LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085927.D
Acq On : 31 Mar 2016 15:04
Operator : UM/SJ
Sample : H2075-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-11

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-BF032416.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	4.973	233	235	241	rBV	59550	87493	3.01%	0.367%
2	5.384	269	271	283	rBV	2411465	2441447	84.09%	10.233%
3	6.424	360	362	365	rBV	2025115	2284911	78.70%	9.577%
4	6.550	371	373	376	rBV	1989569	2576308	88.73%	10.798%
5	6.790	391	394	396	rBV	617274	638151	21.98%	2.675%
6	6.939	405	407	410	rBV	1806013	1940240	66.83%	8.132%
7	7.350	441	443	446	rBV	1243802	1668242	57.46%	6.992%
8	7.465	450	453	458	rVB	51927	76680	2.64%	0.321%
9	8.070	504	506	509	rBV	905575	847248	29.18%	3.551%
10	9.156	598	601	603	rBV	2499178	2903449	100.00%	12.169%
11	9.545	633	635	638	rBV	433887	400455	13.79%	1.678%
12	9.762	652	654	656	rBV	63540	54549	1.88%	0.229%
13	9.831	657	660	662	rVB	854743	898291	30.94%	3.765%
14	10.265	696	698	699	rVB	80003	81550	2.81%	0.342%
15	10.482	714	717	718	rBV	33576	48725	1.68%	0.204%
16	10.619	726	729	731	rBV	1790030	1775363	61.15%	7.441%
17	10.733	737	739	746	rVB	117951	140010	4.82%	0.587%
18	11.179	776	778	779	rBV	86432	71209	2.45%	0.298%
19	11.305	787	789	792	rBV2	726876	849121	29.25%	3.559%
20	11.374	792	795	798	rVB2	12392	30736	1.06%	0.129%
21	11.602	814	815	818	rVB	42041	38973	1.34%	0.163%
22	11.842	834	836	847	rBV	118474	160759	5.54%	0.674%
23	12.619	902	904	909	rBV2	23787	50567	1.74%	0.212%
24	12.768	914	917	922	rVB2	18441	34340	1.18%	0.144%
25	12.894	925	928	930	rBV	2515836	2258510	77.79%	9.466%
26	13.785	1004	1006	1012	rVV	136719	212662	7.32%	0.891%
27	13.945	1017	1020	1022	rBV	650856	591978	20.39%	2.481%
28	14.688	1083	1085	1088	rBV2	42895	81561	2.81%	0.342%
29	14.780	1091	1093	1096	rVB	54631	73811	2.54%	0.309%
30	15.363	1141	1144	1150	rBV	374086	541767	18.66%	2.271%

Sum of corrected areas: 23859106

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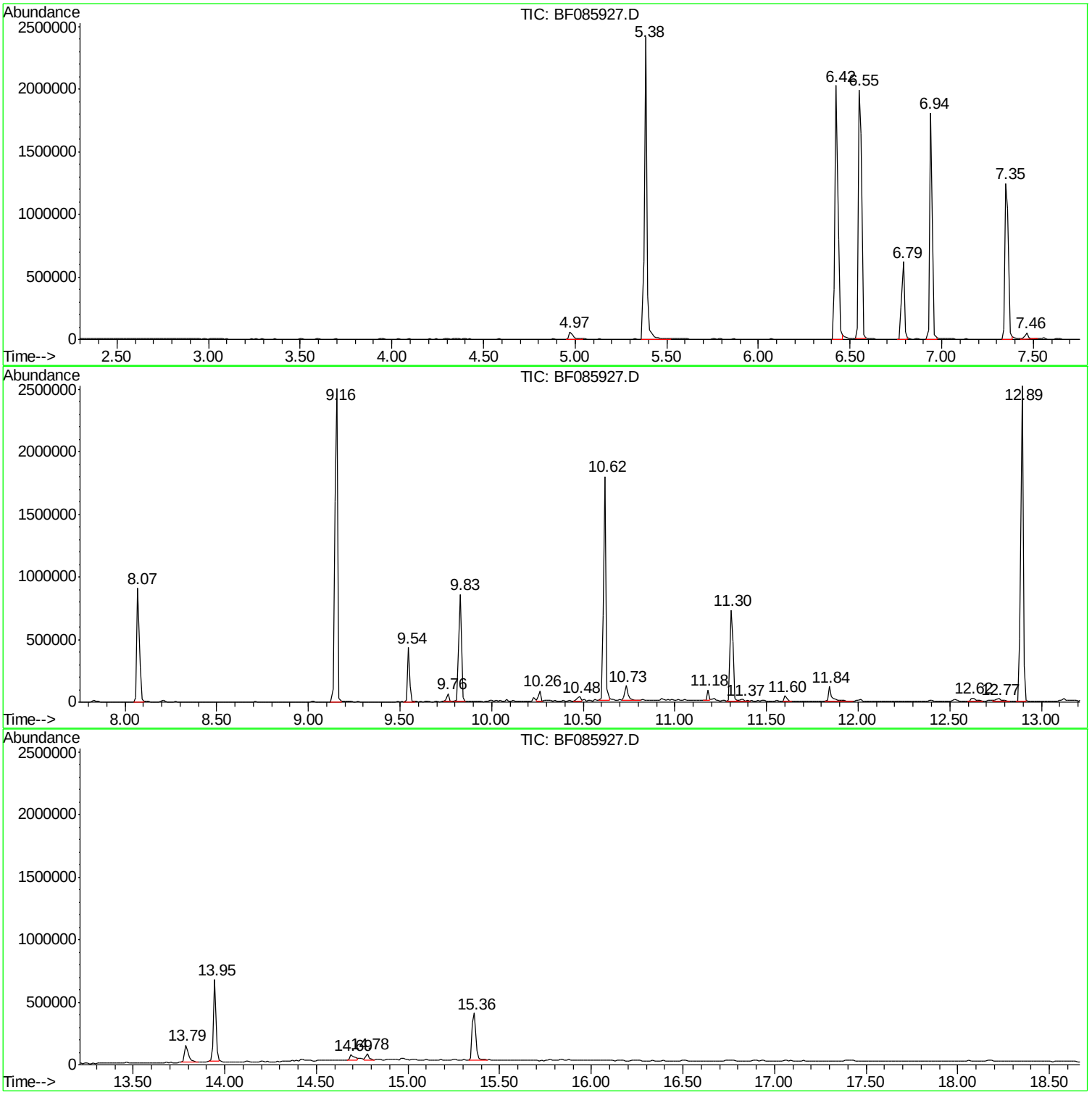
Instrument :
BNA_F
ClientSampleId :
SP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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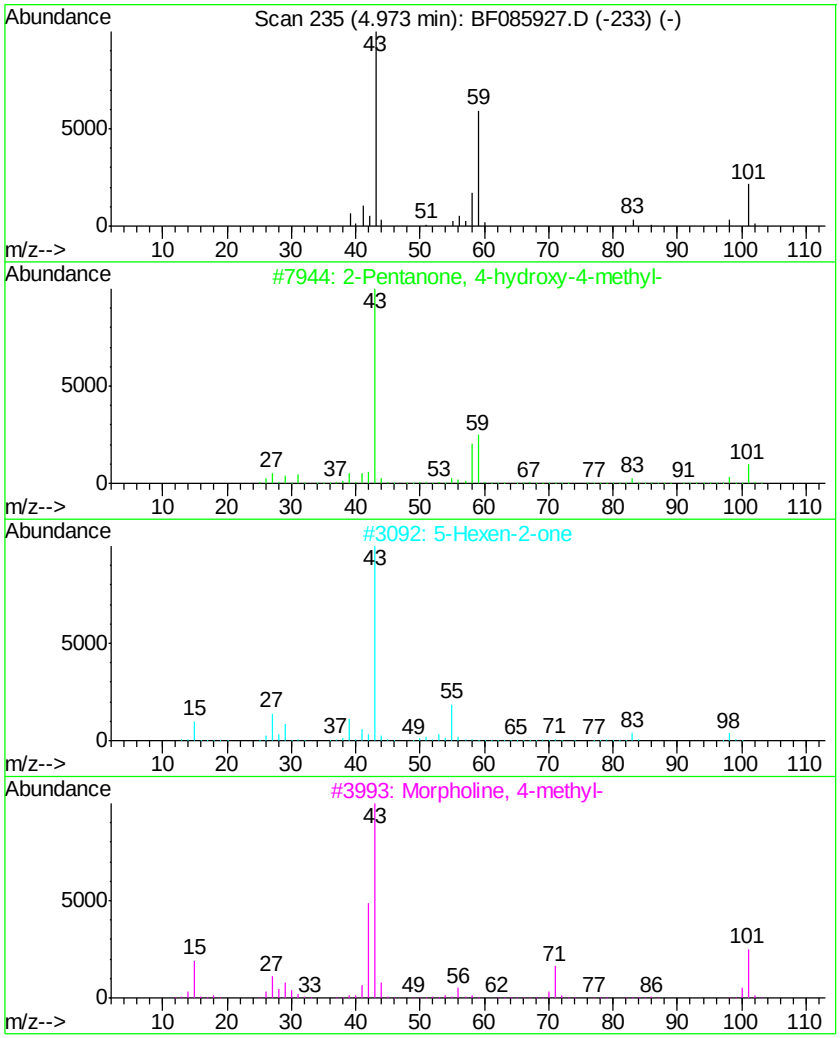
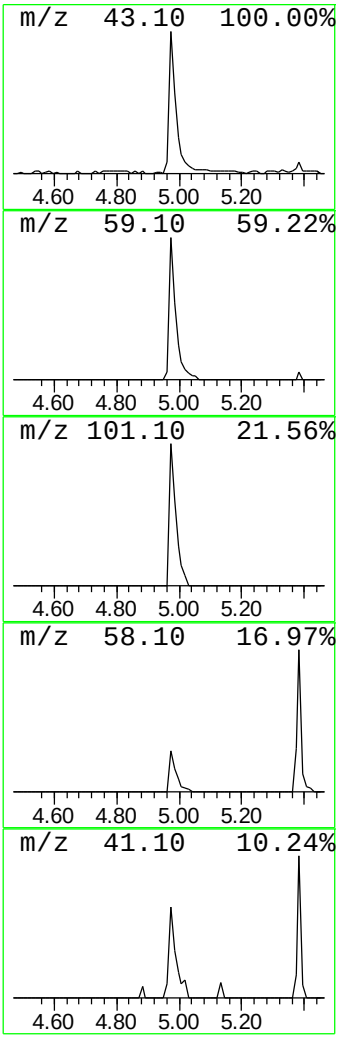
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.74 ng	87493	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : UM/SJ
Sample : H2075-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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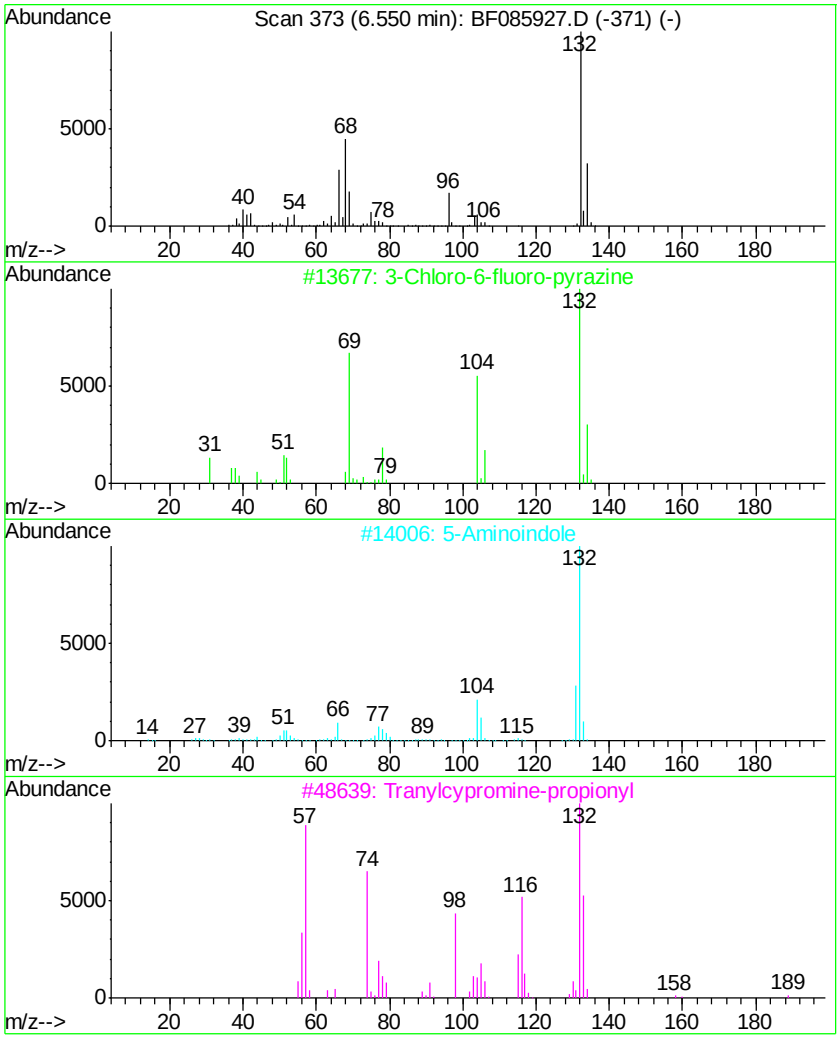
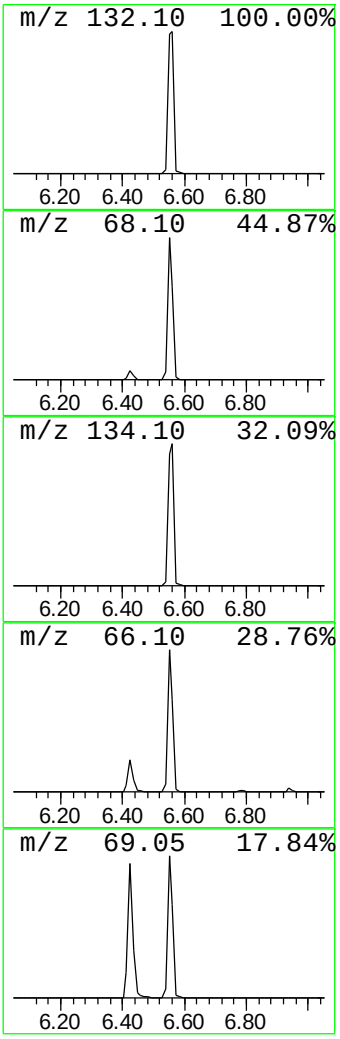
Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	80.74 ng	2576310	1,4-Dichlorobenzene-d4	6.79

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085927.D
Acq On : 31 Mar 2016 15:04
Operator : UM/SJ
Sample : H2075-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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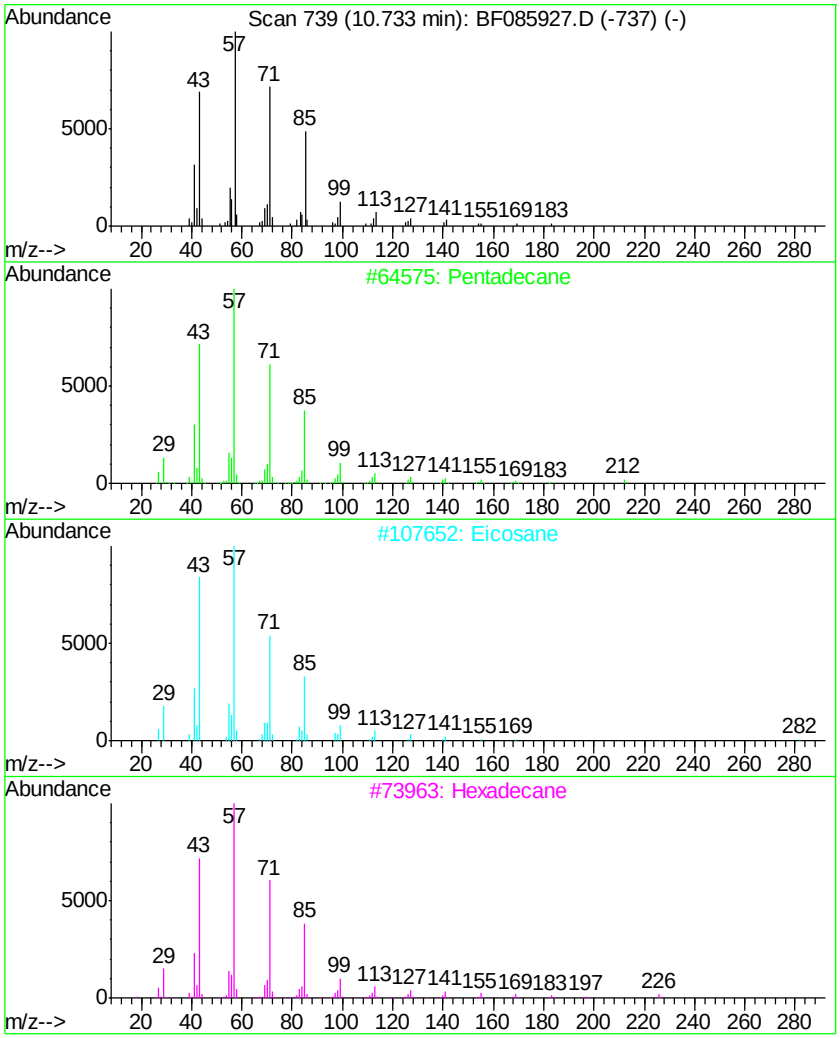
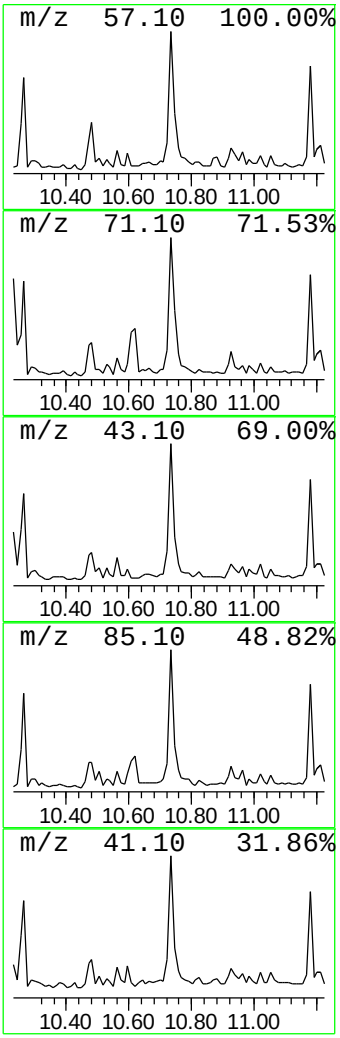
Peak Number 4 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.30 ng	140010	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Tetradecane	198	C14H30	000629-59-4	91





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Data File : BF085927.D
Acq On : 31 Mar 2016 15:04
Operator : UM/SJ
Sample : H2075-03
Misc :
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Instrument : BNA_F
ClientSampleId : SP-11

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

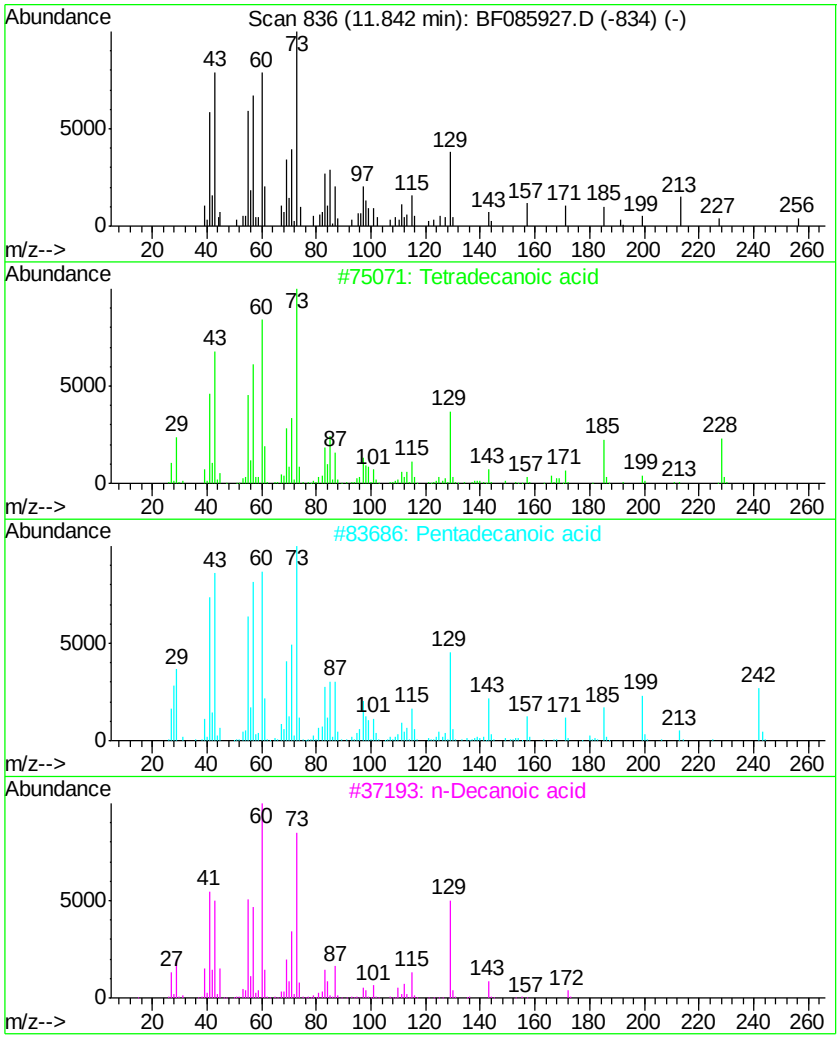
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

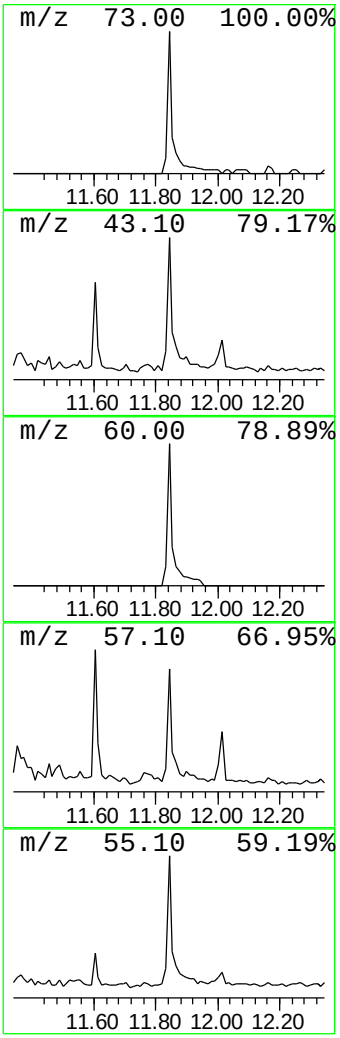
****

Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.79 ng	160759	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
5	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
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Operator : UM/SJ
Sample : H2075-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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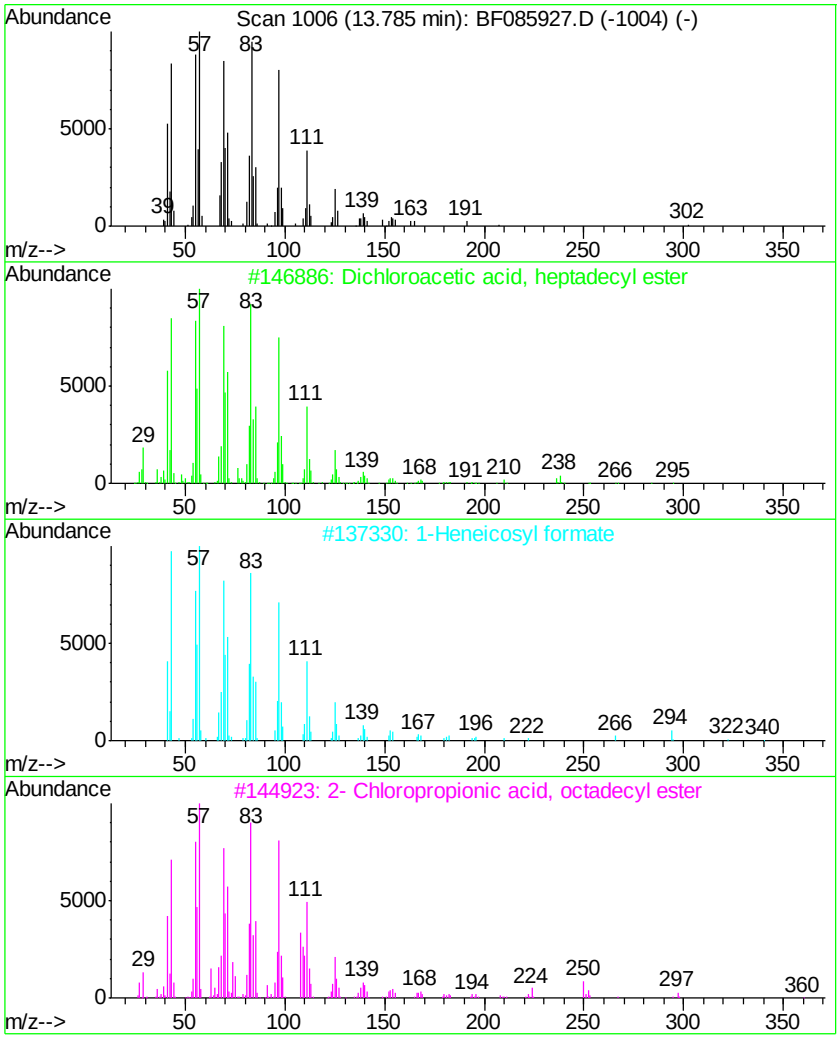
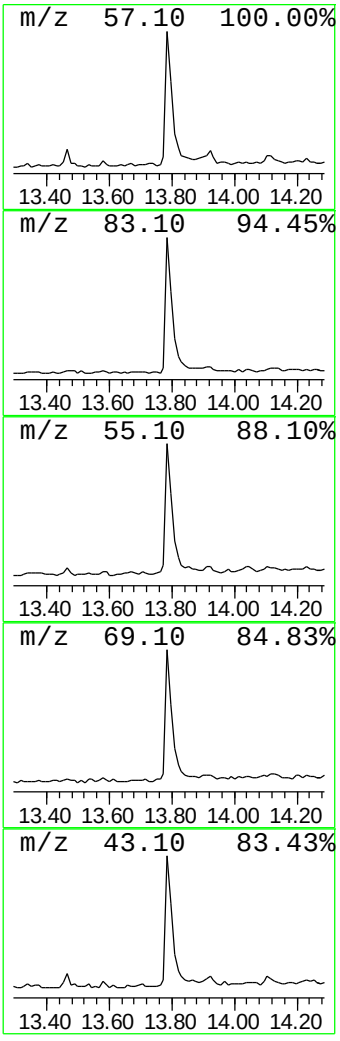
Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.18 ng	212662	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	1-Nonadecanol	284	C19H40O	001454-84-8	93
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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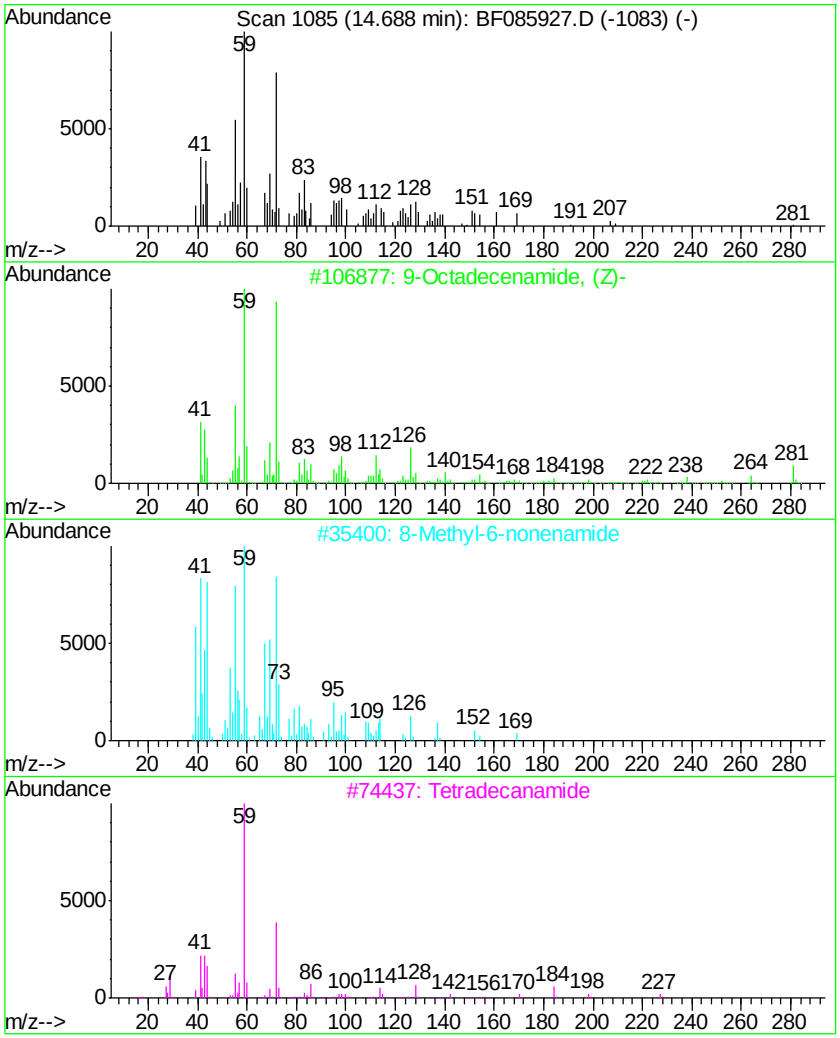
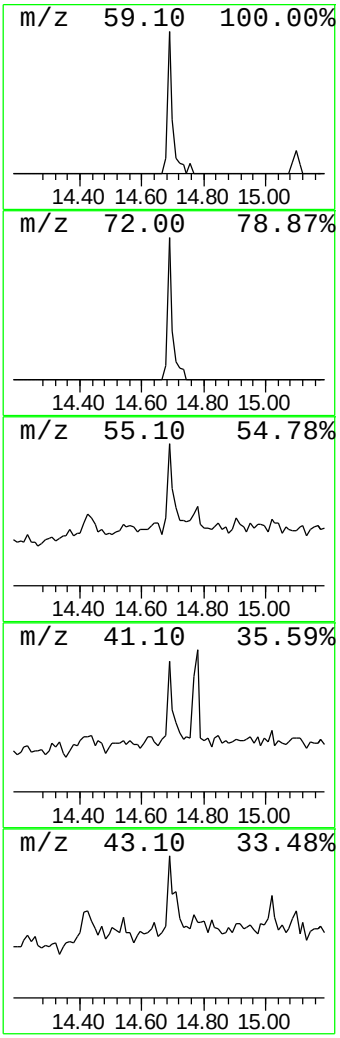
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	3.01 ng	81561	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	8-Methyl-6-nonenamide	169	C10H19NO	1000293-20-9	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	38
4	N'-(4-Nitrobenzylidene)-2-pentyl...	303	C16H21N3O3	339027-09-7	38
5	Hexadecanamide	255	C16H33NO	000629-54-9	32





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

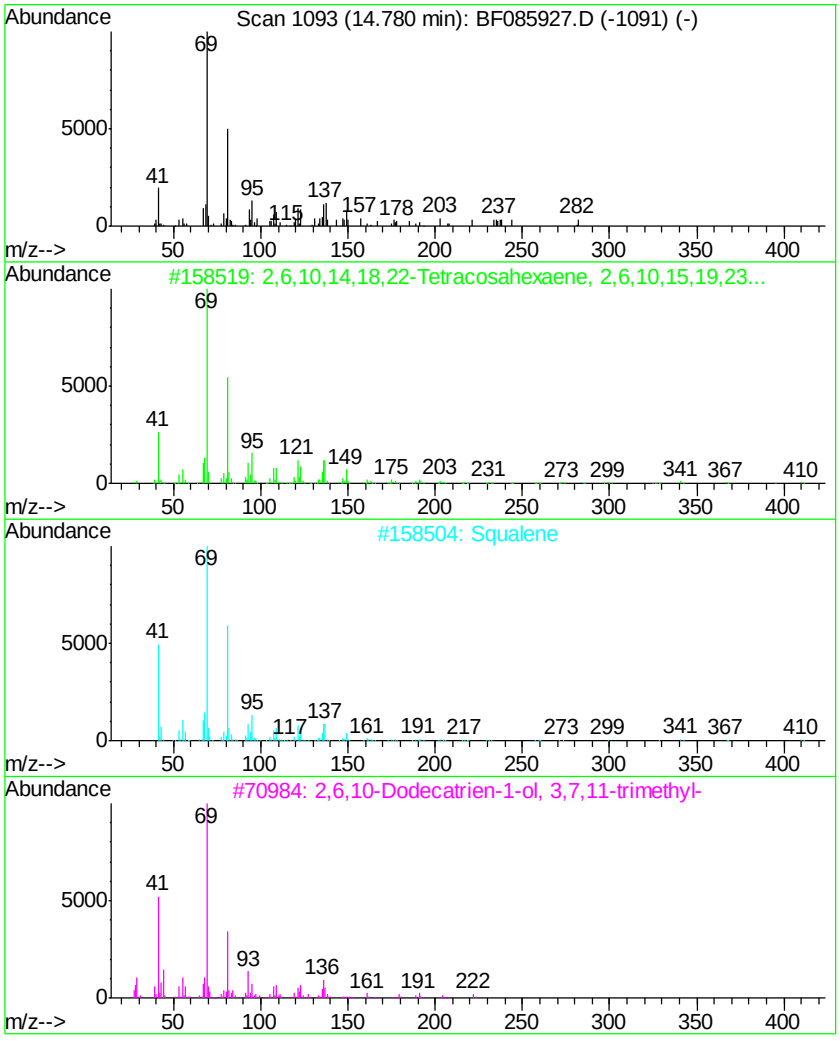
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

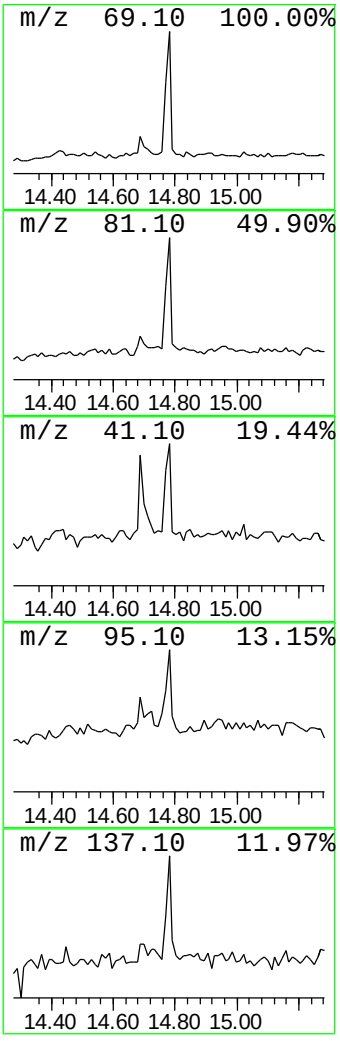
****

Peak Number 8 2,6,10,14,18,22-Tetracosahe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.72 ng	73811	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
2	Squalene	410	C30H50	007683-64-9	87
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

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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...	4.97	2.7	ng	87493	1	6.79	638151	20.0
unknown6.55	6.55	80.7	ng	2576310	1	6.79	638151	20.0
Pentadecane	10.73	3.3	ng	140010	4	11.31	849121	20.0
Tetradecanoic acid	11.84	3.8	ng	160759	4	11.31	849121	20.0
Dichloroacetic ac...	13.79	7.2	ng	212662	5	13.95	591978	20.0
9-Octadecenamide,...	14.69	3.0	ng	81561	6	15.36	541767	20.0
2,6,10,14,18,22-T...	14.78	2.7	ng	73811	6	15.36	541767	20.0