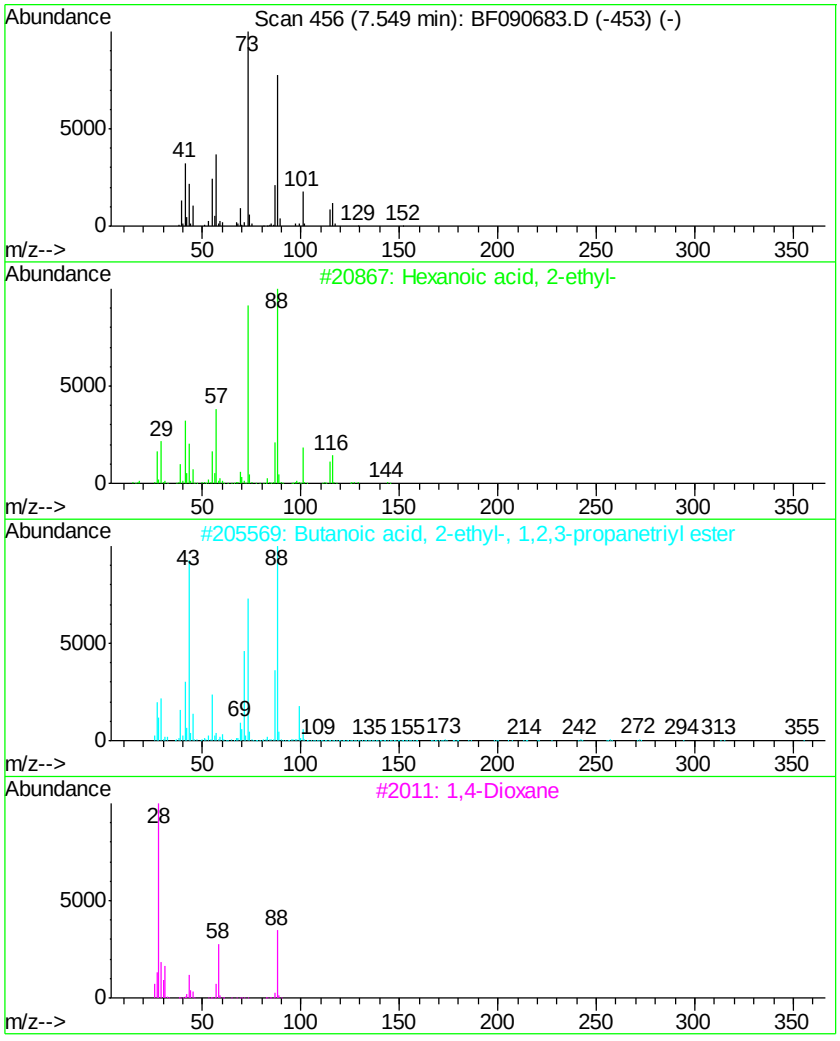
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

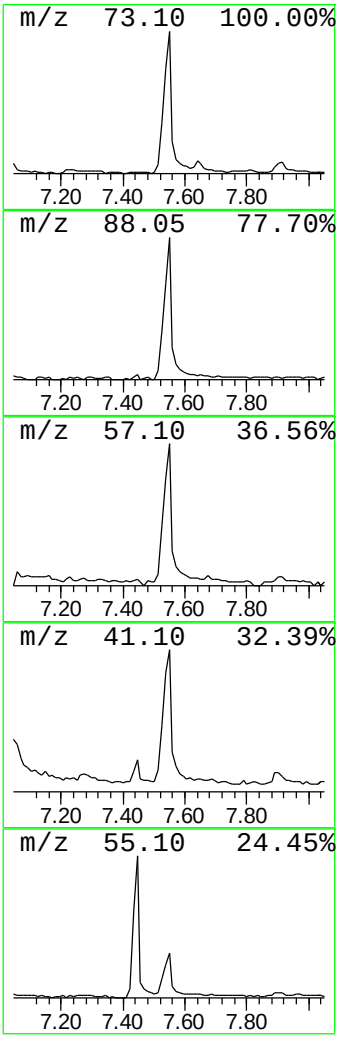
****

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	3.09 ng	352040	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
3	1,4-Dioxane	88	C4H8O2	000123-91-1	43
4	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	36
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	36





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Data File : BF090683.D
Acq On : 20 Oct 2016 15:42
Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

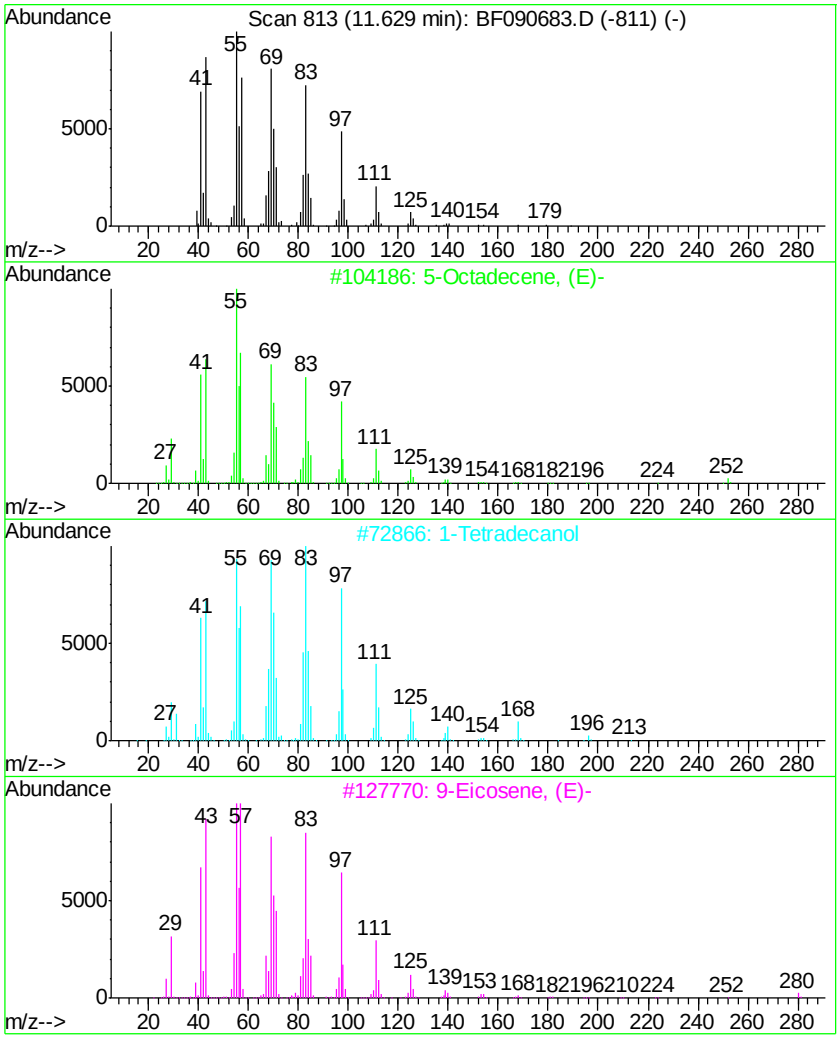
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

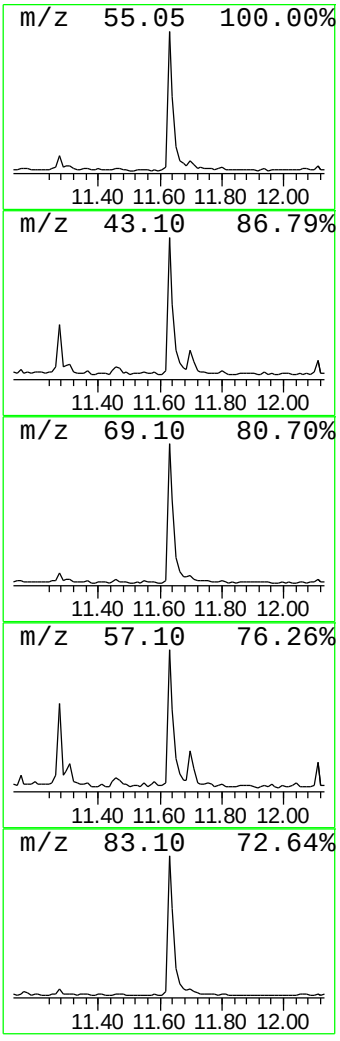
****

Peak Number 5 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	5.10 ng	609867	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	1-Tetradecanol	214	C14H30O	000112-72-1	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102016\
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Operator : UM/SJ
Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

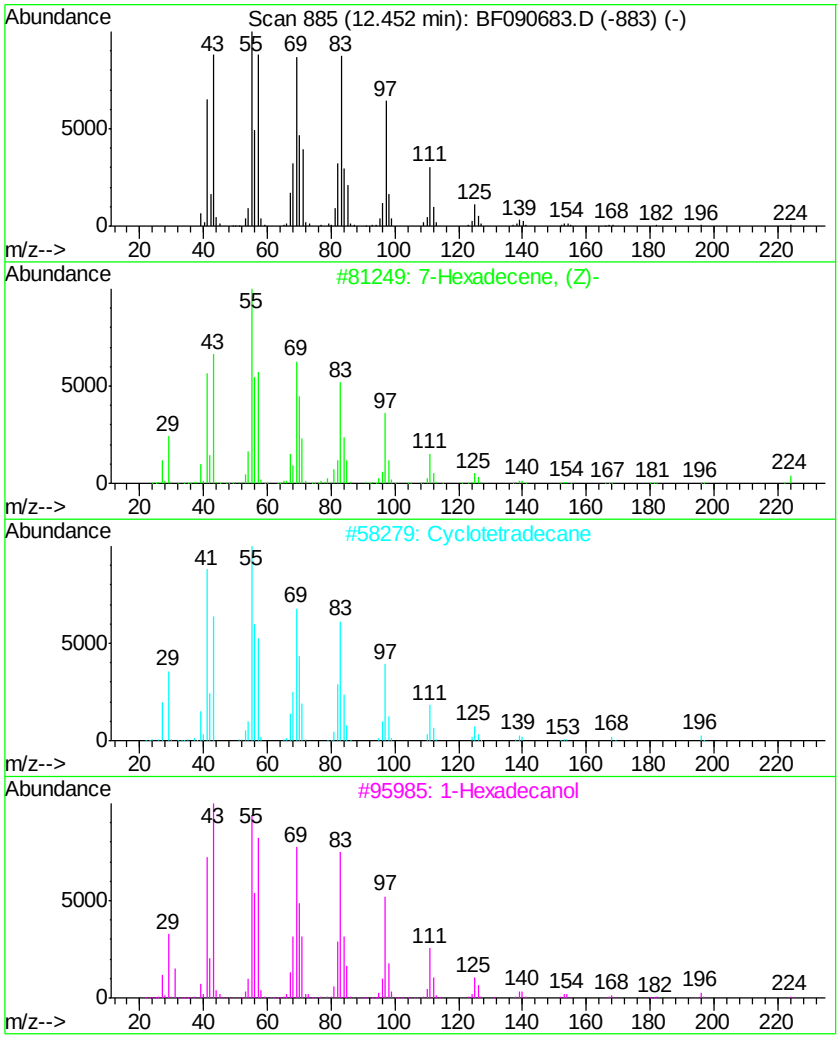
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

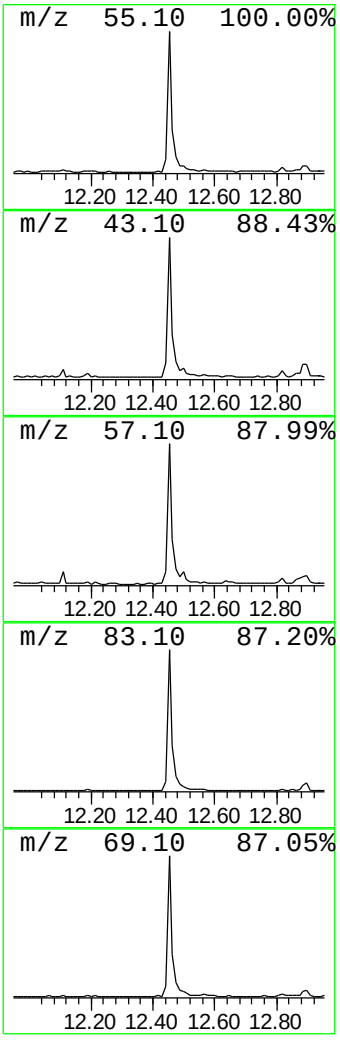
****

Peak Number 6 7-Hexadecene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	9.16 ng	1094110	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	97
2	Cyclotetradecane	196	C14H28	000295-17-0	97
3	1-Hexadecanol	242	C16H34O	036653-82-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	94





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Sample : H5315-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

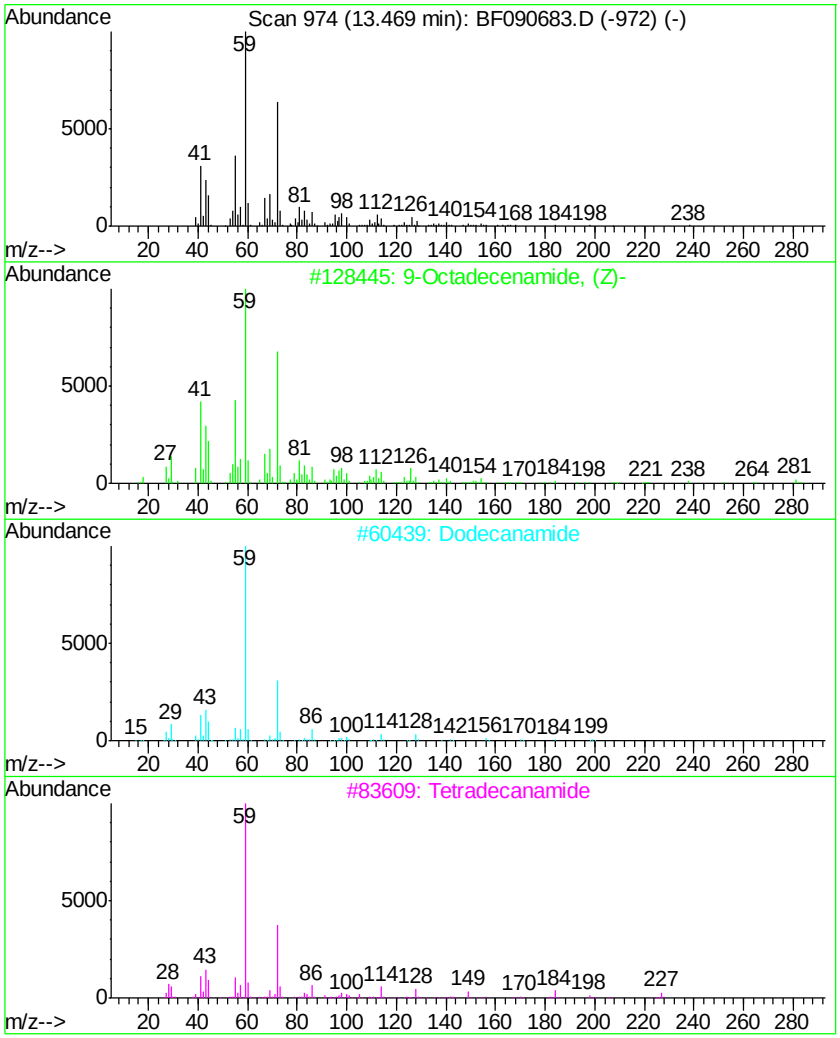
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

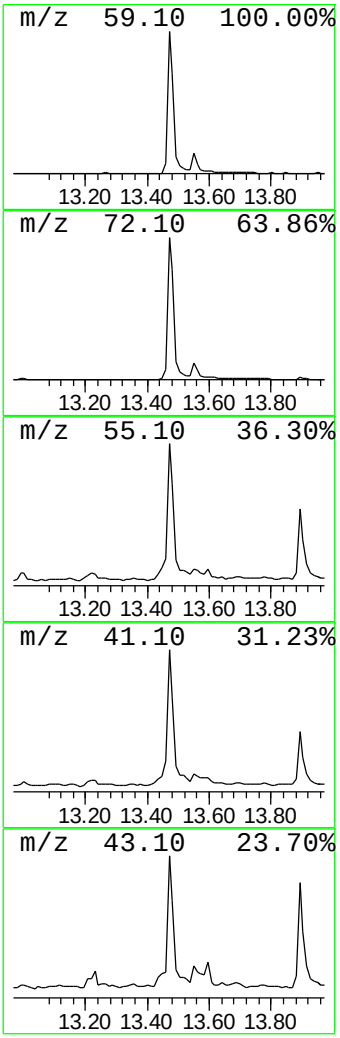
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.92 ng	578436	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Dodecanamide	199	C12H25NO	001120-16-7	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	56
4	Decanamide-	171	C10H21NO	002319-29-1	56
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	46





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Misc :
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Instrument : BNA_F
ClientSampleId : FO-TANK-END-EAST

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

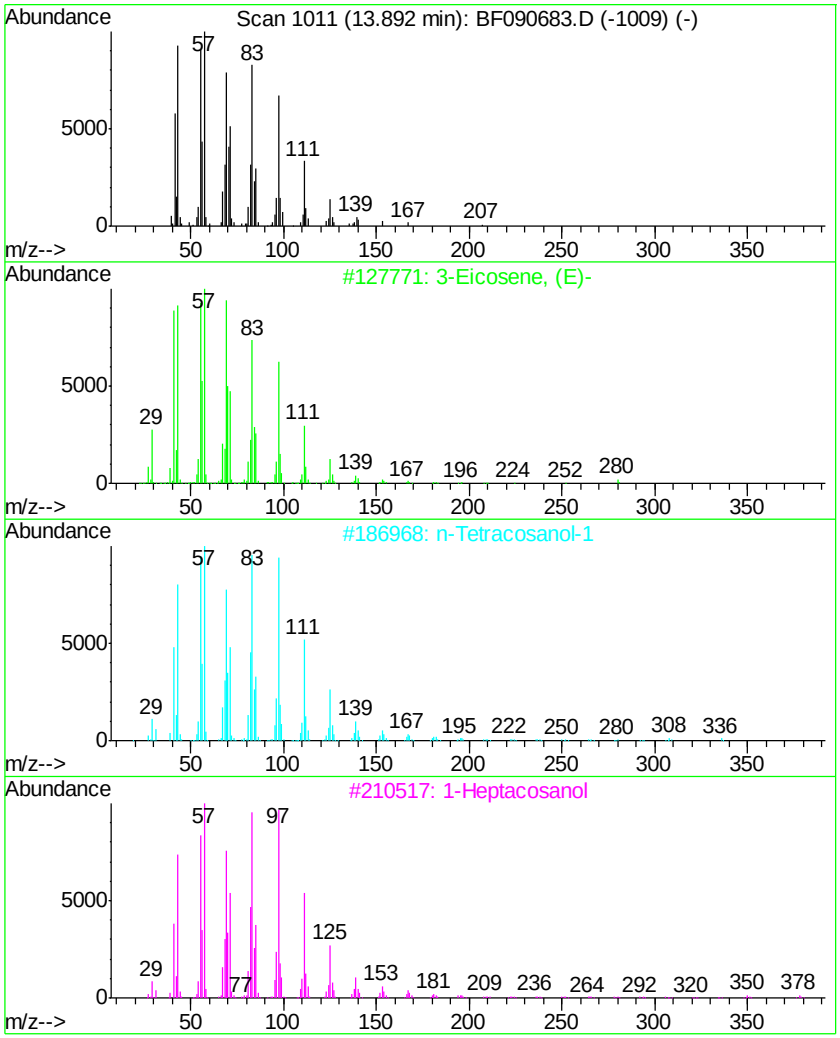
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

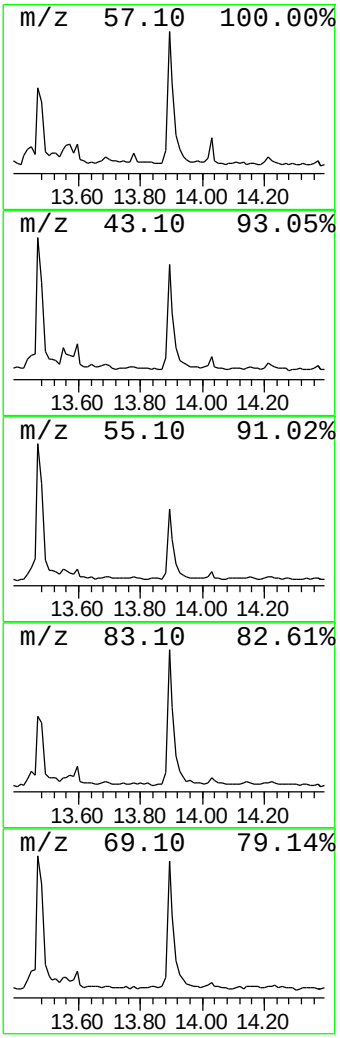
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.14 ng	306761	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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...	5.07	19.3	ng	1596230	1	6.87	1652900	20.0
unknown6.65	6.65	74.8	ng	6178610	1	6.87	1652900	20.0
Hexanoic acid, 2-...	7.55	3.1	ng	352040	2	8.17	2281540	20.0
5-Octadecene, (E)-	11.63	5.1	ng	609867	4	11.41	2389300	20.0
7-Hexadecene, (Z)-	12.45	9.2	ng	1094110	4	11.41	2389300	20.0
9-Octadecenamide,...	13.47	5.9	ng	578436	5	14.05	1952760	20.0
3-Eicosene, (E)-	13.89	3.1	ng	306761	5	14.05	1952760	20.0