LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088929.D
Acq On : 12 Jul 2016 20:00
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

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-BF063016.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	1.667	5	7	16	rVV	144483	209998	11.57%	1.938%
2	1.792	16	18	41	rVB	181626	399563	22.02%	3.687%
3	4.501	253	255	260	rBB	16365	20198	1.11%	0.186%
4	4.878	283	288	291	rBV	905309	1778198	98.00%	16.408%
5	5.301	323	325	327	rVB	84956	70627	3.89%	0.652%
6	6.341	414	416	419	rVB	121224	101247	5.58%	0.934%
7	6.467	425	427	429	rBV	250371	202211	11.14%	1.866%
8	6.696	445	447	449	rBV	317197	355637	19.60%	3.282%
9	6.856	459	461	463	rVB	1218399	1097253	60.47%	10.125%
10	7.267	494	497	499	rBV	958025	931041	51.31%	8.591%
11	7.987	557	560	562	rVB	588787	502982	27.72%	4.641%
12	8.696	620	622	625	rBV	45996	53403	2.94%	0.493%
13	9.073	652	655	657	rBV	1390988	1814415	100.00%	16.742%
14	9.462	687	689	691	rBB	71981	54713	3.02%	0.505%
15	9.553	694	697	700	rVB	12427	19681	1.08%	0.182%
16	9.736	711	713	716	rVB	603472	503470	27.75%	4.646%
17	10.513	780	781	783	rBV	46632	55034	3.03%	0.508%
18	10.650	792	793	798	rBV	16832	22130	1.22%	0.204%
19	10.971	818	821	824	rVB	93721	123559	6.81%	1.140%
20	11.096	830	832	834	rBV	36403	40916	2.26%	0.378%
21	11.211	840	842	844	rVB	446551	376825	20.77%	3.477%
22	11.279	844	848	852	rVB2	8550	20807	1.15%	0.192%
23	11.816	893	895	898	rVB	40904	55572	3.06%	0.513%
24	12.799	978	981	983	rBV	1232382	1163327	64.12%	10.734%
25	13.702	1058	1060	1067	rBV	68303	81799	4.51%	0.755%
26	13.839	1069	1072	1074	rBV	343446	388160	21.39%	3.582%
27	14.479	1126	1128	1130	rVB	19335	18580	1.02%	0.171%
28	14.685	1144	1146	1149	rBV	41295	44074	2.43%	0.407%
29	15.211	1189	1192	1194	rBV	284967	332083	18.30%	3.064%

Sum of corrected areas: 10837503

LSC Report - Integrated Chromatogram

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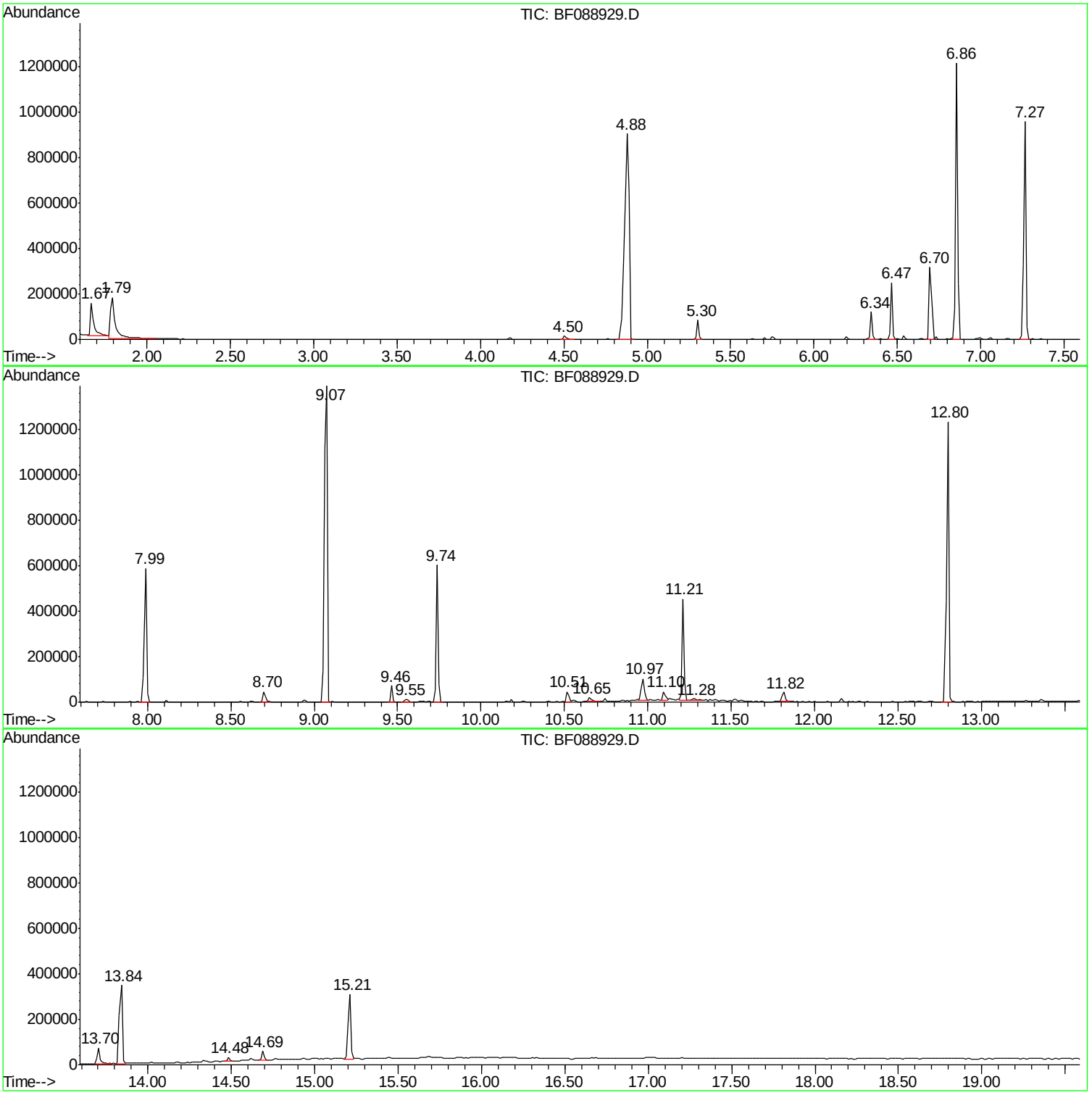
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088929.D
Acq On : 12 Jul 2016 20:00
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

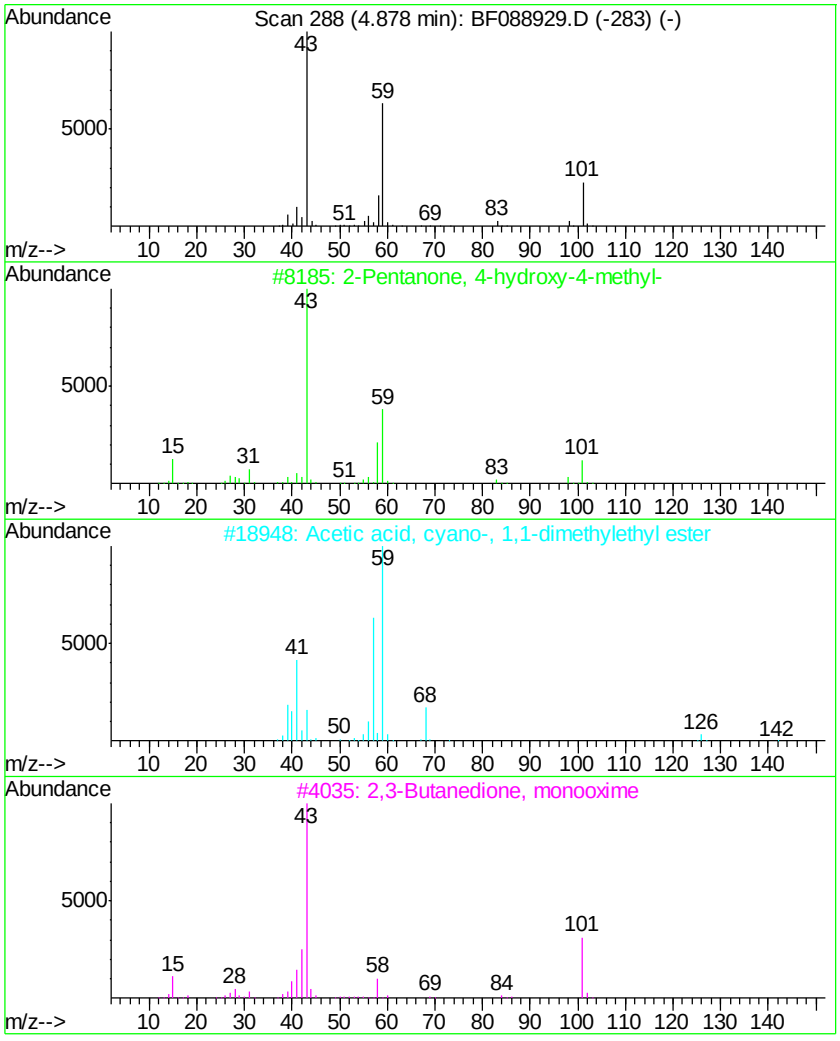
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

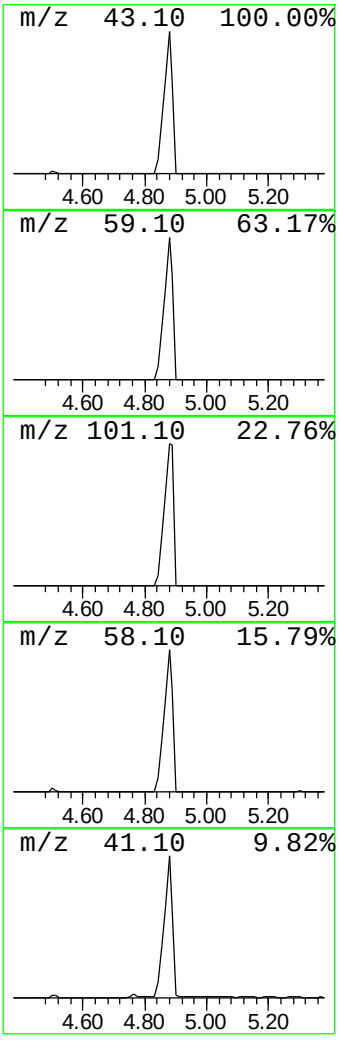
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	100.00 ng	1778200	1,4-Dichlorobenzene-d4	6.70

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	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF088929.D
Acq On : 12 Jul 2016 20:00
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

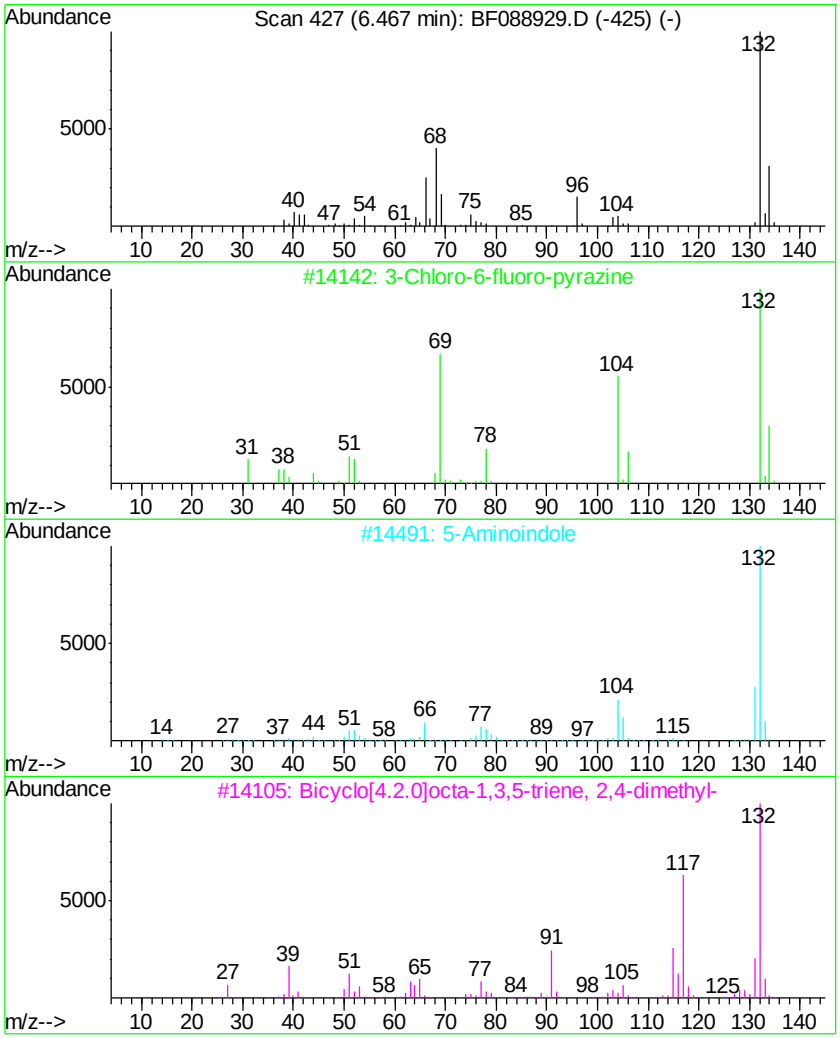
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

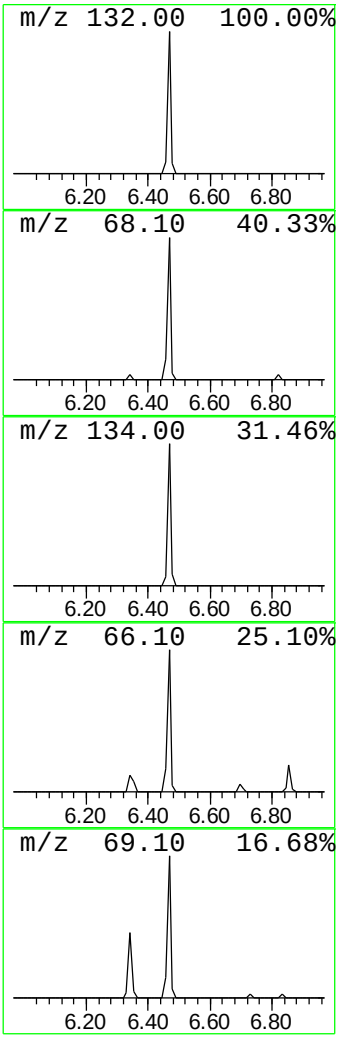
****

Peak Number 4 unknown6.47 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	11.37 ng	202211	1,4-Dichlorobenzene-d4	6.70

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	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088929.D
Acq On : 12 Jul 2016 20:00
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

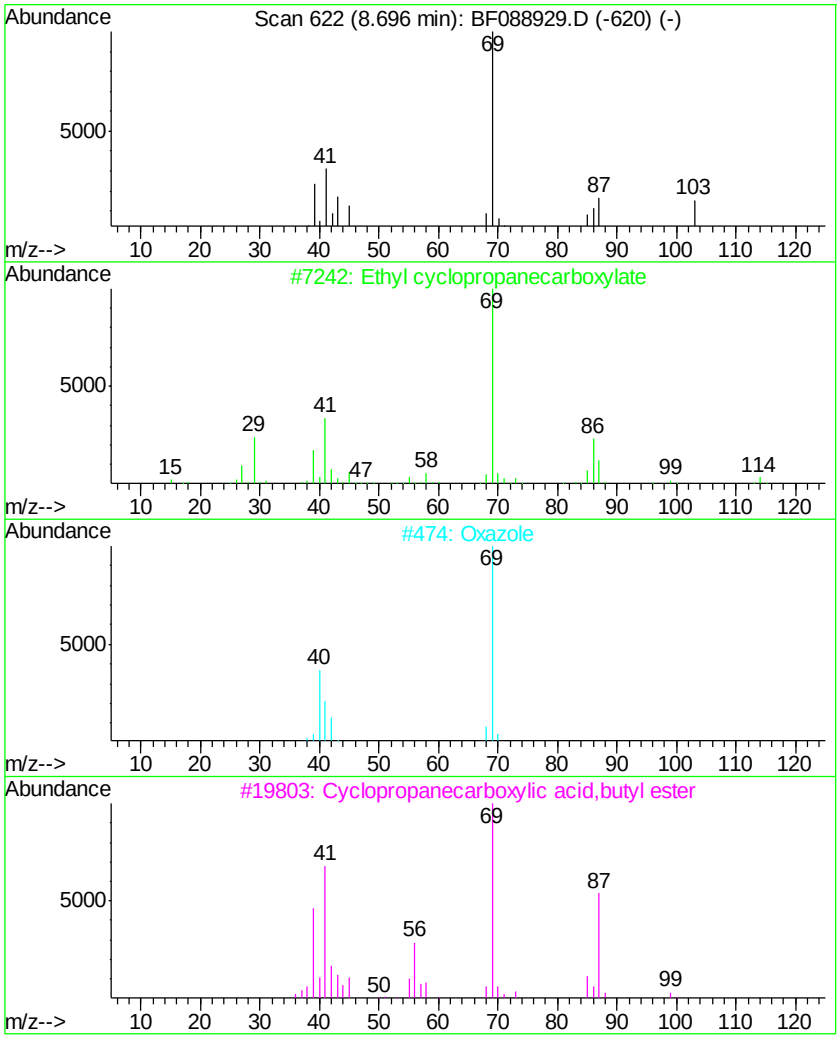
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

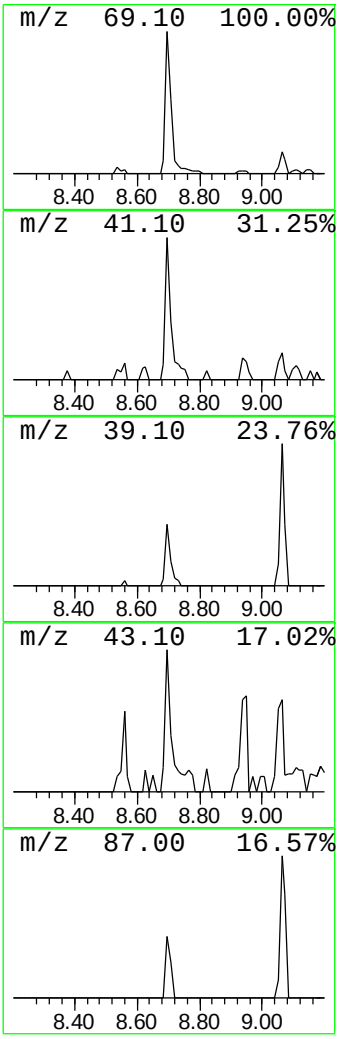
****

Peak Number 6 unknown8.70 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	2.12 ng	53403	Naphthalene-d8	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	40
2	Oxazole	69	C3H3NO	000288-42-6	9
3	Cyclopropanecarboxylic acid,butyl...	142	C8H14O2	054947-39-6	9
4	1-Octyn-4-ol	126	C8H14O	052517-92-7	9
5	2-Pentanol, 1-(2-methylenecyclop...	154	C10H18O	1000161-07-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088929.D
Acq On : 12 Jul 2016 20:00
Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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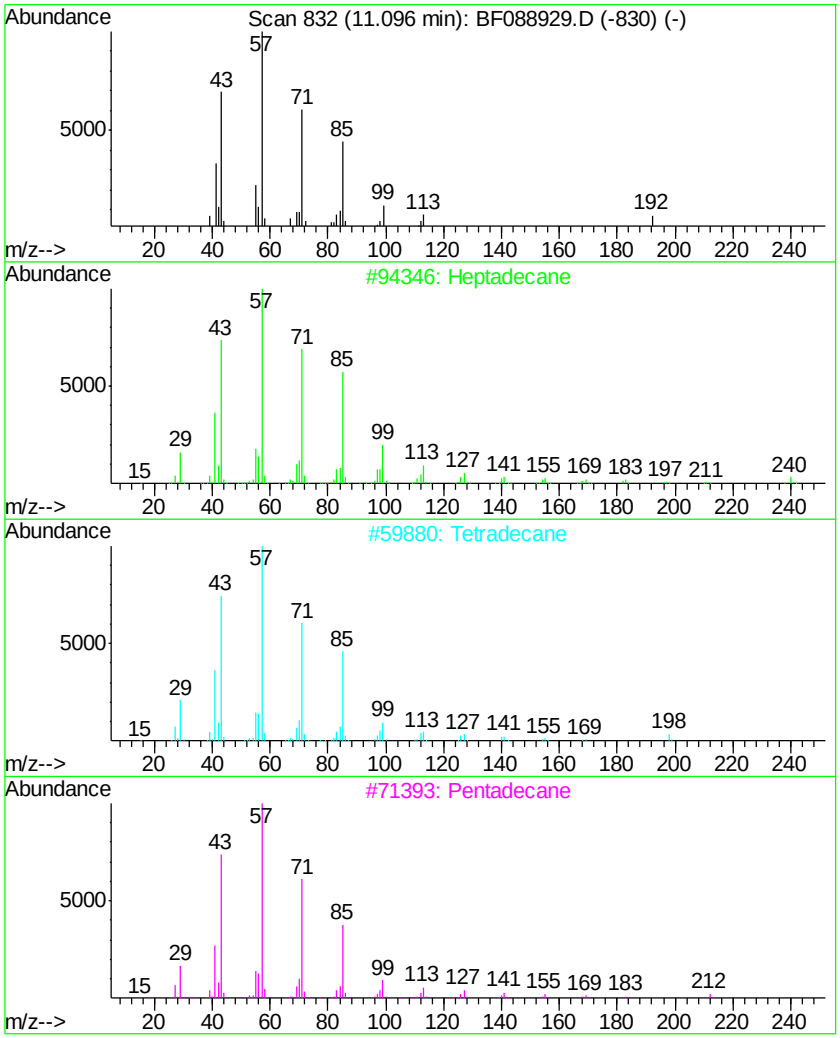
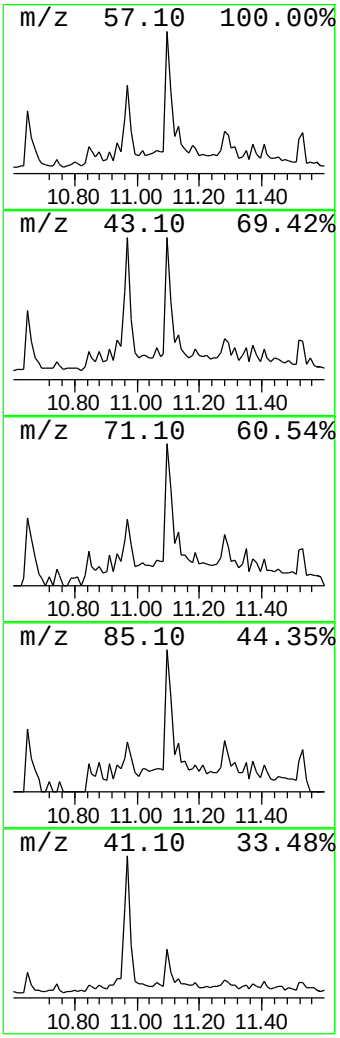
Peak Number 8 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.17 ng	40916	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Hexadecane	226	C16H34	000544-76-3	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
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Acq On : 12 Jul 2016 20:00
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Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

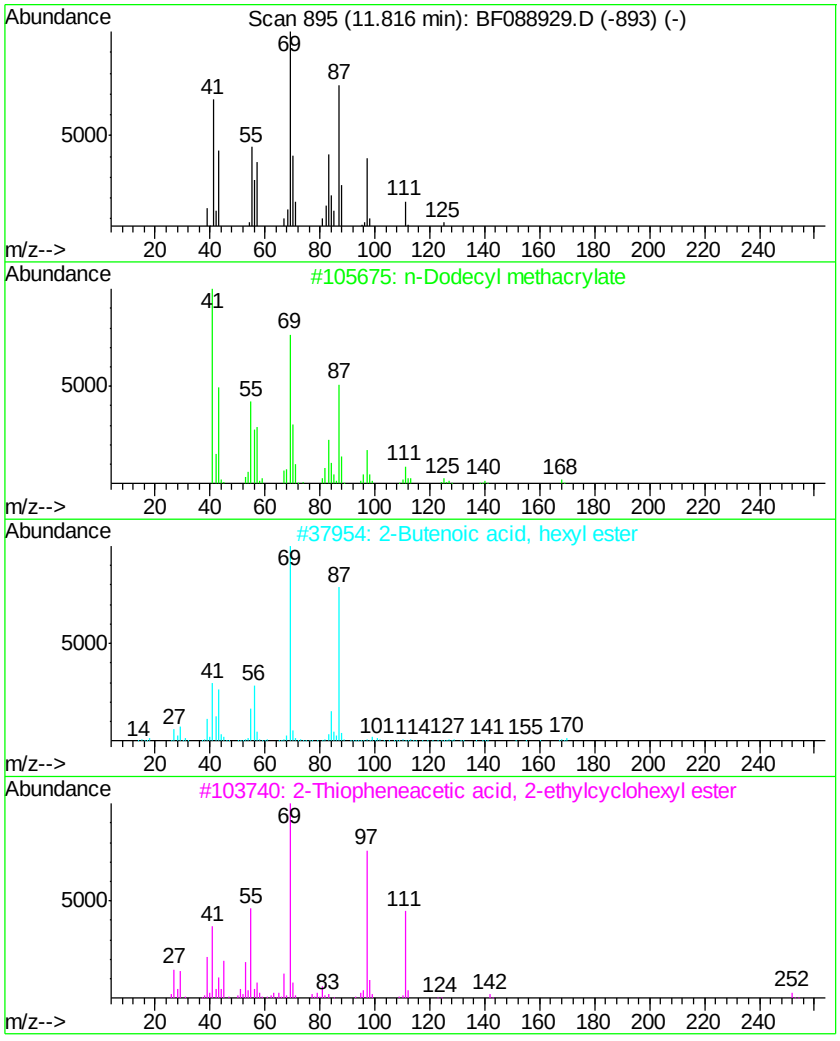
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

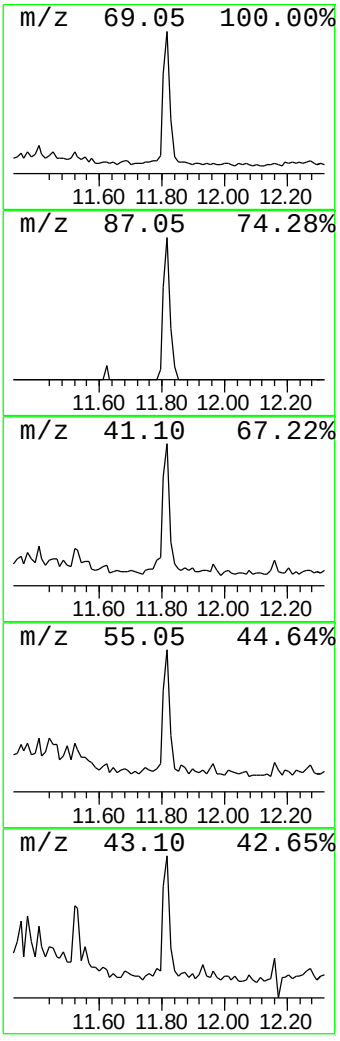
****

Peak Number 9 n-Dodecyl methacrylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.95 ng	55572	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	90
2	2-Butenoic acid, hexyl ester	170	C10H18O2	019089-92-0	37
3	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	27
4	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	22
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	22





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Operator : UM/SJ
Sample : H3999-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

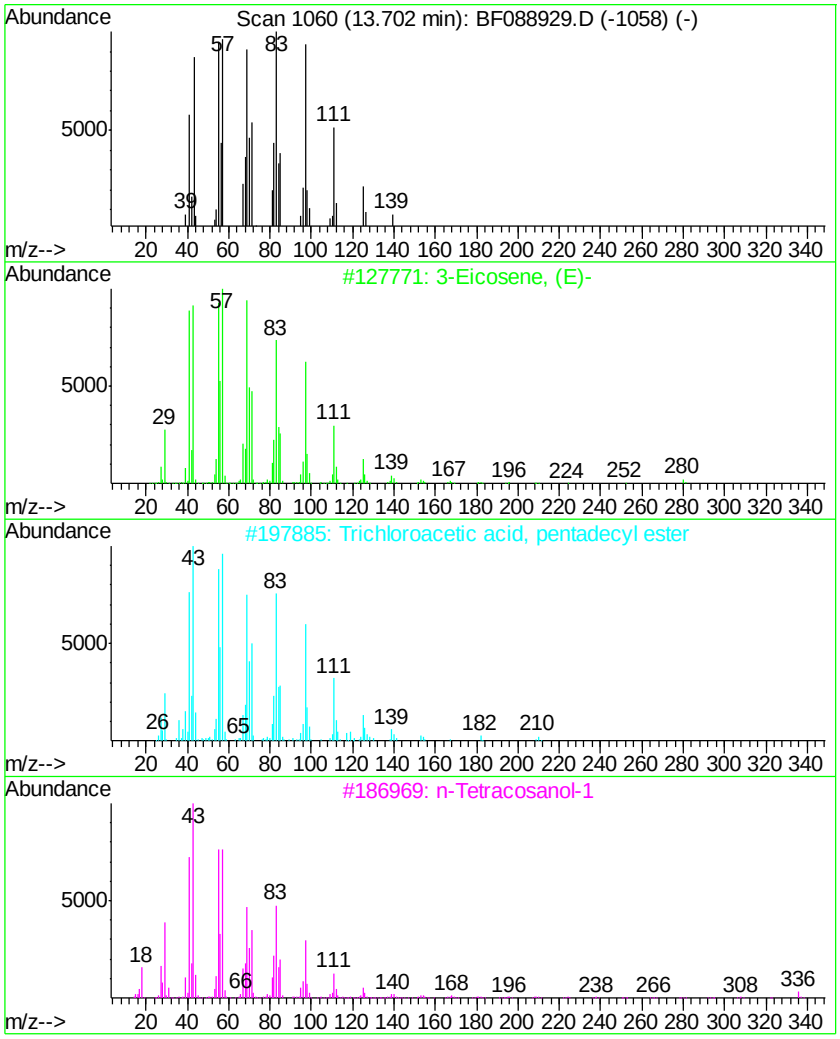
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

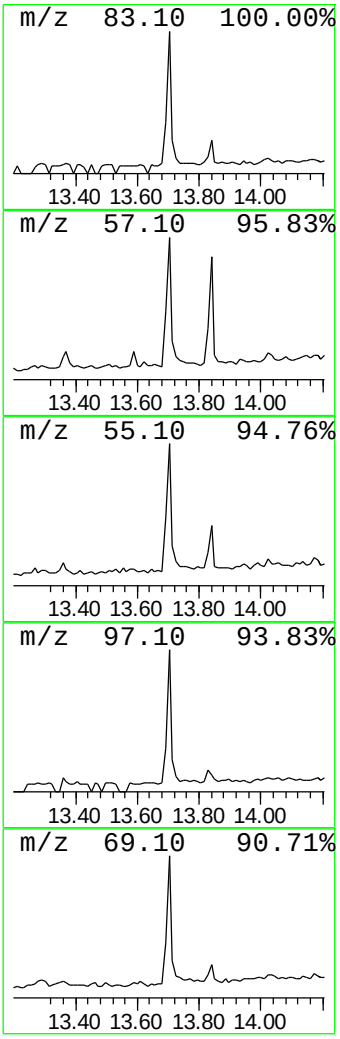
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.21 ng	81799	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	1-Hexadecanol	242	C16H34O	036653-82-4	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	83





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Instrument : BNA_F
ClientSampleId : SES-MS-PH3-COA-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

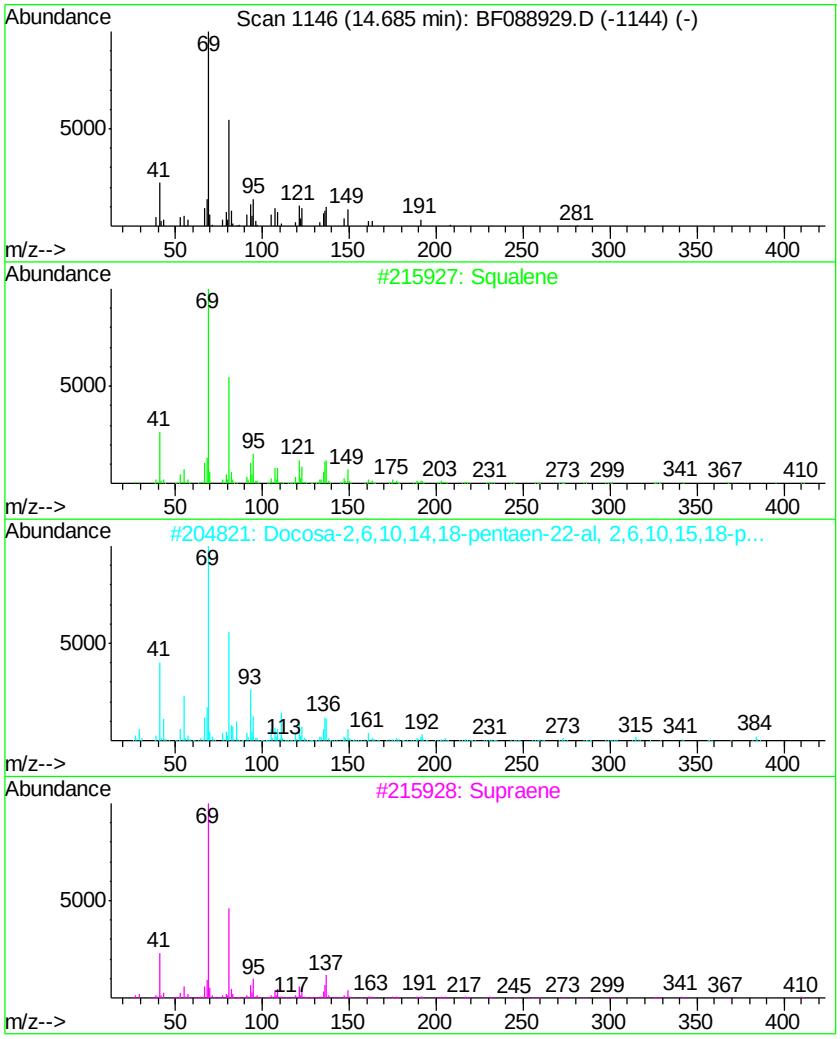
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

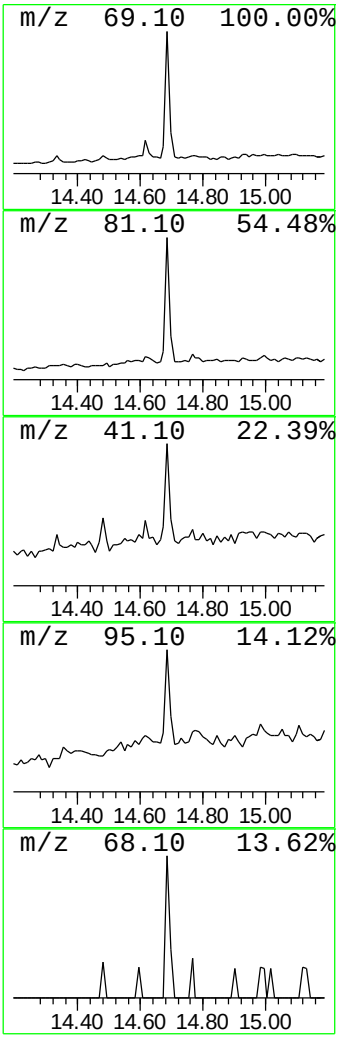
****

Peak Number 11 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.65 ng	44074	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3	Supraene	410	C30H50	007683-64-9	80
4	trans-Farnesol	222	C15H26O	000106-28-5	78
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





Tentatively Identified Compound (LSC) summary

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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...	4.88	100.0	ng	1778200	1	6.70	355637	20.0
unknown6.47	6.47	11.4	ng	202211	1	6.70	355637	20.0
unknown8.70	8.70	2.1	ng	53403	2	7.99	502982	20.0
Heptadecane	11.10	2.2	ng	40916	4	11.21	376825	20.0
n-Dodecyl methacr...	11.82	3.0	ng	55572	4	11.21	376825	20.0
3-Eicosene, (E)-	13.70	4.2	ng	81799	5	13.84	388160	20.0
Squalene	14.69	2.6	ng	44074	6	15.21	332083	20.0